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Ageing and dynamical scaling behaviour far from equilibrium

Florian Baumann

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**Alterung und dynamisches Skalenverhalten
fern des Gleichgewichts**

Den Naturwissenschaftlichen Fakultäten
der Friedrich-Alexander-Universität Erlangen-Nürnberg

zur

Erlangung des Doktorgrades

vorgelegt von

Florian BAUMANN

aus Mannheim

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Chapter 1

Introduction

1.1 Physical ageing

Physical ageing of a material means very broadly that its physical properties change with time. For instance, everybody will probably know the phenomenon that a rubber band loses more and more of its elasticity when it gets older. Effects of this kind can occur in out-of-equilibrium systems in which slow modes exist which prevent the system from relaxing exponentially towards its equilibrium (or stationary) state¹. They have been observed in many systems, a classical example being glass-forming materials which are quenched from a high-temperature molten state to a low temperature below the so-called 'glass-transition temperature' T_g . Early experiments on the mechanical properties

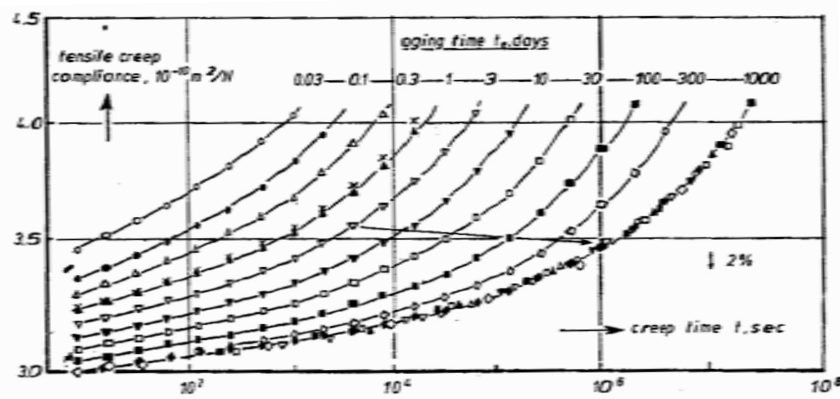


Figure 1.1: Small-strain tensile creep curves of PVC quenched from 90°C to 20°C . The arrow indicates the almost horizontal shift performed to obtain the data collapse. The crosses were found when, after 1000 days of ageing, the sample was reheated to the original temperature, requenched and then remeasured for $t_e = 1$ day. The image is taken from [224].

of polymeric glasses (and similar materials) identified several important features of ageing as described in [224]. Various materials were prepared above T_g and then quenched below

¹This is not the only mechanism which can prevent a system from reaching its equilibrium state. This can for example also happen if external driving forces are present. In this thesis however we will focus on the case of slow relaxation.

the glass transition temperature. After a certain waiting time t_e the sample was subjected to a constant stress and the tensile creep compliance $J_{t_e}(t)$ was measured. In figure 1.1 the creep curves for PVC are shown as a function of the creep time for several ageing times t_e . Now, several important observations can be made. First, the mechanical state of the polymer, as measured through the compliance, slowly changes over time-scales of 10^6 seconds or over several weeks. This is much larger than the usual microscopic time scales. Second, for different waiting times t_e different curves are obtained, hence the state of the system does not only depend on the time since the quench, but also on the waiting time t_e . Therefore, time-translation invariance is broken. Third, the shape of the curves is similar and one can collapse all curves onto one common master curve by (almost) horizontal shifts. This implies that for a constant rescaling factor a , one has the *dynamical scaling behaviour* $J_{at_e}(t) = J_{t_e}(at)$. These three properties are the basic properties of ageing systems.

Furthermore, the same kind of experiment has been performed for various kinds of materials. As shown in figure 1.2 the master curves for materials as different as PVC, PMMA, shellac and lead can even be collapsed onto one *universal* master curve. This experimental

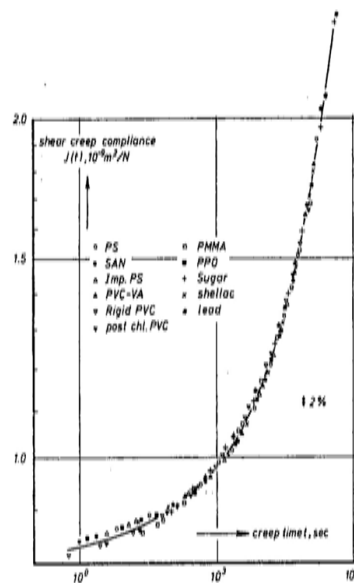


Figure 1.2: Master creep curve for various materials. The curve can be described by $J(t) = J_0 \exp(t/t_0)^{1/3}$ for constants J_0 and t_0 . The image is taken from [224]

observation - dynamical scaling behaviour and universality - strongly suggests that there might be underlying very general properties connecting physical systems, which are at the first glance very different. We shall suggest in this work, that one of these general features might be a 'hidden' non-trivial local scale-invariance, which is at least partially responsible for the observed universal behaviour.

Another important aspect of physical ageing is its reversibility. Reconsider figure 1.1 for PVC and take t_e equal to one day. After 1000 days of ageing, the sample was reheated to the molten phase, allowed to equilibrate there and then quenched again. After waiting for $t_e = 1$ day, the same stress as before was applied and the compliance measured (crosses in figure 1.1). As one can see, the results are identical to the first run.

1.1.1 Phase-ordering kinetics

In order to gain a better theoretical insight into the observed concepts of scaling and universality, we look at somewhat simpler systems. Appropriate examples are for instance the ordering kinetics of systems which undergo a disorder-order phase transition. Conceptually simple examples are magnetic systems which are prepared in an unmagnetised (disordered) high-temperature state and then quenched to below the critical temperature T_c . Magnetic domains will start forming and for larger times, *coarse-graining* occurs: For

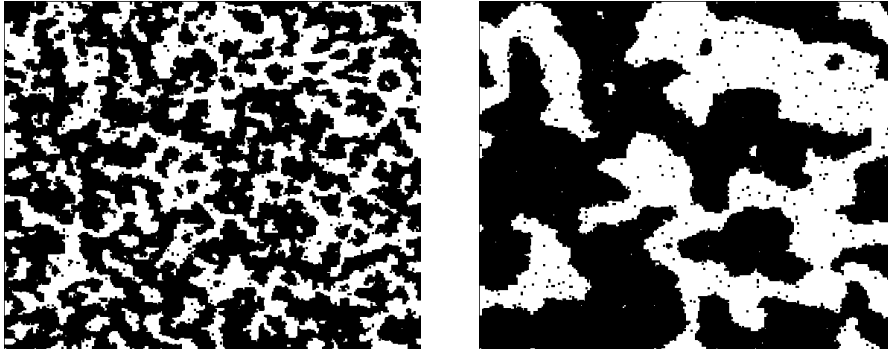


Figure 1.3: Snap-shot of a Monte-Carlo simulation of the Ising model quenched to below the critical point. In white areas spins point upwards, in black areas downwards. The left picture shows the system a relative short time after the quench, the right picture at a later stage. Both pictures courtesy of M. Pleimling.

a spatially infinite system, ordered domains form and grow, their size being characterised by a time-dependent length scale $L = L(t)$. This is illustrated in figure 1.3 by snapshots of a Monte Carlo simulation in the 2D Ising model quenched to below the critical temperature. The typical form of the free energy in this kind of system is shown in figure 1.4.

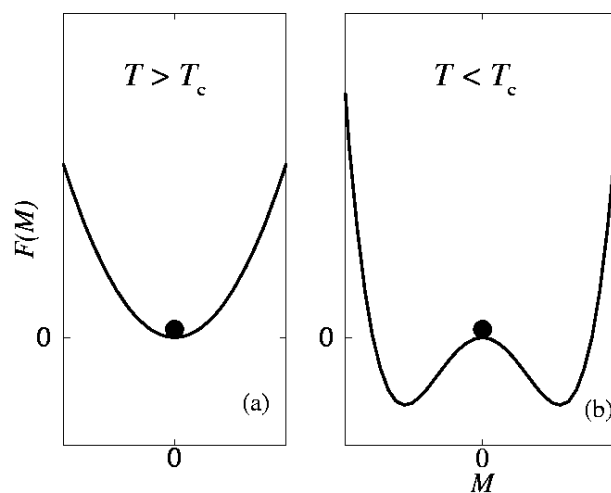


Figure 1.4: Typical form of the free energy $F(M)$ of a magnetic system undergoing phase-ordering. Whereas above the critical temperature only one, unique minimum exists (a), there are two local minima below the critical temperature (b).

Before the quench the system 'sits' in the unique global minimum of the free energy. After

the quench however, there are two equivalent local minima, which reflects the up-down symmetry of the model. Due to the existence of these two competing stationary states the system evolves slowly and depends non-exponentially on time.

Suppose the system is described by an order parameter ϕ and that we want to look at the correlation function $C(t, \mathbf{r}) := \langle \phi(t, \mathbf{0})\phi(t, \mathbf{r}) \rangle$ (where the angular brackets indicate an average over initial conditions and over the noise, see section 1.2 for an exact definition). One possibility to proceed would be to use a *stochastic Langevin equation* for the description of the temporal evolution of the order parameter [226]. This is a *mesoscopic* description of the system, which assumes that some sort of coarse-graining has already taken place. Another essential assumption for this approach is that there is a separation of time scales between the *slow* dynamics of the order parameter and the fast degrees of freedom, which can be modelled by a *stochastic* term. The ansatz for the temporal evolution of the order parameter $\phi = \phi(t, \mathbf{r})$ is ²

$$\partial_t \phi(t, \mathbf{r}) = \mathcal{F}[\phi](t, \mathbf{r}) + \eta(t, \mathbf{r}) \quad (1.1)$$

where $\mathcal{F}[\phi]$ is some functional of ϕ and represents the *deterministic* part of the equation. We concentrate on the simplest case of purely *relaxational* dynamics [45, 226], in which case

$$\mathcal{F}[\phi](t, \mathbf{r}) = -\mathcal{D}[\phi(t, \mathbf{r})] \frac{\delta \mathcal{H}[\phi](t, \mathbf{r})}{\delta \phi(t, \mathbf{r})}. \quad (1.2)$$

Here the functional $\mathcal{D}[\phi]$ will either be a constant or proportional to the Laplace operator. $\mathcal{H}[\phi]$ is the effective Hamiltonian governing the phase-transition, which has typically a form as depicted in 1.4.

On the other hand $\eta(t, \mathbf{r})$ is a random variable, which is supposed to be Gaussian with the two first moments [226]

$$\langle \eta(t, \mathbf{r}) \rangle = 0, \quad \langle \eta(t, \mathbf{r})\eta(t', \mathbf{r}') \rangle = 2\mathfrak{L} \delta(\mathbf{r} - \mathbf{r}')\delta(t - t'). \quad (1.3)$$

Here \mathfrak{L} is an operator, which will in practise typically be equal to the identity operator times the temperature or the Laplace operator (again with the temperature as a prefactor). It is justified to assume a Gaussian distribution if we suppose that the underlying microscopic processes for the fast degrees of freedom can be described by stochastic processes, whose first two moments exist. In this case the central limit theorem applies and leads to a Gaussian distribution of the noise term, which is uniquely characterised by its first two moments.

In general, the functional $\mathcal{F}[\phi]$ has a rather involved form [37, 176, 146] and even with the further simplification of a quench to zero temperature, this approach can only be treated perturbatively and leads very quickly to complicated calculations [176, 146]. We will come back to this approach in section 1.2. Instead of using the temporal evolution of the order parameter as a starting point, one can use the so-called *scaling hypothesis* in order to learn more about the behaviour of $C(t, \mathbf{r})$ [37].

The scaling hypothesis has been brought forward (see [37] and references therein) in order to analyse the dynamics of a system undergoing phase-ordering. It states that at

²The treatment can also be done for an order parameter with several components. As we deal almost always with a one-component order parameter this simple treatment suffices.

late times, there is only one single characteristic length scale $L(t)$ such that the domain structure is (in a statistical sense) independent of time when lengths are scaled by $L(t)$. This hypothesis has been proven in some exactly solvable models [33, 55, 3] and there is very strong numerical and experimental evidence [131, 87, 164, 28, 218] in favour of it. We stress however, that it has not yet been proven in complete generality. The scaling hypothesis asserts for $C(t, \mathbf{r})$ and its Fourier transform $S(t, \mathbf{k})$ (the so-called *dynamical structure factor*)

$$C(t, \mathbf{r}) = f\left(\frac{r}{L}\right), \quad S(t, \mathbf{k}) = L^d g(kL) \quad (1.4)$$

with $k = |\mathbf{k}|$, $r = |\mathbf{r}|$ and two scaling functions $f(u)$ and $g(u)$. For systems with sharp interfaces between the domains, one generally expects [37] the so-called Porod law to hold, which states that for a n -component order parameter with $O(n)$ -symmetry

$$S(t, \mathbf{k}) \sim \frac{1}{Lk^{d+n}}, \quad \text{for } kL \gg 1 \quad (1.5)$$

Combining dynamical scaling and (1.5) a consideration of energy conservation of the stochastic equations of motion (1.1) [38] allows to derive the time-dependent form of $L(t)$. In most cases one indeed finds that for late times

$$L(t) \sim t^{1/z} \quad (1.6)$$

Here z is the so-called *dynamical exponent*, which is a characteristic number for the system under consideration. It depends on the kind of dynamics and the number of components n of the order parameter [38].

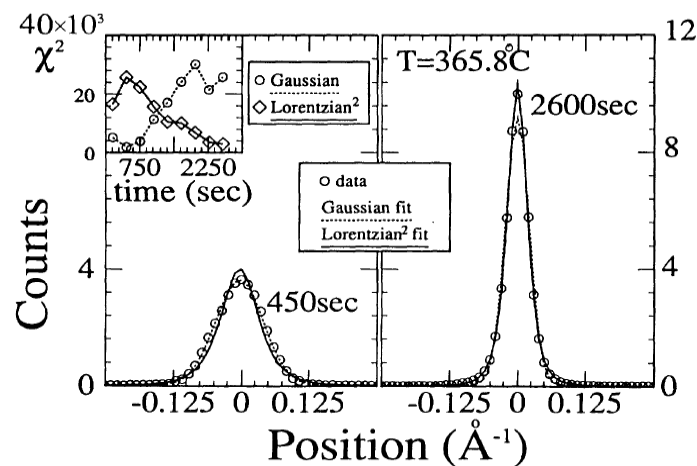


Figure 1.5: Change in the line shape after a quench of Cu_3Au below the critical temperature. Solid (dotted) line is a Lorentzian-squared (Gaussian) convolution least-squares fit. Image taken from [218]

As an example for the experimental observation of these phenomena, let us mention the systems treated in [218]. The binary alloy Cu_3Au has an order-disorder transition at a critical temperature of about $T_c = 390^\circ\text{C}$. We do not enter into the microscopic details of this phase-transition, for which we defer the reader to [218], where they have been

discussed thoroughly. We only state that the order parameter ϕ is linearly related to the concentrations of atoms [153] and that the structure factor $S(t, \mathbf{k})$ can be measured directly by x-ray scattering. One has therefore the possibility to verify experimentally the predictions inferred from the scaling hypothesis as described above. One of the results of the measurements of $S(t, \mathbf{k})$ is shown in figure 1.5: For relatively short times after the quench the data is fitted best by a Gaussian curve, whereas for latter times a squared Lorentzian

$$S(t, \mathbf{k}) = S_0 \left(1 + \left(\frac{\mathbf{k} - \mathbf{k}_0}{\Lambda(t)} \right)^2 \right)^{-2} \quad (1.7)$$

becomes more appropriate and the time dependence enters through the function $\Lambda(t)$. Here S_0 and \mathbf{k}_0 are parameters. This late-time form is clearly compatible with the Porod law (1.5) and figure 1.5 demonstrates nicely the crossover into the coarse-graining regime. Also the scaling hypothesis (1.4) and the growth law (1.6) with $z = 2$ are confirmed in

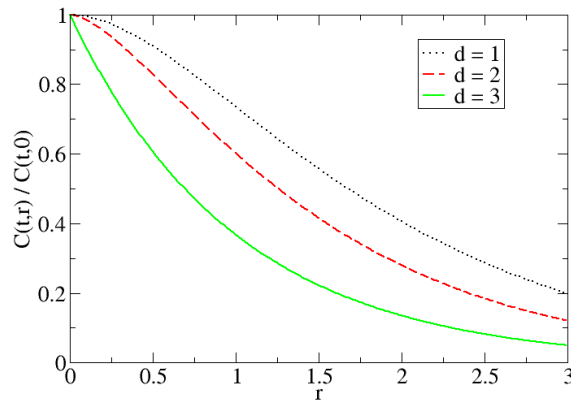


Figure 1.6: Form of the one-time correlator in direct space, if the structure factor is given by a squared Lorentzian (1.7) with $\Lambda(t) = 1$. The picture shows the dependence on $r = |\mathbf{r}|$.

the experiments [218]. It is also instructive to consider the form of the correlator in direct space, if the structure factor is given by (1.7). For $\mathbf{k}_0 = \mathbf{0}$ one finds [127]

$$\frac{C(t, \mathbf{r})}{C(t, \mathbf{0})} = \begin{cases} e^{-r\Lambda(t)}(1 + r\Lambda(t)) & d = 1 \\ r\Lambda(t)K_1(r\Lambda(t)) & d = 2 \\ e^{-r\Lambda(t)} & d = 3 \end{cases} \quad (1.8)$$

where $r = |\mathbf{r}|$ and $K_1(z)$ is a modified Bessel-function. Figure 1.6 illustrates the dependence on r for $\Lambda(t) = 1$.

As we stated before, in systems undergoing ageing time translation-invariance is broken. This fact cannot be captured by simple one-time quantities. This is the reason why it is necessary to look at two-time quantities for the theoretical description of ageing phenomena. One typically considers the autoresponse function $R(t, s)$ and the autocorrelation

function $C(t, s)$, which are defined by

$$C(t, s) := \langle \phi(t, \mathbf{x}) \phi(s, \mathbf{x}) \rangle, \quad R(t, s) := \left. \frac{\delta \langle \phi(t, \mathbf{x}) \rangle}{\delta h(s, \mathbf{x})} \right|_{h=0}. \quad (1.9)$$

Here $h(s, \mathbf{x})$ is an external perturbation (magnetic field) and spatial translation invariance was assumed, so that both quantities do not depend on \mathbf{x} . $R(t, s)$ measures the response of the system to small external perturbation. Generally we assume $t > s$ and call s the *waiting time* and t the *observation time*. With the help of these two quantities, we can now say more precisely what we mean by ageing. By definition, the system undergoes ageing if at least one of the quantities $C(t, s)$ or $R(t, s)$ does not merely depend on the difference $t - s$. In other words, the system undergoes ageing, if time-translation invariance is broken. Dynamical scaling behaviour occurs typically in the *scaling regime* where

$$t, s, \text{ and } t - s \gg t_{\text{micro}} \quad (1.10)$$

for some microscopic time-scale t_{micro} . One expects the following scaling behaviour in this regime [123, 45, 60, 94]

$$C(t, s) = s^{-b} f_C \left(\frac{t}{s} \right), \quad R(t, s) = s^{-a-1} f_R \left(\frac{t}{s} \right) \quad (1.11)$$

which defines the ageing exponents a and b . The scaling functions $f_C(y)$ and $f_R(y)$ behave for large arguments as

$$f_C(y) \stackrel{y \rightarrow \infty}{\sim} y^{-\lambda_C/z}, \quad f_R(y) \stackrel{y \rightarrow \infty}{\sim} y^{-\lambda_R/z} \quad (1.12)$$

so that we have altogether the exponents $z, a, b, \lambda_C, \lambda_R$ which characterise the out-of-equilibrium dynamics. For phase-ordering kinetics, one has found $b = 0$ in all concrete examples. The value for a depends on the behaviour of the *equilibrium* correlator [112, 117]. If it behaves as $C_{\text{eq}}(\mathbf{r}) \sim \exp(-|\mathbf{r}|/\xi)$ for a finite ξ , it is said to be in *class S*, but if it behaves as $C_{\text{eq}}(\mathbf{r}) \sim |\mathbf{r}|^{-(d-2+\eta)}$ (with the standard equilibrium critical exponent η), it is said to be in *class L*. Then

$$a = \begin{cases} 1/z & \text{for class } S \\ (d-2+\eta)/z & \text{for class } L \end{cases} \quad (1.13)$$

Furthermore, one can show for decorrelated initial correlations [192, 37] that $\lambda_R = \lambda_C$, but this does not need to hold for long-range initial correlations [191] or when some randomness is present [214, 121, 125].

1.1.2 Critical dynamics

A physically completely different example, in which ageing can also be observed, are systems undergoing *critical dynamics*. Consider for instance the Ising magnet described above, but this time the quench is performed *onto* the critical point. Also in this case, there is a diverging length scale, but this time it is the correlation length $\xi(t)$ which behaves as

$$\xi(t) \sim t^{1/z}. \quad (1.14)$$

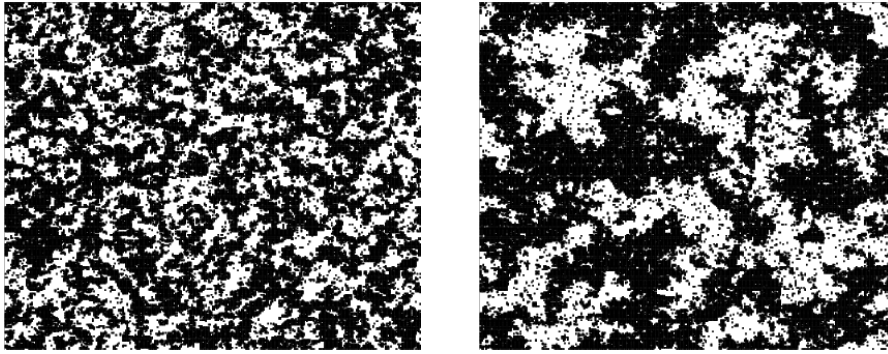


Figure 1.7: Snap-shot of a Monte-Carlo simulation of the Ising model quenched onto the critical point. White areas have spin up, black areas spin down. The left picture shows the system a relative short time after the quench, the right picture at a later stage. Both pictures courtesy of M. Pleimling

This defines the (critical) dynamical exponent z . We stress that the value of z for the case of critical quenches is in general different from the value of z for quenches below the critical temperature. In picture 1.7 we shown again snapshots from a Monte-Carlo simulation to illustrate this. The fact, that also in this situation, one has one relevant length scale ($\xi(t)$ instead of $L(t)$) entails, that the formal description of scaling behaviour is very similar to the case of phase-ordering kinetics described above, although the physical situation is very different. In fact, it is possible by using the dynamical renormalisation group [45] to prove, at least for a very large class of magnetic systems, that scaling behaviour occurs and that also for this case the scaling forms (1.11) and (1.12) hold for the two-time quantities (1.9). One still has $\lambda_R = \lambda_C$ [192, 45] (for decorrelated initial correlations) but as opposed to the case of phase-ordering, one has for the magnetic systems discussed up until here the equality [137, 45]

$$a = b = \frac{2\beta}{\nu z} = \frac{d - 2 + \eta}{z} \quad (1.15)$$

where β, ν and η are the usual static critical exponents (and d the dimensionality). For critical dynamics, there is another important quantity, the so-called *fluctuation-dissipation ratio* $X(t, s)$ which is defined as

$$X(t, s) := TR(t, s)/(\partial_s C(t, s)) \quad (1.16)$$

For equilibrium critical dynamics, where time-translation invariance holds, this quantity would be equal to one $X(t, s) = 1$. This statement is the famous *fluctuation-dissipation theorem*. For non-equilibrium dynamics, where time-translation invariance is broken, this is not true any more. On the one hand, one expects to recover an asymptotic value of one for $X(t, s)$, when fixing $t - s$ and taking the limit $s \rightarrow \infty$ [93]. On the other hand, in the ageing regime (1.10), one defines the limit fluctuation dissipation ratio

$$X_\infty := \lim_{s \rightarrow \infty} \left(\lim_{t \rightarrow \infty} X(t, s) \right) \quad (1.17)$$

which will, in general, not be equal to one. This quantity is essentially an amplitude ratio and is universal [45], that is it characterises the universality class of the system together

with the ageing exponents and the scaling functions. Let us make already at this point an important remark: If one requires, that X_∞ should be a nontrivial value (nonvanishing and finite) it follows [80] that necessarily $a = b$ and $\lambda_C = \lambda_R$, which can be verified by using the scaling forms (1.11) and (1.12).

However, the phenomenon of critical dynamics is not restricted to magnetic systems. Reaction-diffusion systems, which will be introduced in section 1.3 and treated in detail in chapter 4, can also display critical behaviour. In these systems $a \neq b$ may happen and this makes a modification of the definition of $X(t, s)$ necessary. As an example for a

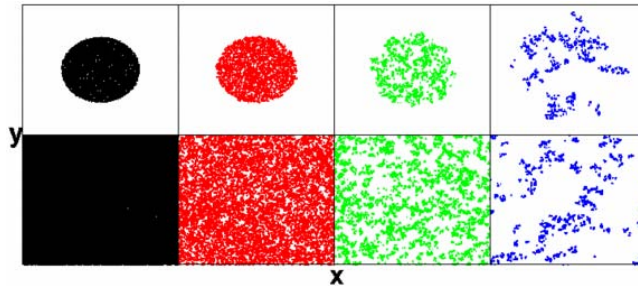


Figure 1.8: Cluster dissolution in the critical 2D contact process for two different initial conditions. The picture is taken from [203]

system of this kind, let us mention the two-dimensional fermionic contact process, which will be treated in detail in section 4.1. One has a two-dimensional lattice and particles A which occupy the lattice sites with the restriction, that at most one particle per site is allowed. Particles undergo diffusion and in addition particle creation and annihilation processes can occur. If the annihilation rate is strong enough compared to the creation rate, the particle density will drop to zero exponentially for $t \rightarrow \infty$. In the opposite case when particle creation is stronger than particle annihilation, the particle density will have a nonvanishing value for all times t . There is a critical point in between these two regimes, where the particle density also vanishes for $t \rightarrow \infty$, but algebraically. The microscopic evolution taking place in this system is illustrated in figure 1.8, where snapshots from a Monte-Carlo simulation are shown. One can see that the particle clusters dissolve gradually with time, which is markedly different from what is happening in the critical magnetic systems shown in 1.7.

1.2 Formal description of non-equilibrium dynamics

1.2.1 Field-theoretical formalism

In order to formally describe the phenomena presented in the last subsection, we shall use a field theoretical formalism, introduced in [165, 134, 24, 64, 65, 66], which has by now become standard. In what follows we briefly sketch a standard derivation of the formalism, which can be found in many books and reviews [45, 226]. We use the so-called $\hat{\text{Ito}}$ prescription, which amounts to assuming $\Theta(0) = 0$ for the Heaviside step function. In this case, it is justified [226] to drop the functional determinants, which would actually crop up during the following derivation.

The formalism starts with the stochastic Langevin equation (1.1) and considers the average of an observable \mathcal{O} . It is defined as an average over the noise η and over all $\phi(t, \mathbf{x})$ satisfying (1.1) for a given realisation of the noise [45]:

$$\langle \mathcal{O} \rangle := \int \mathcal{D}[\phi] \mathcal{O} \left[\int \mathcal{D}[\eta] \delta(\partial_t \phi - \mathcal{F}[\phi] - \eta) \mathcal{W}[\eta] \right] \quad (1.18)$$

where $\mathcal{W}[\eta]$ denotes the Gaussian functional probability distribution of the noise [226]

$$\mathcal{W}[\eta] \propto \exp \left(-\frac{1}{4} \int_{\mathbb{R}^d} d\mathbf{r} \int_0^\infty dt \eta(t, \mathbf{r}) [(\mathcal{L})^{-1} \eta(t, \mathbf{r})] \right). \quad (1.19)$$

$(\mathcal{L})^{-1}$ is the inverse of the operator \mathcal{L} introduced in (1.3). One may express the (functional) delta function in (1.18) as an integral

$$\delta(\partial_t \phi - \mathcal{F}[\phi] - \eta) = \int \mathcal{D}[\tilde{\phi}] \exp \left(\int_{\mathbb{R}^d} d\mathbf{r} \int_0^\infty dt \tilde{\phi} [\partial_t \phi - \mathcal{F}[\phi] - \eta] \right) \quad (1.20)$$

for a complex field $\tilde{\phi}$. In the resulting expression the integral over the noise can be performed and one obtains

$$\langle \mathcal{O} \rangle = \int \mathcal{D}[\phi] \mathcal{D}[\tilde{\phi}] \mathcal{O} \exp \left(-\mathcal{J}[\phi, \tilde{\phi}] \right) \quad (1.21)$$

with the *Janssen- De Dominics* response functional

$$\mathcal{J}[\phi, \tilde{\phi}] = \int_{\mathbb{R}^d} d\mathbf{r} \int_0^\infty dt \left[\tilde{\phi} (\partial_t \phi - \mathcal{F}[\phi]) - \tilde{\phi} \mathcal{L} \tilde{\phi} \right] \quad (1.22)$$

The noisy initial state is taken into account by the term

$$\mathcal{J}_{init}[\tilde{\phi}] = -\frac{1}{2} \int_{\mathbb{R}^d \times \mathbb{R}^d} d\mathbf{r} d\mathbf{r}' \tilde{\phi}(0, \mathbf{r}) a(\mathbf{r}, \mathbf{r}') \tilde{\phi}(0, \mathbf{r}'). \quad (1.23)$$

which is added to $\mathcal{J}[\phi, \tilde{\phi}]$. Here $a(\mathbf{r}, \mathbf{r}') := \langle \phi(0, \mathbf{r}) \phi(0, \mathbf{r}') \rangle$ is the *initial correlator*. The form (1.23) was introduced in [170], but Janssen had already introduced it earlier [137] in a slightly different form. The latter can be shown to be equivalent to (1.23), as Janssen proved [137] that at $t = 0$ the order parameter field is proportional to $\tilde{\phi}(0, \mathbf{r})$.

The functional (1.22) is the starting point for the field-theoretical description of the dynamics of a physical system. Although the response field $\tilde{\phi}$, introduced as an auxiliary field to simplify the calculations, has no direct physical interpretation, its usefulness becomes apparent when considering the *response function*, which we define as

$$R(t, s; \mathbf{x}, \mathbf{y}) := \left. \frac{\delta \langle \phi(t, \mathbf{x}) \rangle}{\delta h(s, \mathbf{y})} \right|_{h=0}. \quad (1.24)$$

It describes the linear response of the system to the external perturbation. On the level of the Langevin equation (1.1), an external perturbation can be introduced by adding the term $h(t, \mathbf{x})$ to the righthand side of (1.1). On the field-theoretical level, this amounts

to adding the term $-\int_{\mathbb{R}^d} d\mathbf{r} \int_0^\infty dt h(t, \mathbf{r}) \tilde{\phi}(t, \mathbf{r})$ to the functional $\mathcal{J}[\phi, \tilde{\phi}]$, as can be seen directly from (1.22). Then it follows from the definition (1.24) that

$$R(t, s; \mathbf{x}, \mathbf{y}) = \langle \phi(t, \mathbf{x}) \tilde{\phi}(s, \mathbf{y}) \rangle \quad (1.25)$$

For $\mathbf{x} = \mathbf{y}$ this reduces to the *autoresponse function*, which was already introduced above. The correlation function is defined as

$$C(t, s; \mathbf{x}, \mathbf{y}) := \langle \phi(t, \mathbf{x}) \phi(s, \mathbf{y}) \rangle \quad (1.26)$$

which also reduces for $\mathbf{x} = \mathbf{y}$ to the *autocorrelation function* defined above. The two quantities $C(t, s; \mathbf{x}, \mathbf{y})$ and $R(t, s; \mathbf{x}, \mathbf{y})$ will be the principal objects of interest for us.

1.2.2 Schrödinger invariance and local-scale invariance (LSI)

In general, the functional $\mathcal{F}[\phi]$ is rather complicated and besides a few exactly solvable models, one usually has to resort to perturbative methods in order to compute response and correlation function. However in this thesis we shall present a different approach which uses the local symmetries of $\mathcal{J}[\phi, \tilde{\phi}]$ and $\mathcal{J}_{init}[\tilde{\phi}]$. The essential idea, which will be explained in more detail in chapter 2, is the following: As the full functional $\mathcal{J}[\phi, \tilde{\phi}]$ does not have nontrivial symmetry properties, we split it up in the following way [192]

$$\mathcal{J}[\phi, \tilde{\phi}] = \mathcal{J}_0[\phi, \tilde{\phi}] + \mathcal{J}_{th}[\phi, \tilde{\phi}] \quad (1.27)$$

where

$$\mathcal{J}_0[\phi, \tilde{\phi}] = \int_{\mathbb{R}^d} d\mathbf{r} \int_0^\infty dt \left[\tilde{\phi} (\partial_t \phi - \mathcal{F}[\phi]) \right] \quad (1.28)$$

is the 'deterministic' part and

$$\mathcal{J}_{th}[\tilde{\phi}] = - \int_{\mathbb{R}^d} d\mathbf{r} dt \tilde{\phi}(t, \mathbf{r}) \left(\mathcal{L} \tilde{\phi}(t, \mathbf{r}) \right) \quad (1.29)$$

together with $\mathcal{J}_{init}[\tilde{\phi}]$ are the 'noise' parts. One proceeds now in the following way

1. Treatment of the deterministic theory: One considers the dynamical symmetries of the functional $\mathcal{J}_0[\phi, \tilde{\phi}]$ only. This theory we will also call *noiseless* or *deterministic theory*. For the simple case of $\mathcal{F}[\phi] = (2\mathcal{M})^{-1} \nabla_{\mathbf{r}}^2 \phi$ the equation of motion for ϕ deduced from $\mathcal{J}_0[\phi]$ is the well-known diffusion equation

$$\partial_t \phi = (2\mathcal{M})^{-1} \nabla_{\mathbf{r}}^2 \phi. \quad (1.30)$$

where the 'mass' \mathcal{M} is related to the diffusion constant. The symmetries of this equation are well understood [158, 177, 106, 223]. The largest group of space-time transformations $(t, \mathbf{r}) \rightarrow (t', \mathbf{r}') = g(t, \mathbf{r})$ transforming solutions of (1.30) into other solutions is called the Schrödinger group $Sch(d)$. An element of $g \in Sch(d)$ transforms the spacetime coordinates as $(t, \mathbf{r}) \rightarrow (t', \mathbf{r}') = g(t, \mathbf{r})$ with

$$t' = \frac{\alpha t + \beta}{\gamma t + \delta}, \quad \mathbf{r}' = \frac{\mathcal{R}\mathbf{r} + \mathbf{v}t + \mathbf{a}}{\gamma t + \delta}, \quad \alpha\delta - \gamma\beta = 1. \quad (1.31)$$

A solution $\phi(t, \mathbf{r})$ of (1.30) is transformed as

$$\phi(t, \mathbf{r}) \rightarrow (T_g \phi)(t, \mathbf{r}) = f_g[g^{-1}(t, \mathbf{r})]\phi(g^{-1}(t, \mathbf{r})) \quad (1.32)$$

where the factor $f_g(t, \mathbf{r})$ is given by [177]

$$f_g(t, \mathbf{r}) = (\gamma t + \delta)^{-d/2} \exp \left[-\frac{\mathcal{M}}{2} \frac{\gamma \mathbf{r}^2 + 2\mathcal{R}\mathbf{r} \cdot (\gamma \mathbf{a} - \delta \mathbf{v}) + \gamma \mathbf{a}^2 - t\delta \mathbf{v}^2 + 2\gamma \mathbf{a} \cdot \mathbf{v}}{\gamma t + \delta} \right]$$

A scaling operator transforming like (1.32) is called *quasiprimary*. In one space dimension $d = 1$ the Lie algebra \mathfrak{sch}_1 corresponding to $Sch(1)$ is spanned by set of operators $X_{-1}, X_0, X_1, Y_{-1/2}, Y_{1/2}$ and M_0 , the explicit form of which is given in the *fixed mass representation* by [106]

$$\begin{aligned} X_{-1} &= -\partial_t && \text{time translation} \\ X_0 &= -t\partial_t - \frac{1}{2}r\partial_r - \frac{x}{2} && \text{scale dilatation} \\ X_1 &= -t^2\partial_t - tr\partial_r - \frac{\mathcal{M}}{2}r^2 - xt && \text{special Schrödinger transformation} \\ Y_{-1/2} &= -\partial_r && \text{space translation} \\ Y_{1/2} &= -t\partial_r - \mathcal{M}r && \text{Galilei transformation} \\ M_0 &= -\mathcal{M} && \text{phase shift} \end{aligned} \quad (1.33)$$

which satisfy the nonvanishing commutation relations [106] (with $n \in \{-1, 0, 1\}$ and $m \in \{-1/2, 1/2\}$).

$$[X_n, X_{n'}] = (n-n')X_{n+n'}, \quad [X_n, Y_m] = (n/2-m)Y_{n+m}, \quad [Y_{1/2}, Y_{-1/2}] = M_0 \quad (1.34)$$

A quasiprimary field ϕ , that is a field transforming as (1.32), transforms under infinitesimal transformations as

$$\delta_X \phi = -\epsilon X_n \phi, \quad \delta_Y \phi = -\epsilon Y_m \phi, \quad (1.35)$$

(where ϵ is a small parameter) and it is characterised by its 'mass' \mathcal{M} and its 'scaling dimension' x . An important assumption at this point is to assume the order parameter ϕ of the system and also the corresponding response field $\tilde{\phi}$ to be quasiprimary. Looking at the equations of motion for ϕ and $\tilde{\phi}$, which can be obtained from the action $\mathcal{J}_0[\phi, \tilde{\phi}]$, one finds

$$\partial_t \phi = (2\mathcal{M})^{-1} \nabla_{\mathbf{r}}^2 \phi, \quad \text{and} \quad \partial_t \tilde{\phi} = -(2\mathcal{M})^{-1} \nabla_{\mathbf{r}}^2 \tilde{\phi} \quad (1.36)$$

This suggests that if we assign the mass \mathcal{M} to the field ϕ , we should assign the mass $-\mathcal{M}$ to $\tilde{\phi}$. For a n -point function built from quasiprimary fields one can show that

$$\sum_{i=1}^n \mathcal{X}_i \langle \phi_1(t_1, \mathbf{r}_1) \dots \phi_n(t_n, \mathbf{r}_n) \rangle_0 = 0 \quad (1.37)$$

where \mathcal{X}_i is one of the generators (1.33) acting on the coordinates of the i -th field. By $\langle \dots \rangle_0$ we mean that the average is computed with respect to $\mathcal{J}_0[\phi, \tilde{\phi}]$ only. This equation provides a set of partial differential equations which allow to fix (at least

partially) the n -point function of the deterministic theory. For instance the two-point function is given by [106]

$$\langle \phi_1(t_1, \mathbf{r}_1) \phi_2(t_2, \mathbf{r}_2) \rangle_0 = \delta_{x_1, x_2} \delta_{\mathcal{M}_1, -\mathcal{M}_2} (t_1 - t_2)^{-x_1} \exp\left(-\frac{\mathcal{M}_1 (\mathbf{r}_1 - \mathbf{r}_2)^2}{2(t_1 - t_2)}\right). \quad (1.38)$$

From this one can see, that the critical exponent in this case is $z = 2$. One can even extend these considerations further by considering the dimensionful constant \mathcal{M} as a variable [111], but we shall not enter into the details of this. We defer the interested reader to [126].

2. Reduction of the noisy theory: From the operator M_0 and the condition (1.37) one can deduce that an n -point function built of quasiprimary fields is zero, unless the sum of the masses of the fields is zero. This is the so-called *Bargmann superselection rule* [11, 106]. From this it follows that

$$\underbrace{\langle \phi \dots \phi \rangle}_n \underbrace{\langle \tilde{\phi} \dots \tilde{\phi} \rangle}_m = 0 \quad \text{unless} \quad n = m \quad (1.39)$$

Notice, that it is only necessary to assume invariance under $Y_{-1/2}$ and $Y_{1/2}$ (translation invariance and Galilei invariance) in order to obtain this rule. This fact allows to reduce the full theory to quantities, which can be determined in the deterministic theory. More precisely one has [192]

$$\begin{aligned} R(t, s; \mathbf{x}, \mathbf{y}) &= \langle \phi(t, \mathbf{x}) \tilde{\phi}(s, \mathbf{y}) \rangle \\ &= \left\langle \phi(t, \mathbf{x}) \tilde{\phi}(s, \mathbf{y}) \exp\left(-\mathcal{J}_{th}[\tilde{\phi}]\right) \exp\left(-\mathcal{J}_{init}[\tilde{\phi}]\right) \right\rangle_0. \end{aligned} \quad (1.40)$$

Each exponential is now developed into a series. Taking into account the explicit form of $\mathcal{J}_{th}[\tilde{\phi}]$ and $\mathcal{J}_{init}[\tilde{\phi}]$ and the Bargmann superselection rule (1.39) one realises that only the first term of the series survives and therefore [192]

$$R(t, s; \mathbf{x}, \mathbf{y}) = \left\langle \phi(t, \mathbf{x}) \tilde{\phi}(s, \mathbf{y}) \right\rangle_0. \quad (1.41)$$

The quantity on the righthand side is computed with respect to the deterministic part of the theory. Similar considerations yield for the correlation function [192]

$$\begin{aligned} C(t, s; \mathbf{x}, \mathbf{y}) &= \int_{\mathbb{R}^d} d\mathbf{R} \int_0^\infty du \left\langle \phi(t, \mathbf{x}) \phi(s, \mathbf{y}) \mathcal{L} \tilde{\phi}^2(u, \mathbf{R}) \right\rangle_0 \\ &+ \frac{1}{2} \int_{\mathbb{R}^d \times \mathbb{R}^d} d\mathbf{R} d\mathbf{R}' \left\langle \phi(t, \mathbf{x}) \phi(s, \mathbf{y}) \tilde{\phi}(0, \mathbf{R}) \tilde{\phi}(0, \mathbf{R}') \right\rangle_0 a(\mathbf{R}, \mathbf{R}') \end{aligned} \quad (1.42)$$

We have therefore expressed the two quantities of interest through two-, three- and fourpoint functions of the deterministic theory, which can be (at least partially) fixed by symmetries with the help of (1.37).

For the above considerations a comparatively simple form of the functional $\mathcal{F}[\phi] = (2\mathcal{M})^{-1} \nabla_{\mathbf{r}}^2 \phi$ was used (which leads to the value $z = 2$), which amounts to a linear equation of motion for ϕ . There have been however extensive comparisons with numerical results from nonlinear models [112, 110, 114], which yielded an excellent agreement. For

this reason the predictions coming from Schrödinger invariance are expected to hold for a much larger range of models with $z = 2$, but we stress that this has not been proven yet. A natural question is how the approach can be extended to include also more general forms of $\mathcal{F}[\phi]$. To do this for the case $z = 2$, one has to consider nonlinear Schrödinger equations and their symmetries. One goal of this thesis is to use recent work of Stoimenov [222, 223] to make progress into this direction.

Another question is, how one can generalise this approach to values of z different from 2. A first step has been done in [109], which allowed for a prediction of the autoresponse function also for values $z \neq 2$. Several tests for $z \neq 2$ have been performed (see [126, 124] for recent reviews), but a complete generalisation of the above ideas to systems with $z \neq 2$ is still lacking and it will be another goal of this thesis to provide such a generalisation.

1.3 Objectives of this thesis

The first objective of this thesis is to generalise the considerations of the last section to an arbitrary value of z . The idea how to generalise the treatment of the deterministic part of the theory has already been proposed in [109]. It is a purely algebraic construction generalising the generators (1.33), which is based on special cases known from the past like Schrödinger invariance and conformal invariance. This theory, which plays a crucial rôle in this work is called *theory of local scale invariance* and we will refer to it with the shorthand LSI from now on. The construction of the generators is based on the following axioms, which will be introduced in more detail in chapter 2.

1. Möbius transformations of the time coordinate occur, i. e.

$$t \rightarrow t' = \frac{\widehat{\alpha}t + \widehat{\beta}}{\widehat{\gamma}t + \widehat{\delta}}; \quad \text{with} \quad \widehat{\alpha}\widehat{\delta} - \widehat{\beta}\widehat{\gamma} = 1 \quad (1.43)$$

where $\widehat{\alpha}, \widehat{\beta}, \widehat{\delta}, \widehat{\gamma}$ are real parameters. The infinitesimal generators of these transformations are denoted by X_n (with $n \in \{-1, 0, 1\}$) and the commutator between these generators is given by

$$[X_n, X_m] = (n - m)X_{n+m}. \quad (1.44)$$

Scaling operators which transform covariantly under (1.43) are called *quasiprimary* in analogy to the notion of conformal quasiprimary operators [26].

2. The generator of scale transformations X_0 is given by

$$X_0 = -t\partial_t - \frac{1}{z}r \cdot \partial_r - \frac{x}{z}. \quad (1.45)$$

Here, x is the scaling dimension of the quasiprimary field on which X_0 acts.

3. Spatial translation invariance is required.
4. When acting on quasiprimary fields ϕ , extra terms coming from the scaling dimension of ϕ must be present in the generators and be compatible with (1.45).

5. By analogy with Schrödinger invariance, mass terms should be present.
6. Application of the generators yields a *finite* number of independent conditions for the two-point functions built from quasiprimary fields. This will usually be achieved by the requirement that the generators form a finite-dimensional Lie algebra.

These axioms have allowed for a systematic construction of infinitesimal generators, which we will recall in chapter 2.

Although this theory has been successfully applied to the autoresponse function of systems with $z \neq 2$ (see [124, 126] for reviews), it is at present plagued with several problems:

- The generalisation of the Bargmann superselection rule (1.39) has only been given for two-point functions. Therefore the treatment of noisy systems was not possible yet and the predictions for the autoresponse function lack an important justification.
- The computation of three- or fourpoint functions has not been possible yet. They are however needed for the computation of correlation functions by LSI.
- We have realised [21, 20], that for long-range spherical model the LSI- prediction of the response function is incorrect. The question is whether the theory can be modified as to yield a correct prediction.

In this thesis, we will provide an answer to all these questions by proposing a new version of LSI. We will modify the construction of the mass terms, which should be present according to fifth axiom of LSI. This new version of LSI is formulated in chapter 2, where we also compute the new LSI-predictions for response and correlation functions.

These predictions will be thoroughly compared to concrete models in chapter 3. These will be for example certain magnetic models such as the long-range spherical model, the spherical model with conserved order parameter or the diluted Ising model. For the long-range spherical model we shall also address the question whether the composite fields are quasiprimary or not.

We shall see in the same chapter that the magnetic systems considered up until now are not the only physical systems which display dynamical scaling. A completely different type of system occurs during surface growth processes or interface fluctuations [208]. These phenomena can be observed in many experimental situations, for instance in biological systems [78] or atomic deposition processes [6]. As an experimental example for a one-dimensional fluctuation surface, we show in the left panel of figure 1.9 a STM-picture of a gold sample, which has been cut nearly parallel to the (110)-surface. The surface then has steps with the height of a monolayer, one of which is shown in the picture. The microscopic processes which can take place at this step are depicted in the right panel of figure 1.9: (1) New particles can attach to or detach from the step by evaporation or condensation, (2) particles can undergo diffusion on the surface or (3) particles can undergo diffusion along the step. When looking at the STM-picture, one can clearly see that the step gets rougher when the temperature is increased. These type of system can be described on a mesoscopic level by Langevin equations [150] similar to the ones encountered for the description of magnetic systems. The order parameter is simply the height field $h(t, \mathbf{x})$ which describes the height of the surface over the substrate at time

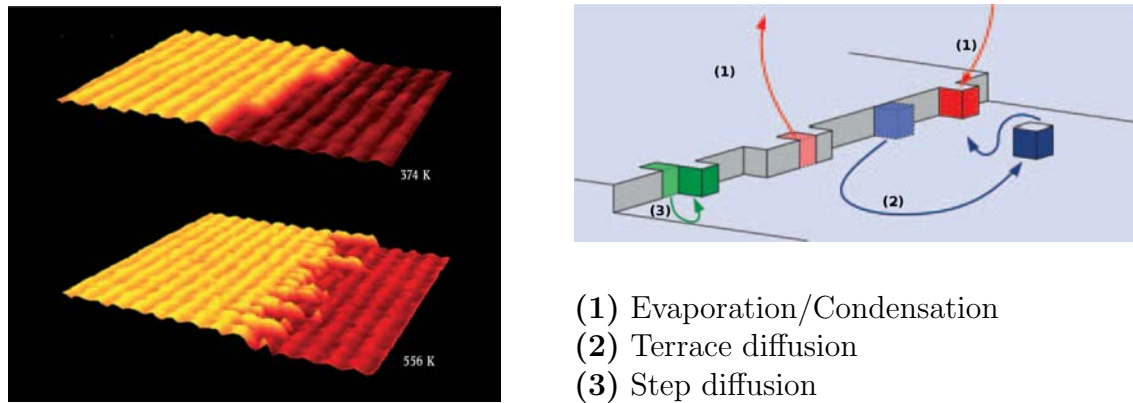


Figure 1.9: Left panel: STM-picture of a $Au(110)$ -surface with a step and two kinks at temperature $374K$ (top) and $556K$ (bottom). One can observe the roughening of the step. Right panel: Microscopic processes which can occur during the kinetic roughening. **(1)** Evaporation or condensation of particles, **(2)** terrace diffusion of particles and **(3)** step diffusion along the step. Pictures are taken from [216]

t and place \mathbf{x} . The most famous Langevin equation describing these phenomena is the KPZ-equation [141](after **K**ardar, **P**arisi and **Z**hang) or its modified version for a conserved order parameter [226]. These equations are fairly difficult to treat, but as a first step we look at linearised versions of them: The Edward-Wilkinson equation [79] and the Mullins-Herring equation [175, 231] which turn out to display ageing behaviour and to be suitable for the treatment with LSI. This is described in section 3.1.

Still another type of system is provided by so-called *reaction-diffusion* systems, which will be considered in chapter 4. These systems can be considered as simple examples for chemical reactions, but are also used to model traffic problems or the propagation of diseases or fires. Their investigation is the second objective of this thesis.

Reaction-diffusion systems, as opposed to magnetic systems, in general do not satisfy the detailed balance condition, that is there is no local time-reversal symmetry. This entails that these systems never tend to an equilibrium state. The general setup we shall consider in chapter 4 is the following: On a d -dimensional cubic lattice particles A undergo diffusion³ and at the same time, particle creation or annihilation processes can occur. The system can be either *fermionic*, which means, that only one particle per site is allowed, or *bosonic*, which means that there is no restriction on the number of particles on one site.

The most prominent reaction-diffusion system is the fermionic contact process (CP), which allows (apart from particle diffusion) for spontaneous particle desintegration ($A \rightarrow \emptyset$) and the particle creation process $A \rightarrow 2A$, where the offspring particle is placed randomly at an empty nearest neighbour site (if there is any). The universality class of this system is the *directed percolation* universality class (DP), which is arguably the most important universality class in theoretical studies of out-of-equilibrium systems [139, 227, 228, 102, 178]. The importance of this universality class is also due to its robustness with respect

³We shall restrict ourselves to one type of particles only, although systems with several sorts of particles have also been considered, see for instance [227, 228] and references therein

to the microscopic details of the underlying physical process. As a matter of fact, a very long list of examples could be given for systems belonging to this universality class. The Janssen-Grassberger conjecture [135, 98] states that a model should belong to the DP universality class provided it (i) has a scalar, positive order parameter, (ii) displays a continuous phase transition from a fluctuating active phase into a unique absorbing state, (iii) the dynamic rules are short-ranged and (iv) there are no further attributes like additional symmetries or randomness involved. Therefore the directed percolation process is central to the understanding of non-equilibrium phenomena. In this sense, the DP universality class plays a somewhat analogous rôle to the Ising model for equilibrium dynamics. We will look closer at the ageing behaviour of this system in section 4.1 of chapter 4.

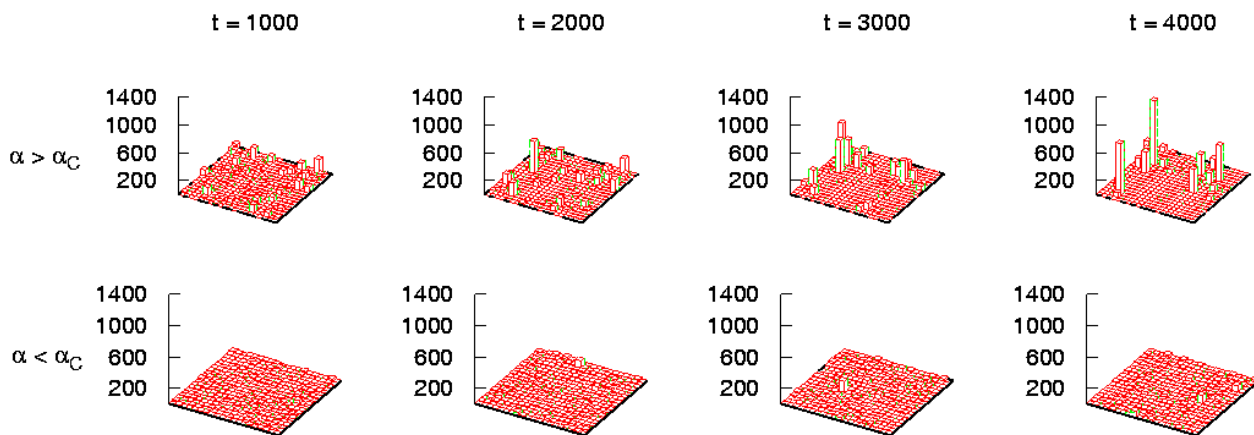


Figure 1.10: Illustration of the phase transition occurring in the bosonic pair contact process (BPCPD). The system is a cube of $20 \times 20 \times 20$ sites (with periodic boundary conditions). Initially each site was occupied by ten particles. The pictures show the number of particles on the sites of one layer of the cube at different times (in Monte Carlo steps). The situation for dominant reactions ($\alpha > \alpha_c$, upper line) and for dominant diffusion ($\alpha < \alpha_c$, lower line) are compared. For the former situation, the pile-up of particles on few lattice sites is nicely observed, whereas for the latter case, the system stays essentially homogeneous.

In spite of its simple microscopic rules, the fermionic contact process can not be solved exactly. One can however consider the bosonic version of this process, the bosonic contact process with diffusion (BCPD) [129, 184, 15], which is exactly solvable. It has been used in [129] to study clustering phenomena in biological systems. Particles undergo diffusion (with constant D) and the processes $A \rightarrow \emptyset$ and $A \rightarrow 2A$ take place on *one* site with rates λ and μ respectively. Offspring particles are placed on the same site as the original particle. The system can be solved exactly and one realises [129, 184] that for $\mu = \lambda$,

i.e. if creation and annihilation processes balance each other, the particle density remains constant, provided a homogeneous initial particle distribution was chosen. In this case it turns out [129, 184], that for $d \leq 2$ the system shows a *clustering transition*, which means that particles start piling up on very few lattice sites. For $d > 2$ this is not the case and the system stays homogeneous. Another example for a system of this type is the bosonic pair-contact process with diffusion (BPCPD) [184, 185, 15]. Here the reactions $2A \rightarrow A$ and $2A \rightarrow 3A$ can take place with rates λ and μ respectively. As outlined in section 4.2 this model is also exactly solvable if creation and annihilation processes occur with the same rate $\mu = \lambda$, which entails that the particles density remains constant for a homogeneous initial distribution. For $d \leq 2$ clustering occurs, whereas for $d > 2$, the control parameter $\alpha = \mu/D$ plays a crucial rôle (with the diffusion constant D). For small α (i.e. if diffusion dominates reactions) the system remains homogeneous, whereas for α larger than a certain critical value α_c a clustering transition occurs. In picture 1.10 we show for illustrational purposes a Monte-Carlo simulation of this system, at which we will look more closely in section 4.2. We shall derive the two-time quantities and show in 4.3 that the exact results thus obtained can be understood by an extension of LSI to nonlinear situations. However it will also be shown that in other systems like in the fermionic contact process new problems arise which can not yet be tackled by LSI in a satisfying way.

Up until now, only systems were considered, in which spatial translation invariance holds. All real systems will of course have surfaces, edges and corners, which can change the physical behaviour. As a first step towards a more realistic situation one can consider semi-infinite magnetic systems with a surface. It is for instance known that in such a system at the critical temperature, the static universality class of the system splits up into different surface universality classes. Much less is known about the ageing dynamics of such systems, even though some works have been done in the past [195, 45]. In [195, 45] it was shown that one can reasonably define a *surface autoresponse function* and a *surface autocorrelation function* by considering the quantities (1.9) close to the surface. This in turn allows for the definition of a *surface ageing exponents*, *surface scaling functions* and a *surface fluctuation-dissipation ratio* in a similar way as done in (1.11),(1.12) and (1.16) for a bulk system. These surface quantities do not necessarily need to agree with the corresponding bulk quantities, as was already shown in [195, 45]. A third objective of this thesis is to address this situation and provide additional results to what was already stated in [195, 45].

To sum up, the aim of this thesis is threefold

1. We want to generalise, starting from earlier works [109], the existing theory of local scale invariance (LSI) to the case of arbitrary dynamical exponent z . This will include a generalisation of the Bargmann superselection rule which allows for an reduction of the noisy theory to expressions computed in the noiseless theory. The formulation of this theory will be given in chapter 2, before it will be compared to concrete examples in chapter 3. In section 3.1 we will consider surface-growth models, whereas in 3.2 the spherical model with conserved order parameter will be looked at. In section 3.3 we will then consider the spherical model with long range interaction and shall also address the question whether composite fields are quasiprimary or not.

2. We want to extend the investigation of ageing phenomena in reaction-diffusion system. The results of this will be presented in chapter 4. In section 4.1 we will add some results obtained from renormalisation group techniques, before we look at two exactly solvable models in section 4.2. Finally, in section 4.3 we show how the existing theory for $z = 2$ can be extended to nonlinear theories and be used to describe the reaction-diffusion systems considered in 4.2.
3. Lastly, we wish to extend the study of non-equilibrium phenomena at surfaces of semi-infinite systems, which will be done in chapter 5. First we will provide an exactly solvable case in section 5.1. In section 5.2 we will then provide some more exact result but also simulational results, which help to provide a fairly complete picture about ageing in semi-infinite geometries.

To a very large extend the results presented in what follows have already been published in scientific journals. Others have already appeared as preprints. For space considerations, some of these articles have been included in a slightly shortened form. In particular many appendices have been dropped. They can be found in the original papers, a complete list of which is given below.

1. F. Baumann, M. Henkel, M. Pleimling and J. Richert, *Ageing without detailed balance in the bosonic contact and pair-contact processes: Exact results*. J. Phys. A: Math. Gen. **38**, 6623 (2005).
2. F. Baumann and M. Pleimling, *Out-of-equilibrium properties of the semi-infinite kinetic spherical model*. J. Phys. A: Math. Gen. **39**, 1981 (2006).
3. F. Baumann, S. Stoimenov and M. Henkel, *Local scale-invariances in the bosonic contact and pair-contact processes*. J. Phys. A: Math. Gen. **39**, 4095 (2006).
4. F. Baumann, *Ageing without detailed balance: local scale-invariance applied to two exactly solvable models*. J. Phys.: Conf. Ser. **40**, 86 (2006).
5. A. Röthlein, F. Baumann and M. Pleimling, *Symmetry based determination of space-time functions in nonequilibrium growth processes*. Phys. Rev. **E 74**, 061604 (2006); erratum: Phys. Rev. **E 76**, 019901(E) (2007).
6. F. Baumann and A. Gambassi, *Ageing in the contact process: Scaling behaviour and universal features*. J. Stat. Mech., P01002 (2007).
7. F. Baumann and M. Henkel, *Kinetics of phase-separation in the critical spherical model and local scale-invariance*, J. Stat. Mech., P01012 (2007).
8. M. Henkel and F. Baumann, *Autocorrelation functions in phase-ordering kinetics from local-scale invariance*, J. Stat. Mech., P07015 (2007).
9. F. Baumann, S.B. Dutta and M. Henkel, *Kinetics of the long-range spherical model* J. Phys. A: Math. Theor. **40**, 7389 (2007)
10. F. Baumann and M. Pleimling, *Local aging phenomena close to magnetic surfaces*, Phys. Rev. **B 76**, 104422 (2007).

11. F. Baumann and M. Henkel, *Towards a theory of local scale-invariance: non-equilibrium systems with an arbitrary dynamical exponent z* , submitted to Nucl. Phys. B
12. F. Baumann, M. Henkel and M. Pleimling, *Phase-ordering kinetics of two-dimensional disordered Ising models*, submitted to Europhys. Lett.

Chapter 2

Theory of local scale-invariance (LSI)

2.1 Introduction

We have outlined in chapter 1 that we are interested in the long-time dynamics of systems undergoing *ageing* behaviour, that is, systems with (i) a slow, non-exponential dynamics, (ii) dynamical scaling and (iii) breaking of time-translation invariance. They are conveniently described by the two-time response and correlation functions of its time-dependent order-parameter $\phi = \phi(t, \mathbf{r})$ for which one usually assumes the scaling forms (1.11) and (1.12) in the scaling regime. We quote a slightly more general form, which also includes the space-dependence [37, 94, 60, 45, 122]

$$R(t, s; \mathbf{r}) = \left. \frac{\delta \langle \phi(t, \mathbf{r}) \rangle}{\delta h(s, \mathbf{0})} \right|_{h=0} \sim s^{-a-1} f_R \left(\frac{t}{s}, \frac{\mathbf{r}}{s^{1/z}} \right) \quad ; \quad f_R(y, \mathbf{0}) \stackrel{y \rightarrow \infty}{\sim} y^{-\lambda_R/z} \quad (2.1)$$

$$C(t, s; \mathbf{r}) = \langle \phi(t, \mathbf{r}) \phi(s, \mathbf{0}) \rangle \sim s^{-b} f_C \left(\frac{t}{s}, \frac{\mathbf{r}}{s^{1/z}} \right) \quad ; \quad f_C(y, \mathbf{0}) \stackrel{y \rightarrow \infty}{\sim} y^{-\lambda_C/z} \quad (2.2)$$

where h is the magnetic field conjugate to ϕ and the initial conditions are assumed to be such that $\langle \phi(t, \mathbf{r}) \rangle = 0$ for all times. Space-translation invariance will be assumed throughout this chapter and we recall that in writing these scaling forms, one assumes the existence of a single time-dependent length scale $L = L(t) \sim t^{1/z}$ which defines the dynamical exponent z .

Present attempts to calculate the exponents and the corresponding scaling functions usually [128] start from a master equation for the probability distribution or else from a stochastic Langevin equation for the order-parameter

$$2\mathcal{M} \frac{\partial \phi(t, \mathbf{r})}{\partial t} = \Delta \phi(t, \mathbf{r}) - \frac{\delta \mathcal{V}[\phi]}{\delta \phi(t, \mathbf{r})} + \eta(t, \mathbf{r}) \quad (2.3)$$

where \mathcal{V} is a Ginzbourg-Landau potential, the ‘mass’ \mathcal{M} plays the rôle of the kinetic coefficient and η is a Gaussian noise with zero average and variance $\langle \eta(t, \mathbf{r}) \eta(t', \mathbf{r}') \rangle = 2T \delta(t - t') \delta(\mathbf{r} - \mathbf{r}')$ where T is the temperature of the heat bath. In the classification of Hohenberg and Halperin [128], the above Langevin equation with a non-conserved order-parameter is called ‘model A’, the conserved case (‘model B’) is obtained by applying an extra $-\nabla^2$ operator to the right-hand-side of (2.3). We consider n -point observables (n -point functions)

$$F^{(n)}(t_1, \dots, t_n; \mathbf{r}_1, \dots, \mathbf{r}_n) = \langle \psi_1(t_1, \mathbf{r}_1) \dots \psi_n(t_n, \mathbf{r}_n) \rangle \quad (2.4)$$

where ψ can stand either for an order-parameter field ϕ or else for the associate response field $\tilde{\phi}$ of non-equilibrium field-theory [66, 137, 226]. This equation is to be completed by stochastic initial conditions representing the disordered initial state. In the context of non-equilibrium field-theory correlation functions $C(t, s) = \langle \phi(t)\phi(s) \rangle$ and response functions $R(t, s) = \langle \phi(t)\tilde{\phi}(s) \rangle$ can be treated simultaneously. Dynamical scaling is then expressed through the relation

$$F^{(n)}(b^z t_1, \dots, b^z t_n; b\mathbf{r}_1, \dots, b\mathbf{r}_n) = b^{-(x_1 + \dots + x_n)} F^{(n)}(t_1, \dots, t_n; \mathbf{r}_1, \dots, \mathbf{r}_n) \quad (2.5)$$

where b is a constant rescaling factor and x_i the scaling dimension of the fields ψ_i . Motivated by an analogy with conformal invariance [26], it has been suggested to generalise dynamical scaling to a *local* scaling where $b = b(t, \mathbf{r})$ may depend on time and on space [106, 109]. Indeed, the best known examples of such local scale-transformations are for $z = 1$ conformal transformations and for $z = 2$ the elements of the Schrödinger group [177, 99, 142]. Starting from those, it was shown earlier [109] that infinitesimal local scale transformations can be constructed for any given value of z and that these are indeed dynamical symmetries of certain linear partial differential equations. Assuming that the response functions $R(t, s; \mathbf{r})$ transform covariantly under local scale-transformations, its form is fixed through certain linear (fractional) differential equations whereas the exponents $a, \lambda_R/z$ have to be determined independently. In particular, the form of the resulting autoresponse function $R(t, s) := R(t, s; \mathbf{0})$ has been confirmed for a large class of models, both with $z = 2$ and $z \neq 2$, including simple and disordered magnets [125] and kinetics of models without detailed balance [125]. Conceptually, however, the agreement of the prediction of a dynamical symmetry of a *deterministic* equation and the results of *stochastic* models is surprising, since it is easy to see that the noise terms in the stochastic Langevin equation destroy almost all dynamical symmetries the ‘deterministic part’ alone might have. For the special case $z = 2$, this problem was solved [192] in realising that because of the Bargmann superselection rules which follow from the assumed Galilei-invariance of the deterministic part an exact reduction formula for the average of any observable to an average within the deterministic part alone can be derived. In particular, this not only explains why $R(t, s)$ could be successfully tested but is also enough to explain the available results for the space-time response function $R(t, s; \mathbf{r})$ in several exactly solvable models as well as in non-integrable models such as $2D/3D$ Ising models and $2D$ q -states Potts models quenched to $T < T_c$ as reviewed in detail in [125, 124]. On the other hand, a quantitative prediction for the autocorrelation function $C(t, s) := C(t, s; \mathbf{0})$ can only be obtained for $z = 2$ if one further assumes that the Schrödinger-invariance of the deterministic part may be extended to a new type of conformal invariance in $d + 2$ dimensions [111, 192]. This extension could be tested and confirmed in the $2D$ Ising [114] and Potts models [161] quenched to $T < T_c$ and is compatible with the results in several exactly solvable models, see [126] for a recent review.

In this chapter, we present the extension of LSI to *stochastic* Langevin equation satisfying dynamical scaling with a dynamical exponent $z \neq 2$. In section 2.2, we recall first some standard facts about conformal invariance ($z = 1$), Schrödinger-invariance ($z = 2$) and a further non-trivial dynamical symmetry, again with $z = 1$. We then recall the basic axioms of local scale-invariance (LSI) [109] and recall the main features of it. However, motivated by specific model results with $z < 2$ on the space-time response $R(t, s; \mathbf{r})$ [19], we reconsider the details of the construction of so-called ‘mass terms’ in the infinitesimal generators of LSI which requires the construction of a new type of fractional derivative the

properties of which are derived in appendix A. We then write down *linear* deterministic equations on which the new generators of LSI acts as dynamical symmetries and then derive, for the first time, generalised Bargmann superselection rules valid for $z \neq 2$. Remarkably, these imply a factorisation property for the n -point function $F^{(n)}$ which looks quite analogous to requirements seen in integrable systems, see e.g. [235, 236]. In section 2.3, we combine local scale-transformations with non-equilibrium field-theory, split the action $\mathcal{J}[\phi, \tilde{\phi}] = \mathcal{J}_0[\phi, \tilde{\phi}] + \mathcal{J}_b[\tilde{\phi}]$ into a ‘deterministic part’ \mathcal{J}_0 and a ‘noise part’ \mathcal{J}_b and derive exact reduction formulæ for the average $\langle \mathcal{O} \rangle = \langle \mathcal{O} e^{-\mathcal{J}_b} \rangle_0$ to the ‘noiseless’ average implying only the action \mathcal{J}_0 , for any observable \mathcal{O} . In section 2.4, we calculate the two- and four-point functions for the ‘deterministic’ theory and use the results in section 2.5 to derive the LSI-predictions for the two-time response function $R(t, s; \mathbf{r})$ and the two-time correlation function $C(t, s; \mathbf{r})$. In particular, it will be shown that the predicted autoresponse function $R(t, s)$ is identical to the form found from our earlier formulation [109]. This means that all tests performed on LSI using $R(t, s)$, see [125, 124], do remain valid, with the bonus that we now understand how to treat stochastic problems which was not possible before. The tests of these predictions are deferred to chapter 3. The conclusions of this chapter are given in section 2.6 and some technical points of the calculations can be found in the appendices of [20].

2.2 Local scale-invariance

In this section, we recall first some background material on local scale-invariance (LSI), namely two kinds of conformal invariance as well as Schrödinger-invariance, before recalling the basic axioms of LSI. The LSI-construction of infinitesimal generators without mass terms [109] is repeated and for reference we briefly review the main results of the older formulation of local scaling. We then introduce our new generators and derive some basic consequences, notably the invariant linear deterministic equations and the generalised Bargmann superselection rules.

2.2.1 Background on local scale-transformations

We briefly recall some known groups of local scale-transformations, either with $z = 1$ (usual conformal invariance as well as a variant more appropriate for dynamics) or with $z = 2$ (Schrödinger-invariance).

Conformal invariance

Let us recall some basic aspects of conformal invariance, for later convenience in $(1+1)D$, with directions labelled as ‘time’ t and ‘space’ r . We shall be brief and refer to the literature e.g. [51, 72, 107] for further information. In terms of the complex variables

$$z = t + ir, \quad \bar{z} = t - ir \quad (2.6)$$

conformal transformation include the projective transformations (which have analogues in $(1+d)$ dimensions)

$$z \rightarrow z' = \frac{\hat{\alpha}z + \hat{\beta}}{\hat{\gamma}z + \hat{\delta}}, \quad \hat{\alpha}\hat{\delta} - \hat{\beta}\hat{\gamma} = 1 \quad (2.7)$$

for z and similarly for \bar{z} . Writing $z' = z + \epsilon(z)$, the infinitesimal generators of this transformations read for ($n \in \{-1, 0, 1\}$)¹

$$\ell_n = -z^{n+1}\partial_z, \quad \bar{\ell}_n = -\bar{z}^{n+1}\partial_{\bar{z}}. \quad (2.8)$$

and satisfy

$$[\ell_n, \ell_m] = (n-m)\ell_{n+m}, \quad [\ell_n, \bar{\ell}_m] = 0, \quad [\bar{\ell}_n, \bar{\ell}_m] = (n-m)\bar{\ell}_{n+m} \quad (2.9)$$

Now consider the 2D Laplace equation

$$\mathcal{S}\phi(z, \bar{z}) = 0, \quad \text{with } \mathcal{S} := \partial_z\partial_{\bar{z}} \quad (2.10)$$

where one has the following commutation relations

$$[\mathcal{S}, \ell_n] = -(n+1)z^n\mathcal{S}, \quad [\mathcal{S}, \bar{\ell}_n] = -(n+1)\bar{z}^n\mathcal{S}. \quad (2.11)$$

Hence we recover the well-known facts that (i) the finite transformations (2.7) send a solution of (2.10) into another solution and (ii) that any analytic function $z' = f(z)$ generates a dynamical symmetry of the 2D Laplace equation.

The generators have to be modified when acting on so-called (*quasi*-)primary scaling operators ϕ_i .² By definition, these transform in the simplest possible way [213, 26]

$$\delta\phi_i(z, \bar{z}) = (\Delta_i\epsilon'(z) + \epsilon(z)\partial_z + \bar{\Delta}_i\bar{\epsilon}'(\bar{z}) + \bar{\epsilon}(\bar{z})\partial_{\bar{z}})\phi_i(z, \bar{z}) \quad (2.12)$$

where Δ_i and $\bar{\Delta}_i$ are called the conformal weights of the operator ϕ_i . If $\epsilon(z)$ can stand for any infinitesimal function, then ϕ_i is called *primary*, but if $\epsilon(z)$ is merely an infinitesimal projective transformation, ϕ_i is merely *quasiprimary* [26]. If ϕ_i is a scalar under (space-time) rotations (we shall always assume this to be the case), $\Delta_i = \bar{\Delta}_i = x_i/2$, where x_i is the scaling dimension of ϕ_i . If $\epsilon(z) = \varepsilon z^{n+1}$, one has $\delta\phi_i(z, \bar{z}) = -\varepsilon(\ell_n + \bar{\ell}_n)\phi_i(z, \bar{z})$ where the generators $\ell_n, \bar{\ell}_n$ now read

$$\ell_n = -z^{n+1}\partial_z - \Delta_i(n+1)z^n, \quad \bar{\ell}_n = -\bar{z}^{n+1}\partial_{\bar{z}} - \Delta_i(n+1)\bar{z}^n \quad (2.13)$$

and again satisfy (2.9). The scaling dimension x_i can be considered as quantum number characterising the field ϕ_i . If one would consider for instance the two-point correlator $F^{(2)}(t_1, t_2, r_1, r_2) = \langle\phi_1(t_1, r_1)\phi_2(t_2, r_2)\rangle$, each field would be characterised by its own scaling dimension x_i so that x_1 and x_2 appear as parameters in the two-point function.

In view of the intended generalisations to dynamics, we prefer to work with the generators

$$X_n = \ell_n + \bar{\ell}_n, \quad Y_n = i(\ell_n - \bar{\ell}_n) \quad (2.14)$$

which satisfy the commutation relations

$$[X_n, X_m] = (n-m)X_{n+m}, \quad [X_n, Y_m] = (n-m)Y_{n+m}, \quad [Y_n, Y_m] = -(n-m)X_{n+m} \quad (2.15)$$

The well-known two-point function $F^{(2)}(t_1, t_2; r_1, r_2)$ of quasiprimary scaling operators reads

$$\begin{aligned} F^{(2)}(t_1, t_2; r_1, r_2) &= f_{12}\delta_{x_1, x_2}((z_1 - z_2)(\bar{z}_1 - \bar{z}_2))^{-x_1} \\ &= f_{12}\delta_{x_1, x_2}((t_1 - t_2)^2 + (r_1 - r_2)^2)^{-x_1} \end{aligned} \quad (2.16)$$

with a normalisation constant f_{12} [201].

¹In principle one can write down the generators for all $n \in \mathbb{Z}$. The existence of this infinite-dimensional Lie algebra, known as the Virasoro algebra without central charge, is peculiar to two dimensions

²We follow here the terminology proposed by Cardy [51].

Schrödinger-invariance

The Schrödinger group [177, 99, 142] is the largest group of space-time transformations $(t, \mathbf{r}) \rightarrow (t', \mathbf{r}') = g(t, \mathbf{r})$ which send a solution of the free Schrödinger/diffusion equation (the ‘mass’ \mathcal{M} plays the rôle of a diffusion constant)

$$\mathcal{S}\psi = 0 \quad , \quad \text{where } \mathcal{S} = (2\mathcal{M}\partial_t + \nabla_{\mathbf{r}}^2) \quad (2.17)$$

into another solution through $\psi(t, \mathbf{r}) \rightarrow T_g\psi$ with $(T_g\psi)(t, \mathbf{r}) = f_g(g^{-1}(t, \mathbf{r}))\psi(g^{-1}(t, \mathbf{r}))$. The function $f_g(t, \mathbf{r})$ can be computed explicitly [177] and the space-time transformations are

$$\mathbf{r} \rightarrow \mathbf{r}' = \frac{\mathcal{R}\mathbf{r} + \mathbf{v}t + \mathbf{a}}{\widehat{\gamma}t + \widehat{\delta}} \quad , \quad t \rightarrow t' = \frac{\widehat{\alpha}t + \widehat{\beta}}{\widehat{\gamma}t + \widehat{\delta}} \quad ; \quad \widehat{\alpha}\widehat{\delta} - \widehat{\beta}\widehat{\gamma} = 1 \quad (2.18)$$

where $\widehat{\alpha}, \widehat{\beta}, \widehat{\gamma}, \widehat{\delta}, \mathbf{v}, \mathbf{a}$ are real parameters and \mathcal{R} is a rotation matrix in d spatial dimensions. In $d = 1$ space dimensions, to which we restrict ourselves here for simplicity (then $\mathcal{R} = 1$), the infinitesimal generators read [106]

$$\begin{aligned} X_n &= -t^{n+1}\partial_t - \frac{n+1}{2}t^n r \partial_r - \frac{n(n+1)}{4}\mathcal{M}t^{n-1}r^2 - \frac{x}{2}(n+1)t^n \\ Y_m &= -t^{m+1/2}\partial_r - \left(m + \frac{1}{2}\right)\mathcal{M}t^{m-1/2}r \\ M_n &= -\mathcal{M}t^n \end{aligned} \quad (2.19)$$

and satisfy the commutation relations

$$\begin{aligned} [X_n, X_{n'}] &= (n - n')X_{n+n'} \quad , \quad [X_n, Y_m] = \left(\frac{n}{2} - m\right)Y_{n+m} \quad , \quad [X_n, M_{n'}] = -n'M_{n+n'} \\ [Y_m, Y_{m'}] &= (m - m')M_{m+m'} \quad , \quad [Y_n, M_m] = [M_n, M_{n'}] = 0 \end{aligned} \quad (2.20)$$

The infinitesimal generators of the finite transformations (2.18) form the Schrödinger Lie algebra $\mathfrak{sch}_1 := \langle X_{\pm 1,0}, Y_{\pm 1/2}, M_0 \rangle$ but there also exists the infinite-dimensional Lie algebra $\mathfrak{sv} := \langle X_n, Y_m, M_n \rangle_{n \in \mathbb{Z}, m \in \mathbb{Z} + \frac{1}{2}}$ [106]. Extensions to $d > 1$ are straightforward [109]. Central extensions and deformations of \mathfrak{sv} have recently been studied in detail [209]. From the commutators

$$\begin{aligned} [\mathcal{S}, X_n] &= -(n+1)t^n \mathcal{S} - \frac{1}{2}n(n+1)(2x-1)M_{n-1} + \frac{1}{2}(n^3 - n)t^{n-2}r^2 \mathcal{M}^2 \\ [\mathcal{S}, Y_m] &= 2\left(m^2 - \frac{1}{4}\right)t^{m-3/2}r \mathcal{M}^2 \\ [\mathcal{S}, M_n] &= 2nt^{n-1} \mathcal{M}^2 \end{aligned} \quad (2.21)$$

it is clear that \mathfrak{sch}_1 is a dynamical symmetry of $\mathcal{S}\psi = 0$ while \mathfrak{sv} is not. By analogy with conformal invariance, we call those scaling operators quasiprimary, which transform covariantly in the simplest possible way as $\delta\phi = -\varepsilon\mathcal{X}\phi$, with $\mathcal{X} \in \mathfrak{sch}_1$ [106]. Then a quasiprimary scaling operator is characterised in terms of the pair (x, \mathcal{M}) of its scaling dimension x and its ‘mass’ \mathcal{M} with the physical convention that $\mathcal{M} \geq 0$. We remark that \mathcal{M} is dimensionful and hence non-universal. One also introduces a ‘complex conjugate’ ϕ^* , characterised by the pair $(x, -\mathcal{M})$ the physical meaning of which will be explained below.

Clearly, the algebraic structure of Schrödinger-invariance is quite close to conformal invariance. The Schrödinger-covariant two-point function is [106, 111]

$$\begin{aligned} F^{(2)}(t_1, t_2; \mathbf{r}_1, \mathbf{r}_2) &= \langle \phi(t_1, \mathbf{r}_1) \phi^*(t_2, \mathbf{r}_2) \rangle \\ &= f_{12} \delta_{x_1, x_2} \Theta(t_1 - t_2) \delta_{\mathcal{M}_1, \mathcal{M}_2} (t_1 - t_2)^{-x_1} \exp \left[-\frac{\mathcal{M}_1 (\mathbf{r}_1 - \mathbf{r}_2)^2}{2} \frac{1}{t_1 - t_2} \right] \end{aligned} \quad (2.22)$$

where f_{12} is again a normalisation constant and the Heaviside function $\Theta(u)$ expresses causality.

An alternative local scaling with $z = 1$

In order to discuss a further example of local scaling, again with $z = 1$, we consider the linear advection equation (which might be used to describe the evolution of the density of a material in a medium flowing with constant velocity, e.g. [156]) in $(1+1)D$

$$\mathcal{S}\phi = 0 \quad ; \quad \mathcal{S} = -\mu\partial_t + \partial_r \quad (2.23)$$

where μ is a constant. In order to discuss its dynamical symmetries, consider the generators, with $n \in \mathbb{Z}$ [109]

$$\begin{aligned} X_n &= -t^{n+1}\partial_t - \frac{1}{\mu} [(t + \mu r)^{n+1} - t^{n+1}] \partial_r - (n+1)xt^n - (n+1)\frac{\gamma}{\mu} [(t + \mu r)^n - t^n] \\ Y_n &= -\frac{1}{\mu}(t + \mu r)^{n+1}\partial_r - \frac{\gamma}{\mu}(n+1)(t + \mu r)^n \end{aligned} \quad (2.24)$$

and which satisfy the commutation relations

$$[X_n, X_m] = (n-m)X_{n+m}, \quad [X_n, Y_m] = (n-m)Y_{n+m}, \quad [Y_n, Y_m] = (n-m)Y_{n+m} \quad (2.25)$$

It is easily seen that this (infinite-dimensional) Lie algebra is isomorphic to the double conformal algebra (2.15) [109]. Still, the generators at hand do generate transformations quite different from the usual conformal ones, for example space-time rotations are *not* included here. The generators contain the scaling dimension x , the ‘mass’ μ and the additional parameter γ ; hence a scaling operator ϕ will be characterised by the triplet (x, μ, γ) . The symmetry of eq. (2.23) follows from the commutators

$$\begin{aligned} [\mathcal{S}, Y_n] &= 0 \\ [\mathcal{S}, X_n] &= -(n+1)t^n\mathcal{S} + n(n+1)t^{n-1}\mu \left(x - \frac{\gamma}{\mu} \right) \end{aligned} \quad (2.26)$$

for all $n \in \mathbb{Z}$. Therefore, the operators Y_n yield an infinite family of symmetry operators while a second infinite family of dynamic symmetries is obtained if the scaling dimension satisfies $x = \gamma/\mu$.

From an algebraic point of view, all this looks quite similar to standard conformal invariance. However, the form of the two-point function [109]

$$F^{(2)}(t_1, t_2; r_1, r_2) = \delta_{x_1, x_2} \delta_{\mu_1, -\mu_2} \delta_{\gamma_1, -\gamma_2} (t_1 - t_2)^{-2x_1} f \left(\frac{r_1 - r_2}{t_1 - t_2} \right) \quad (2.27)$$

where the scaling function $\phi(u)$ is given by

$$f(u) = \begin{cases} f_0(1 + \mu_1 u)^{-2\gamma_1/\mu_1} & \text{for } \mu_1 \neq 0 \\ f_0 \exp(-2\gamma_1 u) & \text{for } \mu_1 = 0 \end{cases} \quad (2.28)$$

and where f_0 is a normalisation constant is quite distinct from the usual result (2.16) of conformal invariance.

Axioms of local scale-invariance

The known examples of local scaling suggest that a systematic generalisation to any given value of z should be possible. Indeed, local scale-transformation can be constructed from the following assumptions [109], which are the defining axioms of local scale-invariance.

1. For both for conformal and for Schrödinger invariance Möbius transformations of the time coordinate occur, i. e.

$$t \rightarrow t' = \frac{\hat{\alpha}t + \hat{\beta}}{\hat{\gamma}t + \hat{\delta}}; \quad \text{with } \hat{\alpha}\hat{\delta} - \hat{\beta}\hat{\gamma} = 1 \quad (2.29)$$

where $\hat{\alpha}, \hat{\beta}, \hat{\delta}, \hat{\gamma}$ are constants. We require that these transformations should also be included for the case of general z . The infinitesimal generators of these transformations are denoted by X_n (with $n \in \{-1, 0, 1\}$) and it is also suggested by conformal and Schrödinger invariance that the commutator between these generators should be given by

$$[X_n, X_m] = (n - m)X_{n+m}. \quad (2.30)$$

This should remain valid also after we have included the transformations of the spatial coordinates \mathbf{r} . Scaling operators which transform covariantly under (2.29) are called *quasiprimary* in analogy to the notion of conformal quasiprimary operators [26, 51].

When considering dynamical scaling out of a stationary state (especially ageing phenomena) we have to restrict to the subalgebra without time-translations, hence $\hat{\beta} = 0$ in (2.29) and there are no generators X_n with $n \leq -1$.

2. The generator of scale transformations X_0 is given by

$$X_0 = -t\partial_t - \frac{1}{z}\mathbf{r} \cdot \partial_{\mathbf{r}} - \frac{x}{z}. \quad (2.31)$$

Here, x is the scaling dimension of the scaling operator on which X_0 acts.

By assuming this particular form for X_0 we require indeed simple power-law scaling.

3. Spatial translation-invariance is required.
4. When acting on quasiprimary scaling operators ϕ , extra terms coming from the scaling dimension of ϕ must be present in the generators and be compatible with (2.31).

5. By analogy with Schrödinger-invariance and the generators (2.24) of local scaling with $z = 1$, further ‘mass terms’ describing the transformation of the scaling operators should be present.

It is at this point, in the explicit construction of these ‘mass terms’ when $z \neq 1, 2$, where we shall propose a new construction which improves upon the earlier work [109].

6. Finally we require that the application of the generators yields a *finite* number of independent conditions for the n -point functions built from quasiprimary fields. This will usually be achieved by the requirement that the generators when applied to states built from quasi-primary scaling operators form a representation of a finite-dimensional Lie algebra.

We now show how to construct from these principles a set of generators X_n and Y_m , which generalise the corresponding operators encountered in the cases quoted in the previous sections.

2.2.2 Construction of the generators of LSI

Background

The general ansatz [109] for the construction of the generators X_n is

$$X_n = X_n^{(I)} + X_n^{(II)} + X_n^{(III)} \quad (2.32)$$

where $X_n^{(I)} = -t^{n+1}\partial_t$ is the infinitesimal form of (2.29), $X_n^{(II)}$ will contain the action on \mathbf{r} and the scaling dimension x and $X_n^{(III)}$ will contain the ‘mass’ terms. Likewise, for Y_m one has [109]

$$Y_m = Y_m^{(II)} + Y_m^{(III)} \quad (2.33)$$

where $Y_m^{(II)}$ contains the action on \mathbf{r} and $Y_m^{(III)}$ contains the ‘mass’ terms. It is enough to discuss the case $d = 1$ of one spatial dimensions since extensions to $d > 1$ are straightforward.

The parts $X_n^{(II)}$ and $Y_m^{(II)}$ were constructed from the above axioms in [109] using the ansatz

$$X_n^{(II)} = a_n(t, r)\partial_r + b_n(t, r), \quad Y_m^{(II)} = Y_{k-1/z}^{(II)} = -\frac{z}{k+1} \left(\frac{\partial a_k(t, r)}{\partial r} \partial_r + \frac{\partial b_k(t, r)}{\partial r} \right) \quad (2.34)$$

where $a_n(t, r)$ and $b_n(t, r)$ have to be determined and $k \in \mathbb{Z}$. From the axioms of local scale-invariance, they can be classified, with the following result.

Theorem: [109] *For a given dynamical exponent z , consider the commutation relations*

$$[X_n, X_{n'}] = (n - n')X_{n+n'} \quad , \quad [X_n, Y_m] = \left(\frac{n}{z} - m \right) Y_{n+m} \quad (2.35)$$

where $m = k - 1/z$ and $n, n', k \in \mathbb{Z}$. *These commutators are indeed necessary for the axioms 1) – 4) of local scale-invariance to be valid. Then the only sets of generators which satisfy these are given in table 2.1.*

Table 2.1: Generators X_n and $Y_{-1/z+k}$ of local scale-transformations with a given dynamical exponent z without mass terms, where $n, k \in \mathbb{Z}$ (here for $d = 1$) and B_{10}, B_{20} and A_{10} are constants. The last column gives the dynamical exponent.

(i)	$X_n^{(I)} + X_n^{(II)} = -t^{n+1}\partial_t - \frac{n+1}{z}t^n r \partial_r - \frac{(n+1)x}{z}t^n - \frac{n(n+1)}{2}B_{10}t^{n-1}r^z$ $Y_{-1/z+k}^{(II)} = -t^k \partial_r - \frac{z^2}{2}k B_{10}t^{k-1}r^{-1+z}$	z
(ii)	$X_n^{(I)} + X_n^{(II)} = -t^{n+1}\partial_t - \frac{1}{2}(n+1)t^n r \partial_r - \frac{1}{2}(n+1)xt^n$ $- \frac{n(n+1)}{2}B_{10}t^{n-1}r^2 - \frac{(n^2-1)n}{6}B_{20}t^{n-2}r^4$ $Y_{k-1/2}^{(II)} = -t^k \partial_r - 2k B_{10}t^{k-1}r - \frac{4}{3}k(k-1)B_{20}t^{k-2}r^3$	2
(iii)	$X_n^{(I)} + X_n^{(II)} = -t^{n+1}\partial_t - A_{10}^{-1}[(t + A_{10}r)^{n+1} - t^{n+1}]\partial_r$ $- (n+1)xt^n - \frac{n+1}{2}\frac{B_{10}}{A_{10}}[(t + A_{10}r)^n - t^n]$ $Y_{k-1}^{(II)} = -(t + A_{10}r)^k \partial_r - \frac{k}{2}B_{10}(t + A_{10}r)^{k-1}$	1

We add that in case (i) of table 2.1, we have at this stage $[Y_m, Y_{m'}] = 0$. Both the dynamical exponent z and the constant B_{10} can be freely chosen. In case (ii) we recover for $B_{20} = 0$ the generators of Schrödinger-invariance with $B_{10} = \mathcal{M}/2$ while for $B_{20} \neq 0$ additional generators must be written down to close the algebra, see [109]. Finally, case (iii) corresponds to the local scaling treated in subsection 2.2.1, with the substitution $Y_n \mapsto A_{10}Y_n$ and $A_{10} = \mu$, $B_{10} = 2\gamma$, hence $[Y_n, Y_m] = A_{10}(n-m)Y_{n+m}$ for the generators of table 2.1. We point out that the chosen ansatz for the Y_m excludes the standard conformal transformations since no terms with ∂_t are present.

The ‘old’ formulation of LSI

A physically interesting formulation of local scale-invariance (LSI) requires the construction of mass terms and since we wish to construct a theory for arbitrary z , we concentrate from now on case (i). We shall also set $B_{10} = 0$ as it was already done in [109].

Practical experience suggests that for generic z , such ‘mass terms’ should contain fractional derivatives, either with respect to time or with respect to space. We have shown earlier [194, 109] that mass terms with fractional time-derivatives lead to generators (referred to as ‘Typ I’) which may describe the form of scaling functions of *equilibrium* systems with competing interactions which are at strongly anisotropic critical points, for example Lifshitz points. In this work, we are exclusively interested in the local scaling of time-dependent systems and therefore concentrate on the second alternative, mass terms with fractional derivatives with respect to space, leading to generators referred to as ‘Typ II’ in [109]. In order to prepare our forthcoming construction of the generators of local scale-invariance, we now review briefly the ‘old’ previous construction and discuss some of its successes and in particular several important shortcomings of it.

In the previous formulation of LSI [109], a fractional derivative ∂_r^a was used which was constructed such that the following, apparently ‘natural’, operational rules (in $d = 1$) are valid, namely

$$\partial_r^{a+b} = \partial_r^a \partial_r^b, \quad [\partial_r^a, r] = a \partial_r^{a-1} \quad (2.36)$$

Following [92], such linear operators can be constructed in a distributional sense, see [109] for the precise definition. For our purposes it is enough to state that generators such as X_1 and $Y_{-1/z+1}$ acquire ‘mass’ terms, whereas X_{-1}, X_0 and $Y_{-1/z}$ are unchanged with respect to case (i) of table 2.1, with $B_{10} = 0$. The first few generators read [109]

$$\begin{aligned} X_{-1} &= -\partial_t && \text{time translation} \\ X_0 &= -t\partial_t - \frac{1}{z}r\partial_r - \frac{x}{z} && \text{scale dilatation} \\ X_1 &= -t^2\partial_t - \frac{2}{z}tr\partial_r - \frac{2x}{z}t - \mu r^2\partial_r^{2-z} && \text{generalised Schrödinger} \\ &\quad -2\gamma(2-z)r\partial_r^{1-z} - \gamma(2-z)(1-z)\partial_r^{-z} && \text{transformation} \\ Y_{-1/z} &= -\partial_r && \text{space translation} \\ Y_{-1/z+1} &= -t\partial_r - \mu zr\partial_r^{2-z} - \gamma z(2-z)\partial_r^{1-z} && \text{generalised Galilei} \\ &&& \text{transformation} \end{aligned} \quad (2.37)$$

such that the commutation relations (2.35) remain valid. One interesting aspect of these generators is that if one considers the generalised Schrödinger equation

$$\mathcal{S}\phi = 0, \quad \mathcal{S} = -\mu\partial_t + \frac{1}{z^2}\partial_r^z \quad (2.38)$$

then the generators (2.37) act as dynamical symmetry on the solutions of that equation, provided that $x = \frac{1}{2}(z-1) + (2-z)\gamma/\mu$ [109]. For $z = 2$ and $z = 1$, respectively, one recovers the special cases of local scaling symmetries treated in subsections 2.2.1 and 2.2.1. Generalising the known cases of the previous subsections, we call a scaling operator ϕ quasiprimary, if it transforms as

$$\delta\phi(t, \mathbf{r}) = -\epsilon\mathcal{X}\phi(t, \mathbf{r}) \quad (2.39)$$

where \mathcal{X} is any of the generators (2.37) and ϵ is a small parameter. Hence a quasiprimary ϕ is characterised by the triplet (x, μ, γ) of its scaling dimension x , its ‘mass’ μ and the parameter γ . Although both μ and γ are dimensionful and hence cannot not be universal, their ratio γ/μ is a dimensionless universal quantity. In distinction to the special cases treated above, the commutators $[Y_m, Y_{m'}]$ create further families of generators which only close when applied to certain ‘physical’ states [109]. While the mathematical structure implied by this requirement (axiom 6) is not yet understood, it is enough for the calculation of two-point functions.

The n -point functions of quasiprimary scaling operators (QSOS) ϕ_i are denoted as

$$F^{(n)}(\{t_i, \mathbf{r}_i\}) := \langle \phi_1(t_1, \mathbf{r}_1) \dots \phi_n(t_n, \mathbf{r}_n) \rangle \quad (2.40)$$

and their spatial Fourier transform is denoted by $\widehat{F}^{(n)}(t_1, \mathbf{k}_1, \dots, t_n, \mathbf{k}_n)$. By definition, n -point functions built from quasiprimary operators must satisfy [109]

$$\sum_{i=1}^n \mathcal{X}_i F^{(n)}(\{t_i, \mathbf{r}_i\}) = 0 \quad (2.41)$$

where \mathcal{X}_i is any of the generators (2.49)-(2.54) acting on the i -th coordinate, or a generator built from commutators of them. This leads to a set of linear differential equations for the n -point function. In particular, the two-point functions can be fully specified in this way and the result, using the generators (2.37) is

$$F^{(2)}(t, s; \mathbf{x}, \mathbf{y}) = \delta_{x_1, x_2} \delta_{\mu_1, -(-1)^z \mu_2} \delta_{\gamma_1, -(-1)^z \gamma_2} (t - s)^{-2x_1/z} \mathcal{F}^{(\mu_1, \gamma_1)} \left(\frac{|\mathbf{x} - \mathbf{y}|}{(t - s)^{1/z}} \right) \quad (2.42)$$

where the scaling function $\mathcal{F}^{\mu, \gamma}(\rho)$ satisfies the fractional differential equation

$$(\partial_\rho + z\mu \rho \partial_\rho^{2-z} + 2z(2-z)\gamma \partial_\rho^{1-z}) \mathcal{F}^{(\mu, \gamma)}(\rho) = 0. \quad (2.43)$$

We direct the attention of the reader to the curious relation between the parameters (μ_1, γ_1) and (μ_2, γ_2) of the two quasiprimary scaling operators. Although at first sight this might remind one of the Bargmann superselection rules (see subsection 2.2.3 below), there is no generalisation to n -point functions with $n > 2$. This is just one of the structural problems of the old formulation of LSI which we shall correct shortly.

If $z = N + p/q$, where $N = [z]$ is the largest integer less than or equal to z , and p and q are coprime, equation (2.43) can be solved by series methods, with the result [207, 19]

$$\mathcal{F}^{(\mu, \gamma)}(\rho) = \sum_{m \in \mathcal{E}} c_m \phi^{(m)}(\rho), \quad \text{with} \quad \phi^{(m)}(\rho) = \sum_{n=0}^{\infty} b_n^{(m)} \rho^{(n-1)z + p/q + m + 1}. \quad (2.44)$$

The constants c_m remain arbitrary and the set \mathcal{E} is defined as

$$\mathcal{E} = \begin{cases} -1, 0, \dots, N-1 & p \neq 0 \\ 0, \dots, N-1, & p = 0 \end{cases}. \quad (2.45)$$

Finally, the coefficients $b_n^{(m)}$ read

$$b_n^{(m)} = \frac{(-z^2 \mu)^n \Gamma(p/q + 1 + m) \Gamma(n + z^{-1}(p/q + m) + 2z^{-1}(2-z)\gamma/\mu)}{\Gamma((n-1)z + p/q + m + 2) \Gamma(z^{-1}(p/q + m) + 2z^{-1}(2-z)\gamma/\mu)}. \quad (2.46)$$

such that the resulting series has an infinite radius of convergence when $z > 1$.

When discussing applications to non-stationary ageing systems, it turns out that the two-point functions so calculated really are related to response functions, rather than correlation functions [108, 109, 111, 110]. Furthermore, space-time response functions factorise as follows $R(t, s; \mathbf{r}) = R(t, s) \mathcal{F}^{(\mu, \gamma)}(|\mathbf{r}|(t-s)^{-1/z})$ with the autoresponse function $R(t, s) = s^{-1-a}(t/s)^{1+a'-\lambda_R/z}(t/s-1)^{-1-a'}$, up to normalisation [109, 192, 123]. It has been one of the successes of that formulation of LSI that this prediction for $R(t, s)$ has been confirmed in a large variety of different models, with dynamical exponents in the range $z \simeq 1.7 - 5$, see [125, 124, 126] for detailed reviews. On the other hand, the space-time dependent part of $R(t, s; \mathbf{r})$ had until recently only been tested in several exactly solvable models, all with linear equations of motion, see [94, 191, 15, 207, 123, 19], as well as in the $2D/3D$ Ising model [110] and the $2D$ q -states Potts model [161] which however, have $z = 2$. Remarkably, our recent study of the non-equilibrium kinetics of the long-range spherical model, where $z < 2$, has shown that the above LSI-prediction for the scaling function $\mathcal{F}^{(\mu, \gamma)}(u)$ is *not* reproduced by the exact result in that model [20],

see section 3.3 of chapter 3. This provides a phenomenological motivation to look for an alternative formulation of LSI.

Finally, in the absence of a Bargmann superselection rule, it is not clear how to extend the treatment of the dynamical symmetries of deterministic equations such as $\mathcal{S}\phi = 0$ to the stochastic Langevin equations one is really interested in. As a consequence, we cannot carry over the calculation of the correlation functions from the Schrödinger-invariant case $z = 2$ [192, 126], whereas without either thermal or initial noise, LSI would simply predict vanishing correlation functions, which is absurd.

Improved construction of infinitesimal generators

In conclusion of the above brief summary of the ‘old’ formulation of LSI, in spite of some phenomenological successes, there are several independent motivations to look for a better formulation of the theory. The existing evidence in favour of LSI suggests that a rather small modification of the structure of LSI might be sufficient. Therefore, we attempt in this chapter to maintain the axioms of local scale-invariance as formulated above, but modify the construction of the ‘mass terms’ through the use of a different type of fractional derivative. We denote this new derivative by $\nabla_{\mathbf{r}}^{\alpha}$ and change the properties (2.36) of $\partial_{\mathbf{r}}^{\alpha}$ to

$$\nabla_{\mathbf{r}}^{\alpha}\nabla_{\mathbf{r}}^{\beta} = \nabla_{\mathbf{r}}^{\alpha+\beta}, \quad [\nabla_{\mathbf{r}}^{\alpha}, r_i] = \alpha\partial_{r_i}\nabla_{\mathbf{r}}^{\alpha-2} \quad \text{for } i = 1, \dots, d \quad (2.47)$$

where r_i is the i -th component of the space vector $\mathbf{r} = (r_1, \dots, r_d)$. In appendix A, we give the precise definition and the basic properties of $\nabla_{\mathbf{r}}^{\alpha}$. Notice that $\nabla_{\mathbf{r}}^{\alpha}$ is a *multidimensional* object and that the second property in (2.36) has been changed. Conceptually, (2.47) is distinct from (2.36) since now *two* types of derivatives appear, namely the usual partial derivative ∂_{r_i} and the new fractional derivative $\nabla_{\mathbf{r}}^{\alpha}$.

That the fractional derivative $\nabla_{\mathbf{r}}^{\alpha}$ is *not* equivalent to the old one $\partial_{\mathbf{r}}^{\alpha}$ is already clear from the simple example (see appendix A for the proof)

$$\nabla_{\mathbf{r}}^{\alpha}\exp(\mathbf{i}\mathbf{q}\cdot\mathbf{r}) = \mathbf{i}^{\alpha}|\mathbf{q}|^{\alpha}\exp(\mathbf{i}\mathbf{q}\cdot\mathbf{r}). \quad (2.48)$$

for a constant vector \mathbf{q} , whereas $e^{i\mathbf{q}\cdot\mathbf{r}}$ is not an eigenfunction of $\partial_{\mathbf{r}}^{\alpha}$. In appendix A, we also discuss several other kinds of fractional derivatives which have been introduced in the literature and show that $\nabla_{\mathbf{r}}^{\alpha}$ is distinct from all of them. At present, we do not understand which properties of fractional derivatives should be the ‘correct’ ones to use with local scale-transformations and can only decide *a posteriori*, by comparing the predictions of a certain formulation of LSI with specific model results, what kind of mass terms might be appropriate.

From eq. (2.48) it is clear that the action of $\nabla_{\mathbf{r}}^{\alpha}$ in Fourier space will be simple such that concrete computations are best done in Fourier space. With respect to the ‘old’ formulation of LSI, this gives a new approach to some previously unsolved problems like for instance the calculation of four-point functions. Of considerable consequence is the fact, which we shall prove in section 2.2.3, that the use of $\nabla_{\mathbf{r}}^{\alpha}$ allows to deduce a generalisation of the Bargmann superselection rules, which in turn is a crucial ingredient for the treatment of noisy systems. Finally, the generalisation of the generators to d spatial

dimensions will turn out to be much more natural than for the old type of derivatives [19].

We begin by listing the generators of local scale-invariance in the new formulation. As we shall show in proposition 1 below, their commutation relations (2.37) are retained from the ‘old’ formulation. The generators read ($i = 1, \dots, d$):

$$X_{-1} := -\partial_t \quad \text{time translation} \quad (2.49)$$

$$X_0 := -t\partial_t - \frac{1}{z}(\mathbf{r} \cdot \partial_{\mathbf{r}}) - \frac{x}{z} \quad \text{scale dilatation} \quad (2.50)$$

$$X_1 := -t^2\partial_t - \frac{2(x+\xi)}{z}t - \mu r^2\nabla_{\mathbf{r}}^{2-z} - \frac{2}{z}t(\mathbf{r} \cdot \partial_{\mathbf{r}}) \quad \text{generalised Schrödinger} \\ -2\gamma(2-z)(\mathbf{r} \cdot \partial_{\mathbf{r}})\nabla_{\mathbf{r}}^{-z} - \gamma(2-z)(d-z)\nabla_{\mathbf{r}}^{-z} \quad \text{transformation} \quad (2.51)$$

$$Y_{-1/z}^{(i)} := -\partial_{r_i} \quad \text{space translation} \quad (2.52)$$

$$Y_{-1/z+1}^{(i)} := -t\partial_{r_i} - \mu z r_i \nabla_{\mathbf{r}}^{2-z} - \gamma z(2-z)\partial_{r_i}\nabla_{\mathbf{r}}^{-z} \quad \text{generalised Galilei} \\ \text{transformation} \quad (2.53)$$

$$R^{(i,j)} := r_i\partial_{r_j} - r_j\partial_{r_i} \quad \text{rotation} \quad (2.54)$$

Again, the infinitesimal change of a quasiprimary scaling operator ϕ is given by one of these generators of (iterated) commutators thereof. Hence a quasiprimary operator is characterised by the quartet (x, μ, γ, ξ) . In order to understand the last parameter ξ , some remarks are in order. If time-translation invariance is required (as would be physically sensible for a system in a stationary state) from the commutator $[X_1, X_{-1}] = 2X_0$ the condition $\xi = 0$ follows. Hence $\xi \neq 0$ is only possible if time-translation invariance is broken and this is only possible for non-equilibrium, non-stationary systems (e.g. ageing phenomena).

The physical meaning of ξ can be understood as follows [123, 126]. Consider a system without time-translation invariance but with local scaling. For simplicity we drop spatial dependence of the observables and consequently can leave out those parts of the generators acting on the spatial coordinates \mathbf{r} . Exponentiating the generators $\langle X_n \rangle_{n \geq 0}$, one finds that the primary scaling operator $\phi(t)$ with scaling dimension $x = x_\phi$ transforms as follows [123]

$$\phi(t) = \dot{\beta}(t')^{-x/z} \left(\frac{t'\dot{\beta}(t')}{\beta(t')} \right)^{-2\xi/z} \phi'(t') \quad (2.55)$$

where we have written $t = \beta(t')$ and also requires that $\beta(0) = 0$. The dot denotes the derivative with respect to time. For quasiprimary scaling operators, we restrict to $\beta(t) = t\hat{\delta}^{-1}/(\hat{\gamma}t + \hat{\delta})$. While this is not the usual transformation of a primary scaling operator unless $\xi = 0$, it does suggest to define the scaling operator

$$\Phi(t, \mathbf{r}) := t^{-2\xi/z} \phi(t, \mathbf{r}). \quad (2.56)$$

which transforms indeed as a conventional primary scaling operator, but with a scaling dimension $x_\Phi = x + 2\xi$. In particular, this implies that for non-stationary systems, the relationship between lattice observables and the primary scaling operators might become more subtle than habitual intuition formed on equilibrium systems made one expect.

Since for specific computation it is easier to work in Fourier space, we list in appendix B of [21] the Fourier-transformed generators of LSI, depending on all four parameters x, μ, γ, ξ . The basic algebraic and symmetry properties of the new generators of LSI are stated in the two theorems below. Their proof, using eqs. (A.6)-(A.9), is a matter of direct calculation. We first list the commutation relations.

Proposition 1: *The generators (2.49)-(2.54) satisfy the following commutation relations, with $n \in \{-1, 0, 1\}$ and $m \in \{-1/z, -1/z + 1\}$*

$$[X_n, X_{n'}] = (n - n')X_{n+n'} \quad (2.57)$$

$$[X_n, Y_m^{(i)}] = \left(\frac{n}{z} - m\right) Y_{n+m}^{(i)} \quad (2.58)$$

$$[Y_m^{(i)}, R^{(i,j)}] = -[Y_m^{(i)}, R^{(j,i)}] = Y_m^{(j)} \quad (2.59)$$

$$[R^{(i,j)}, X_n] = 0, \quad [R^{(i,j)}, Y_m^{(k)}] = 0, \quad \text{if } k \neq i, j \quad (2.60)$$

These simply reproduce the commutation relations known from the ‘old’ version of LSI. Our new definition of the generators therefore has the same algebraic properties as those in the earlier construction of LSI [109] reviewed above. The next result considers the dynamical symmetries of certain linear fractional differential equations.

Proposition 2: *Define the generalised Schrödinger operator*

$$\mathcal{S} := -\mu\partial_t + \frac{1}{z^2}\nabla_r^z \quad (2.61)$$

Then the commutator of \mathcal{S} with any one of the generators (2.49)-(2.54) vanishes except for the following two cases:

$$[\mathcal{S}, X_0] = -\mathcal{S} \quad (2.62)$$

$$[\mathcal{S}, X_1] = -2t\mathcal{S} + \frac{1}{z}\left(2\mu(x + \xi) - \mu(z - 2 + d) - 2\gamma(2 - z)\right) \quad (2.63)$$

This means that the generators (2.49)-(2.54) act as dynamical symmetry operators for the equation $\mathcal{S}\phi = 0$ provided that the relation

$$x + \xi = \frac{z - 2 + d}{2} + \frac{\gamma}{\mu}(2 - z) \quad (2.64)$$

for the scaling dimension $x = x_\phi$ of the solution ϕ holds true.

A central property of our reformulation of LSI will become apparent through a generalisation of the Bargmann superselection rule.

2.2.3 Bargmann superselection rule

For Schrödinger-invariance where $z = 2$ or more generally for Galilei-invariance, the so-called Bargmann superselection rule [11] plays an important role. It states that the n -point function of QSOs is zero unless the sum of the mass of the fields involved vanishes, viz. $\sum_{i=1}^n \mu_i = 0$. This well-known property of non-relativistic fields has turned out to

be extremely useful in the context of non-equilibrium field-theory [66, 137, 226], where it suggests to split the action into a Galilei-invariant ‘deterministic part’ and a non-invariant ‘noise part’ [192]. Then from the Bargmann superselection rule exact reduction formulæ for the average of any observable \mathcal{O} to the noiseless average of a related observable \mathcal{O}' can be derived [192]. In this section, we consider now how the Bargmann superselection rule might be generalised to $z \neq 2$ before taking up in section 2.3 the treatment of stochastic equations.

Consider the effect of the LSI-generators on some n -point functions built from quasiprimary scaling operators. Such a n -point function should satisfy the equation (2.41). It is instructive to consider not only the generators Y_m directly, but also to compute the following series of generators. Define, for $d \geq 1$ dimensions

$$M_0 := [Y_{-1/z}^{(i)}, Y_{-1/z+1}^{(i)}] = \mu z \nabla_{\mathbf{r}}^{2-z} \quad (2.65)$$

$$N_0^{(i)} := [M_0, Y_{-1/z+1}^{(i)}] = -z^2(2-z)\mu^2 \partial_{r_i} \nabla_{\mathbf{r}}^{2-2z} \quad (2.66)$$

and then recursively for $\ell \geq 1$

$$M_\ell := \sum_{i=1}^d [N_{\ell-1}^{(i)}, Y_{-1/z+1}^{(i)}] \quad (2.67)$$

$$N_\ell^{(i)} := [M_\ell, Y_{-1/z+1}^{(i)}] \quad (2.68)$$

We find the following general form for these operators

$$M_\ell = a_\ell \mu^{2\ell+1} \nabla_{\mathbf{r}}^{2\ell+2-(2\ell+1)z} \quad (2.69)$$

$$N_\ell^{(i)} = b_\ell \mu^{2\ell+2} \partial_{r_i} \nabla_{\mathbf{r}}^{(2\ell+2)(1-z)} \quad (2.70)$$

where a_ℓ and b_ℓ are constants depending on z and d . They can be computed recursively from the following recursion relations and initial values:

$$a_0 = z \quad , \quad b_0 = -z^2(2-z) \quad (2.71)$$

$$a_{\ell+1} = -b_\ell z [d + (2\ell+2)(1-z)] \quad , \quad b_\ell = a_\ell z [(2\ell+1)z - (2\ell+2)] \quad (2.72)$$

but for what follows, the specific values of these constants are not required. Because of proposition 2, all generators $M_\ell, N_\ell^{(i)}$ commute with \mathcal{S} and hence are related to dynamical symmetries of the equation $\mathcal{S}\phi = 0$.

This set of dynamical symmetries is finite in two special cases. First, if we take $z = (2N+2)/(2N+1)$ (with $N \in \mathbb{N}_0$), then $a_{\ell+1} = 0$ and $b_\ell = 0$ for $\ell \geq N$.³ Second, if we take $z = 1 + d/(2N+2)$ (for $N \in \mathbb{N}$), then $a_\ell = b_\ell = 0$ for $\ell > N$.

Practical calculations are made in Fourier space where the operators (2.69) are given by

$$\widehat{M}_{2\ell-1} = (-1)^{\ell+1} i^{(2\ell+1)z} a_\ell \mu^{2\ell-1} |\mathbf{k}|^{2\ell-(2\ell-1)z} \quad (2.73)$$

If we apply the covariance-condition (2.41) onto the n -point function $\widehat{F}^{(n)}(\{t_i, \mathbf{k}_i\})$. From the operators (2.73), together with spatial translation-invariance (momentum conservation) we obtain the following conditions, for all $\ell \in \mathbb{N}$

³The case $z = 2$ is recovered for $N = 0$.

$$\left(\sum_{i=1}^n \mu_i^{2\ell-1} |\mathbf{k}_i|^{2\ell-(2\ell-1)z} \right) \widehat{F}^{(n)}(\{t_i, \mathbf{k}_i\}) = 0 \quad (2.74)$$

$$\left(\sum_{i=1}^n \mathbf{k}_i \right) \widehat{F}^{(n)}(\{t_i, \mathbf{k}_i\}) = 0 \quad (2.75)$$

This kind of condition is quite similar to constraints found in factorizable scattering of relativistic particles [235, 236]. If one interprets a n -point function to describe a scattering process of m incoming and $n - m$ outgoing particles, the constraints eqs. (2.74, 2.75) mean that the total momentum and the sums of certain powers of the momenta must be conserved. Furthermore, it is well-known that in the presence of a single conserved quantity of the above type, the scattering matrix factorizes into the product of two-particle S -matrices [235, 236]. We make use of this classic result to arrange the mass factors $\mu_i^{2\ell+1}$ such that the conditions (2.74) and (2.75) are satisfied. A generalisation of the Bargmann superselection rules follows:

Proposition 3: (*Generalised Bargmann superselection rule*) *Let a system be given with dynamical exponent $z \neq 2$.⁴ Let $\{\phi_i\}$ be a set of scaling operators transforming covariantly under the action of the generators $Y_{-1/z}^{(i)}$ and $Y_{-1/z+1}^{(i)}$ (for all $i = 1, \dots, d$). Let furthermore each scaling operator be characterised by the set $(x_i, \xi_i, \mu_i, \gamma_i)$. Then the $(2n)$ -point function*

$$F^{(2n)}(\{t_i\}, \{\mathbf{r}_i\}) := \langle \phi_1(t_1, \mathbf{r}_1) \dots \phi_{2n}(t_{2n}, \mathbf{r}_{2n}) \rangle \quad (2.76)$$

vanishes unless the μ_i form n distinct pairs $(\mu_i, \mu_{\tau(i)})$ ($i = 1, \dots, n$), such that for each pair

$$\mu_i = -\mu_{\tau(i)} \quad (2.77)$$

This result is considerably more restrictive than the Bargmann superselection rule for Galilei-invariant systems (where $z = 2$), which merely requires $\sum_{i=1}^{2n} \mu_i = 0$.

The existence of the conditions (2.74) and (2.75) which are reminiscent of similar constraints known from factorizable scattering [236, 235] might point towards interesting connections to this field and towards integrable systems. However, a detailed investigation of this is beyond the scope of this chapter, where we shall be mainly concerned to demonstrate the physical interest of these results by showing how to related them to specific model calculations of noisy non-equilibrium systems.

Graphically, the superselection rule (2.77) may be represented as shown in figure 2.1 for the fourpoint function $\langle \phi_1(1)\phi_2(2)\phi_3(3)\phi_4(4) \rangle$, which will be treated in detail in section 2.4. We consider two of these fields, say field 1 and field 4 as incoming particles, the other two as outgoing particles. Then there only two ways to connect the incoming and outgoing particles if we want to respect momentum conservation (2.75). Together with (2.74) this then yields the ansatz (2.115) for the fourpoint function.

2.3 Field-theoretical formalism

Up until now our considerations were purely algebraic and the dynamical equation involved is *deterministic*. However, the description of non-equilibrium systems typically

⁴If $z \neq \frac{2N+2}{2N+1}$ or $z \neq 1 + \frac{d}{2N+2}$ with $N \in \mathbb{N}$ one has an infinity of conditions (2.74).

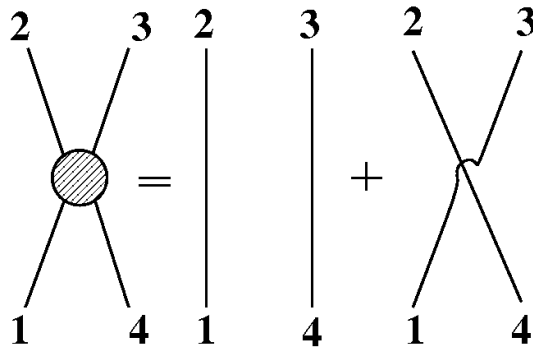


Figure 2.1: Illustration of the generalised Bargmann superselection rule at the example of the four-point function $\langle \phi_1(1)\phi_2(2)\phi_3(3)\phi_4(4) \rangle$. This yields, by using (2.74) and (2.75), the ansatz (2.115) for the fourpoint function.

requires to look at stochastic Langevin equations, to be considered as a coarse-grained equation for the 'slow' degrees of freedom coupled to a heat bath modelled by a set of Gaussian random variables, which mean to describe the 'fast' degrees of freedom. At first sight, this makes our methods from the previous sections inapplicable, as the noise breaks Galilei invariance⁵. However, for $z = 2$ closer inspection shows that with the help of a new decomposition of the associated action of non-equilibrium field-theory into a Galilei-invariant 'deterministic part' and a non-invariant 'noise part' the calculation of averages can be exactly reduced to the computation of certain averages in the deterministic part alone [192].

In this section we outline how to generalise this technique to $z \neq 2$, using proposition 3. We consider the following dynamical equation

$$\mu \partial_t \phi(t, \mathbf{r}) = \frac{1}{z^2} \nabla_{\mathbf{r}}^z \phi(t, \mathbf{r}) - v(t) \phi(t, \mathbf{r}) + \eta(t, \mathbf{r}) \quad (2.78)$$

where we have introduced a time-dependent potential $v(t)$.⁶ The noise $\eta(t, \mathbf{r})$ is a centred Gaussian random variable, with the second moment

$$\langle \eta(t, \mathbf{r}) \eta(t', \mathbf{r}') \rangle = 2T \delta(t - t') b(\mathbf{R} - \mathbf{R}'). \quad (2.79)$$

The usual white noise is recovered if $b(\mathbf{r}) = \delta(\mathbf{r})$. For the computation of response function an external field $h(t, \mathbf{x})$ may be added to the right-hand side of (2.78) and in addition we shall also have to average over the initial conditions.⁷

Noise-less equations (2.78) with time-dependent potentials can be reduced to the invariant equation $\mathcal{S} \bar{\phi}(t, \mathbf{r}) = 0$ with the operator \mathcal{S} as given in equation (2.61) through the gauge transformation [192]

$$\phi(t, \mathbf{r}) = \bar{\phi}(t, \mathbf{r}) \exp \left(-\frac{1}{\mu} \int_0^t du v(u) \right) \quad (2.80)$$

⁵Intuitively, this may be understood as follows. Consider a magnet which is at rest with respect to a homogeneous heat-bath at temperature T . If the magnet is now moved with a constant velocity with respect to the heat-bath, the effective temperature will now appear to be direction-dependent, and the heat-bath is no longer homogeneous. Hence the total system, consisting of the magnet together with the heat-bath is not Galilei-invariant, even if the magnet alone is.

⁶Including such terms is very natural. In section 2.5 we shall see that $v(t)$ is a Lagrangian multiplier coming from the global constraint in the spherical model.

⁷The slight generalisations needed e.g. for a conserved order-parameter or in growth models [19, 207] will be taken up in chapter 3.

Therefore, it is enough to consider the case $v(t) = 0$ explicitly.

In order to treat the noise (both thermal and initial) we adopt the standard set-up of non-equilibrium field-theory [165, 137, 226]. Eq. (2.78) is then converted into the action

$$\mathcal{J}[\phi, \tilde{\phi}] = \mathcal{J}_0[\phi, \tilde{\phi}] + \mathcal{J}_{init}[\tilde{\phi}] + \mathcal{J}_{th}[\tilde{\phi}] \quad (2.81)$$

where the ‘deterministic’ part is given by

$$\mathcal{J}_0[\phi, \tilde{\phi}] = \int du \int d\mathbf{R} \tilde{\phi} \left[\partial_u \phi - \frac{1}{\mu} \nabla_{\mathbf{R}}^z \phi + v(t) \phi \right] \quad (2.82)$$

and the ‘noise’ parts are $\mathcal{J}_{th} + \mathcal{J}_{init}$ where

$$\mathcal{J}_{th}[\tilde{\phi}] = \frac{1}{2} \int dud u' \int d\mathbf{R} d\mathbf{R}' \tilde{\phi}(u, \mathbf{R}) \langle \eta(u, \mathbf{R}) \eta(u', \mathbf{R}') \rangle \tilde{\phi}(u', \mathbf{R}') \quad (2.83)$$

describes the thermal noise and [170, 192]⁸

$$\mathcal{J}_{init}[\tilde{\phi}] = -\frac{1}{2} \int d\mathbf{R} d\mathbf{R}' \tilde{\phi}(0, \mathbf{R}) a(\mathbf{R} - \mathbf{R}') \tilde{\phi}(0, \mathbf{R}') \quad (2.84)$$

describes the initial noise with zero average and correlator

$$a(\mathbf{R} - \mathbf{R}') = \langle \phi(0, \mathbf{R}) \phi(0, \mathbf{R}') \rangle \quad (2.85)$$

For the usually considered un-correlated initial conditions, $a(\mathbf{r}) = \delta(\mathbf{r})$. The average of an observable \mathcal{O} is then given as

$$\langle \mathcal{O} \rangle := \int \mathcal{D}\phi \mathcal{D}\tilde{\phi} \mathcal{O} e^{-\mathcal{J}[\phi, \tilde{\phi}]} \quad (2.86)$$

In what follows, averages with respect to the theory described by $\mathcal{J}_0[\phi, \tilde{\phi}]$ only (the so called noise-free or deterministic theory), will be considered and may be written as

$$\langle \mathcal{O} \rangle_0 := \int \mathcal{D}\phi \mathcal{D}\tilde{\phi} \mathcal{O} e^{-\mathcal{J}_0[\phi, \tilde{\phi}]} \quad (2.87)$$

We are interested in correlation and response functions. While the first one is straightforwardly found from

$$C(t, s; \mathbf{x} - \mathbf{y}) := \langle \phi(t, \mathbf{x}) \phi(s, \mathbf{y}) \rangle \quad (2.88)$$

(where spatial translation-invariance was assumed), the second one is obtained by considering the change of averages with respect to a small external perturbation. A magnetic field conjugate to the order-parameter may be included by adding the term $-\int d\mathbf{R} du \tilde{\phi}(u, \mathbf{R}) h(u, \mathbf{R})$ to the action $\mathcal{J}[\phi, \tilde{\phi}]$. Then one can formally define the response function by

$$R(t, s; \mathbf{x} - \mathbf{y}) := \left. \frac{\delta \langle \phi(t, \mathbf{x}) \rangle_h}{\delta h(s, \mathbf{y})} \right|_{h=0} = \langle \phi(t, \mathbf{x}) \tilde{\phi}(s, \mathbf{y}) \rangle. \quad (2.89)$$

⁸It has been shown by Janssen that, at the initial time $t = 0$, the fields $\phi(0, \mathbf{r})$ and $\tilde{\phi}(0, \mathbf{r})$ are proportional [137].

In what follows, we shall write $\mathbf{r} = \mathbf{x} - \mathbf{y}$ throughout. We suppose throughout this chapter that the averages of the order parameter and the response field vanishes, i.e. $\langle \phi(t, \mathbf{x}) \rangle = 0 = \langle \tilde{\phi}(t, \mathbf{x}) \rangle$. If this is not satisfied and the order parameter has a non-vanishing average (as it is the case in reaction-diffusion systems), new problems can arise [46, 5, 22]. In that case, the theory of LSI as presented in this chapter is not applicable. We now assume that $\phi(t, \mathbf{r})$ and $\tilde{\phi}(t, \mathbf{r})$ are both quasiprimary scaling operators (QSOs) of LSI. If we assign the mass μ to $\phi(t, \mathbf{r})$, from the comparison of the equations of motions coming from $\delta\mathcal{J}[\phi, \tilde{\phi}]/\delta\phi = \delta\mathcal{J}[\phi, \tilde{\phi}]/\delta\tilde{\phi} = 0$ it follows that that $\tilde{\phi}$ should have the mass $\tilde{\mu} = -\mu$. Using the generalised Bargmann superselection rule proposition 3, it further follows that in the noise-free theory

$$\left\langle \underbrace{\phi \dots \phi}_n \underbrace{\tilde{\phi} \dots \tilde{\phi}}_m \right\rangle_0 = 0, \quad \text{unless } n = m \quad (2.90)$$

In order to compute the response function of the full theory, we can now follow [192] and expand the exponential function to obtain

$$\begin{aligned} R(t, s; \mathbf{r}) &= \left\langle \phi(t, \mathbf{x}) \tilde{\phi}(s, \mathbf{y}) \right\rangle = \left\langle \phi(t, \mathbf{x}) \tilde{\phi}(t, \mathbf{y}) e^{-\mathcal{J}_{init}[\tilde{\phi}] - \mathcal{J}_{th}[\tilde{\phi}]} \right\rangle_0 \\ &= \left\langle \phi(t, \mathbf{x}) \tilde{\phi}(s, \mathbf{y}) \right\rangle_0 \end{aligned} \quad (2.91)$$

In other words, the response function is the two-point function of the deterministic theory. Therefore, we may use the dynamic symmetries of the deterministic part in order to derive the full response function. We shall do so in section 2.4.

For the correlation function, we find in a similar way

$$C(t, s, \mathbf{r}) = C_{init}(t, s; \mathbf{r}) + C_{th}(t, s; \mathbf{r}) \quad (2.92)$$

with

$$C_{init}(t, s; \mathbf{r}) = \frac{1}{2} \int d\mathbf{R} d\mathbf{R}' \left\langle \phi(t, \mathbf{x}) \phi(s, \mathbf{y}) \tilde{\phi}(0, \mathbf{R}) \tilde{\phi}(0, \mathbf{R}') \right\rangle_0 a(\mathbf{R} - \mathbf{R}') \quad (2.93)$$

and

$$C_{th}(t, s; \mathbf{r}) = \frac{1}{2} \int d\mathbf{R} d\mathbf{R}' du du' \left\langle \phi(t, \mathbf{x}) \phi(s, \mathbf{y}) \tilde{\phi}(u, \mathbf{R}) \tilde{\phi}(u', \mathbf{R}') \right\rangle_0 \langle \eta(u, \mathbf{R}) \eta(u', \mathbf{R}') \rangle \quad (2.94)$$

We stress that these results are correct provided that translation invariance and generalised Galilei invariance (and by implication (2.90)) hold.

In the next section we extend these invariances to full local scale-invariance in order to fix the remaining two- and four-point response functions.

2.4 Calculation of n -point functions

In this section we shall use the generators (2.49)-(2.54) to fix – as far as it is possible – the two- and fourpoint function of the noiseless theory. As was pointed out above, we can treat the case with $v = 0$ and shall then obtain the case with a non-vanishing potential by applying the gauge transform (2.80). Let us turn to the two-point function first.

2.4.1 Two-point function

We compute the two-point function of two quasiprimary fields ϕ_1 and ϕ_2 . As we have already seen in the last section the Bargmann superselection rule must be fulfilled if we want to have a nontrivial result, hence $\mu_1 = -\mu_2$. We also assume right from the beginning that spatial translation invariance is already implemented and set

$$F^{(2)}(t_1, t_2, \mathbf{r}) := \langle \phi_1(t_1, \mathbf{r}_1) \phi_2(t_2, \mathbf{r}_2) \rangle \quad (2.95)$$

with $\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2$. If the ϕ_i are scalars under rotations, it is enough to restrict to $d = 1$ dimensions, the generalisation to $d > 1$ being obvious. Guided by the result for $z = 2$, we make the following ansatz for $F(t_1, t_2, \mathbf{r})$, in order to obtain homogeneous equations.

$$F^{(2)}(t_1, t_2, \mathbf{r}) = (t_1 - t_2)^{\hat{b}} \left(\frac{t_1}{t_2} \right)^{\hat{a}} t_2^{\hat{c}} G(t_1, t_2, \mathbf{r}) \quad (2.96)$$

with a function $G(t_1, t_2, \mathbf{r})$ which is to be determined. Using this ansatz and covariance under $X_0, Y_{-1/z+1}$ and X_1 , it is easy to see that if one sets

$$\hat{a} = \frac{1}{z} (2\xi_2 + x_2 - x_1), \quad \hat{b} = -\frac{1}{z} \left((2\xi_1 + x_1) + (2\xi_2 + x_2) \right), \quad \hat{c} = \frac{2}{z} (\xi_1 + \xi_2) \quad (2.97)$$

then G satisfies the homogeneous equations

$$\left(t_1 \partial_{t_1} + t_2 \partial_{t_2} + \frac{1}{z} \mathbf{r} \cdot \partial_{\mathbf{r}} \right) G = 0 \quad (2.98)$$

$$\left((t_1 - t_2) \partial_{\mathbf{r}} + z \mu_1 \mathbf{r} \cdot \nabla_{\mathbf{r}}^{2-z} + (\gamma_1^\dagger - \gamma_2^\dagger) \partial_{\mathbf{r}} \nabla_{\mathbf{r}}^{-z} \right) G = 0 \quad (2.99)$$

$$\left((t_1 - t_2)^2 \partial_{t_1} - t_2^2 \partial_{t_2} + \mu_1 \mathbf{r}^2 \nabla_{\mathbf{r}}^{2-z} + \frac{2}{z} (t_1 - t_2) \partial_{\mathbf{r}} \cdot \nabla_{\mathbf{r}}^{-z} + (\gamma_1^* + \gamma_2^*) \nabla_{\mathbf{r}}^{-z} \right) G = 0. \quad (2.100)$$

where we have defined the shorthands

$$\gamma^\dagger = z(2-z)\gamma, \quad \hat{\gamma} = 2(2-z)\gamma, \quad \gamma^* = (2-z)(d-z)\gamma \quad (2.101)$$

$$\beta = -(2-z) \left(1 - 2 \frac{\gamma}{\mu} \right), \quad \alpha = \frac{1}{z^2 \mu^{2-z}} \quad (2.102)$$

They will be used frequently in what follows. Equation (2.98) is readily solved to yield

$$G = H \left(\frac{\mathbf{r}}{(t_1 - t_2)^{1/z}}, \frac{t_1 - t_2}{t_2} \right) \quad (2.103)$$

where from eqs. (2.99,2.100) the function $H = H(\mathbf{u}, v)$ satisfies the following equations

$$\left(\partial_{\mathbf{u}} + z \mu_1 \mathbf{u} \cdot \nabla_{\mathbf{u}}^{2-z} + (\gamma_1^\dagger - \gamma_2^\dagger) \partial_{\mathbf{u}} \nabla_{\mathbf{u}}^{-z} \right) H = 0 \quad (2.104)$$

$$\left(z(v-1) \partial_v + (\gamma_2^\dagger + \gamma_1^\dagger) \partial_{\mathbf{u}} \nabla_{\mathbf{u}}^{-z} + z(\gamma_1^* + \gamma_2^*) \nabla_{\mathbf{u}}^{-z} \right) H = 0 \quad (2.105)$$

Here we have added $-\mathbf{u}$ times equation (2.99) to equation (2.100) in order to get the last equation. Note that equation (2.104) is the analogue of equation (2.43) known from the

old formulation of LSI. These two equations are best solved in Fourier space, where they become

$$\left(z\mu_1 i^{2-z} |\mathbf{k}|^{2-z} \partial_{\mathbf{k}} + \mathbf{k} + (z\mu_1 i(2-z) + (\gamma_1^\dagger - \gamma_2^\dagger)) \mathbf{k} |\mathbf{k}|^{-z} \right) \widehat{H} = 0 \quad (2.106)$$

$$\left(z(v-1) \partial_v - (\gamma_1^\dagger + \gamma_2^\dagger) \mathbf{k} |\mathbf{k}|^{-z} \partial_{\mathbf{k}} \right) \widehat{H} = 0 \quad (2.107)$$

Solving these two equations yields on the one hand the condition $\gamma_1 = -\gamma_2$, and on the other hand for the function \widehat{H} .

$$\widehat{H} = g_0 |\mathbf{k}|^{-(z\mu_1 i^{2-z}(2-z) + (\gamma_1^\dagger - \gamma_2^\dagger) i^{-z}) \alpha_1} \exp(-\alpha_1 |\mathbf{k}|^z) \quad (2.108)$$

Notice that the dependence on v has dropped out. Transforming back to real space and substituting all shorthands, we get therefore as final result:

$$\begin{aligned} F^{(2)}(t_1, t_2; \mathbf{r}) &= g_0 \delta_{\alpha_1, -\alpha_2} \delta_{\beta_1, \beta_2} (t_1 - t_2)^{-((2\xi_1 + x_1) + (2\xi_2 + x_2))/z} \\ &\times \left(\frac{t_1}{t_2} \right)^{(2\xi_2 + x_2 - x_1)/z} t_2^{2(\xi_1 + \xi_2)/z} \mathcal{F}^{(\alpha_1, \beta_1)} \left(\frac{\mathbf{r}}{(t_1 - t_2)^{1/z}} \right) \end{aligned} \quad (2.109)$$

where the space-time part is described by the function $\mathcal{F}^{(\alpha, \beta)}$.

$$\mathcal{F}^{(\alpha, \beta)}(\mathbf{u}) = \int_{\mathbb{R}^d} \frac{d\mathbf{k}}{(2\pi)^d} e^{i\mathbf{u} \cdot \mathbf{k}} |\mathbf{k}|^\beta \exp(-\alpha |\mathbf{k}|^z) \quad (2.110)$$

The Fourier transform depends merely on the absolute value $|\mathbf{k}|$, hence its inverse in real space will only depend on $|\mathbf{r}|$. This is detailed in appendix C of [21], where also some plots of the space-time scaling function $\mathcal{F}^{(\alpha, \beta)}$ can be found.

A remark about the notation: We use here the tuple (x, ξ, α, β) to characterise a quasiprimary field, where α and β have been defined in (2.101). α is related to the mass μ and therefore the Bargmann superselection rule is expressed in the Kronecker delta $\delta_{\alpha_1, -\alpha_2} = \delta_{\mu_1, -\mu_2}$. The parameter β vanishes for $z = 2$ and for $\mu = 2\gamma$. Alternatively one can also use the tuple (x, ξ, μ, γ) or $(x, \xi, \mu, \gamma/\mu)$ to characterise a quasiprimary field.

The case, when one implements as well invariance under time translations works in exactly the same way. In this case one has to set $\xi_1 = \xi_2 = 0$ in the above result and requires in addition that $x_1 = x_2$. We simply quote the result

$$F^{(2)}(t_1 - t_2; \mathbf{r}) = g_0 \delta_{\alpha_1, -\alpha_2} \delta_{x_1, x_2} \delta_{\beta_1, \beta_2} (t_1 - t_2)^{-2x_1/z} \mathcal{F}^{(\mu_1, \gamma_1)} \left(\frac{\mathbf{r}}{(t_1 - t_2)^{1/z}} \right) \quad (2.111)$$

A question which has not at all been addressed here, is whether there are solutions to equations (2.104) and (2.105) which have been lost by passing to Fourier space. This will require further investigation.

2.4.2 Four-point function

We now compute the four-point function of quasiprimary scaling operators

$$F^{(4)}(\{t_i\}, \{\mathbf{r}_i\}) := \left\langle \phi_1(t_1, \mathbf{r}_1) \dots \phi_4(t_4, \mathbf{r}_4) \right\rangle \quad (2.112)$$

Its Fourier transform we denote as usually by $\widehat{F}^{(4)}(\{t_i\}, \{\mathbf{k}_i\})$. The comparatively strict Bargmann rule (2.77) together with spatial translation-invariance suggests the following ansatz

$$\begin{aligned} \widehat{F}^{(4)}(\{t_i\}, \{\mathbf{k}_i\}) &= \delta_{\mu_1, -\mu_2} \delta_{\mu_3, -\mu_4} \delta(\mathbf{k}_1 + \mathbf{k}_2) \delta(\mathbf{k}_3 + \mathbf{k}_4) \widehat{G}_1(\{t_i\}, \{\mathbf{k}_i\}) \\ &+ \delta_{\mu_1, -\mu_2} \delta_{\mu_3, -\mu_4} \delta(\mathbf{k}_1 - \mathbf{k}_2) \delta(\mathbf{k}_3 - \mathbf{k}_4) \delta(\mathbf{k}_1 + \mathbf{k}_3) \widehat{G}_2(\{t_i\}, \{\mathbf{k}_i\}) \\ &+ \{2 \leftrightarrow 3\} + \{2 \leftrightarrow 4\} \end{aligned} \quad (2.113)$$

By the last line we simply mean terms, where the space-time points 2 and 3 and the space-time points 2 and 4 have been exchanged respectively. In this way, all possibilities allowed by the generalised Bargmann superselection rule are covered and momentum conservation (translation invariance) is satisfied.

In order to get clearer on the structure of the solution we start by considering the term $\mu \mathbf{r}^2 \nabla_{\mathbf{r}}^{2-z}$ which is part of the generator X_1 . Notice that it is the only term containing expression of the form \mathbf{r}^2 . Furthermore, we may suppose for the moment, without loss of generality that μ_1 and μ_4 are both positive or both negative. Then the most general ansatz taken from (2.113) is

$$\begin{aligned} F(\{t_i\}, \{\mathbf{r}_i\}) &= \delta_{\mu_1, -\mu_2} \delta_{\mu_3, -\mu_4} G_1(\{t_i\}; \mathbf{r}_{12}, \mathbf{r}_{34}) + \delta_{\mu_1, -\mu_2} \delta_{\mu_3, -\mu_4} \widetilde{G}_1(\{t_i\}; \mathbf{r}_{13}, \mathbf{r}_{24}) \\ &+ \delta_{\mu_1, -\mu_3} \delta_{\mu_2, -\mu_4} G_2(\{t_i\}; \mathbf{r}_{13}, \mathbf{r}_{24}) + \delta_{\mu_1, -\mu_3} \delta_{\mu_2, -\mu_4} \widetilde{G}_2(\{t_i\}; \mathbf{r}_{12}, \mathbf{r}_{34}) \end{aligned} \quad (2.114)$$

where $\mathbf{r}_{ij} := \mathbf{r}_i - \mathbf{r}_j$. If one applies now the operator $\mu \mathbf{r}^2 \nabla_{\mathbf{r}}^{2-z}$ we require that all prefactors of terms like \mathbf{r}_i^2 have to vanish, since the functions G_i and \widetilde{G}_i depend only on the differences \mathbf{r}_{ij} . This leads to the result, that the second and fourth term of the preceding ansatz can be dropped and the ansatz has therefore further been reduced to

$$F(\{t_i\}, \{\mathbf{r}_i\}) = \delta_{\mu_1, -\mu_2} \delta_{\mu_3, -\mu_4} G_1(\{t_i\}; \mathbf{r}_{12}, \mathbf{r}_{34}) + \delta_{\mu_1, -\mu_3} \delta_{\mu_2, -\mu_4} G_2(\{t_i\}; \mathbf{r}_{13}, \mathbf{r}_{24}) \quad (2.115)$$

Furthermore one can show that one can treat each term separately. Hence it is enough to consider

$$F^{(4)}(\{t_i\}, \{\mathbf{r}_i\}) = \delta_{\mu_1, -\mu_2} \delta_{\mu_3, -\mu_4} G(\mathbf{r}, \widetilde{\mathbf{r}}, \{t_i\}) \quad (2.116)$$

with $\mathbf{r} := \mathbf{r}_1 - \mathbf{r}_2$ and $\widetilde{\mathbf{r}} := \mathbf{r}_3 - \mathbf{r}_4$. The other terms can then simply be obtained by permutation of the space-time points. Invariance under $Y_{-1/z}^{(i)}$ is already implemented. The following computations will be done for $d = 1$ for convenience, but the result generalises to arbitrary d . The following equations remain to be solved

$$\left(\sum_{i=1}^4 t_i \partial_{t_i} + \frac{1}{z} \sum_{i=1}^4 \mathbf{r} \cdot \partial_{\mathbf{r}} + \frac{1}{z} \sum_{i=1}^4 x_i \right) G = 0 \quad (2.117)$$

$$\left(\sum_{i=1}^4 t_i \partial_{\mathbf{r}_i} + \sum_{i=1}^4 \mu_i z \mathbf{r}_i \nabla_{\mathbf{r}_i}^{2-z} + \sum_{i=1}^4 \gamma_i^\dagger \partial_{\mathbf{r}_i} \nabla_{\mathbf{r}_i}^{-z} \right) G = 0 \quad (2.118)$$

$$\begin{aligned} \left(\sum_{i=1}^4 t_i^2 \partial_{t_i} + \frac{2}{z} \sum_{i=1}^4 (x_i + \xi_i) t_i + \sum_{i=1}^4 \mu_i \mathbf{r}_i^2 \nabla_{\mathbf{r}_i}^{2-z} + \frac{2}{z} \sum_{i=1}^4 t_i (\mathbf{r}_i \cdot \partial_{\mathbf{r}_i}) \right. \\ \left. + \sum_{i=1}^4 \widehat{\gamma}_i \mathbf{r}_i \partial_{\mathbf{r}_i} \nabla_{\mathbf{r}_i}^{-z} + \sum_{i=1}^4 \gamma_i \nabla_{\mathbf{r}_i}^{-z} \right) G = 0 \end{aligned} \quad (2.119)$$

In order to obtain homogeneous equations, we set

$$G(\{t_i\}; \mathbf{r}, \tilde{\mathbf{r}}) = \prod_{i < j} (t_i - t_j)^{-\rho_{ij}} \prod_{i=1}^4 t_i^{-\sigma_i} \tilde{G}(\{t_i\}; \mathbf{r}, \tilde{\mathbf{r}}) \quad (2.120)$$

Introducing this into (2.117)-(2.119) we obtain on the one hand conditions on the parameters ρ_{ij} and σ_i .

$$\frac{2}{z} \sum_{i=1}^4 (\xi_i + x_i) t_i = \sum_{i=1}^4 \sigma_i t_i + \sum_{i < j} (t_1 + t_2) \rho_{ij} \quad (2.121)$$

$$\sum_{i < j} \rho_{ij} + \sum_{i=1}^4 \sigma_i = \frac{1}{z} \sum_{i=1}^4 x_i \quad (2.122)$$

which must hold true for all possible t_i . On the other hand the function \tilde{G} satisfies the following equations:

$$\left(\sum_{i=1}^4 t_i \partial_{t_i} + \frac{1}{z} \sum_{i=1}^4 \mathbf{r}_i \cdot \partial_{\mathbf{r}_i} \right) \tilde{G} = 0 \quad (2.123)$$

$$\left(\sum_{i=1}^4 t_i \partial_{\mathbf{r}_i} + \sum_{i=1}^4 \tilde{\mu}_i \mathbf{r}_i \nabla_{\mathbf{r}_i}^{2-z} + \sum_{i=1}^4 \gamma_i^\dagger \partial_{\mathbf{r}_i} \nabla_{\mathbf{r}_i}^{-z} \right) \tilde{G} = 0 \quad (2.124)$$

$$\begin{aligned} & \left(\sum_{i=1}^4 t_i^2 \partial_{t_i} + \sum_{i=1}^4 \mu_i \mathbf{r}_i^2 \nabla_{\mathbf{r}_i}^{2-z} + \frac{2}{z} \sum_{i=1}^4 t_i (\mathbf{r}_i \cdot \partial_{\mathbf{r}_i}) \right. \\ & \left. + \sum_{i=1}^4 \hat{\gamma}_i \mathbf{r}_i \partial_{\mathbf{r}_i} \nabla_{\mathbf{r}_i}^{-z} + \sum_{i=1}^4 \gamma_i^* \nabla_{\mathbf{r}_i}^{-z} \right) \tilde{G} = 0 \end{aligned} \quad (2.125)$$

The most frequent case for applications is that one has $x_1 = x_3 =: x$, $\xi_1 = \xi_3 =: \xi$ and $x_2 = x_4 =: \tilde{x}$, $\xi_2 = \xi_4 =: \tilde{\xi}$. This happens for instance for a four-point function of the type $\langle \phi(1) \tilde{\phi}(2) \phi(3) \tilde{\phi}(4) \rangle$, where ϕ is the order parameter field and $\tilde{\phi}$ the response field. In this case one can choose

$$\begin{aligned} \sigma_1 = \sigma_3 &= -\frac{2\xi}{z}, & \sigma_2 = \sigma_4 &= -\frac{2\tilde{\xi}}{z} \\ \rho_{13} &= \frac{2}{z}(2\xi + x) - \frac{2}{z}(2\tilde{\xi} + \tilde{x}), & \rho_{12} = \rho_{14} = \rho_{23} = \rho_{34} &= \frac{1}{z}(2\tilde{\xi} + \tilde{x}) \end{aligned} \quad (2.126)$$

and all other ρ_{ij} are set to zero. We proceed now with the solution of equations (2.123)-(2.125). If the function \tilde{G} depended on all coordinates \mathbf{r}_i , equation (2.123) would have the solution

$$\tilde{G} = H \left(\mathbf{r}_1 \tilde{t}_1^{-1/z}, \mathbf{r}_2 \tilde{t}_1^{-1/z}, \mathbf{r}_3 \tilde{t}_1^{-1/z}, \mathbf{r}_4 \tilde{t}_1^{-1/z}, \frac{\tilde{t}_2}{\tilde{t}_1}, \frac{\tilde{t}_3}{\tilde{t}_1}, \frac{t_4}{\tilde{t}_1} \right) \quad (2.127)$$

where we have introduced the shorthands $\tilde{t}_i := t_i - t_4$ for $i = 1, 2, 3$. But because G and \tilde{G} only depend on the differences \mathbf{r} and $\tilde{\mathbf{r}}$, this rather must have the form

$$H(\mathbf{u}_1, \mathbf{u}_2, \mathbf{v}_1, \mathbf{v}_2, w_2, w_3, w_4) = \tilde{H}(\mathbf{u}, \mathbf{v}, w_2, w_3, w_4) \quad (2.128)$$

where we write $\mathbf{u} = \mathbf{u}_2 - \mathbf{u}_1$ and $\mathbf{v} = \mathbf{v}_2 - \mathbf{v}_1$ and $w_2 = \tilde{t}_2/\tilde{t}_1$, $w_3 = \tilde{t}_3/\tilde{t}_1$, $w_4 = \tilde{t}_4/\tilde{t}_1$. Then one rewrites the remaining two equations (2.124) and (2.125) in terms of the new variables. When doing this, we realise that in order to make disappear an explicit dependence on \mathbf{r}_2 and \mathbf{r}_4 , we have to require the conditions

$$\left((1 - w_2)\partial_{\mathbf{u}} + \mu_1 z \mathbf{r} \nabla_{\mathbf{u}}^{2-z} + (\gamma_1^\dagger - \gamma_2^\dagger)\partial_{\mathbf{u}} \nabla_{\mathbf{u}}^{-z} \right) \tilde{G} = 0 \quad (2.129)$$

$$\left(w_3 \partial_{\mathbf{v}} + \mu_3 z \mathbf{v} \nabla_{\mathbf{v}}^{2-z} + (\gamma_3^\dagger - \gamma_4^\dagger)\partial_{\mathbf{v}} \nabla_{\mathbf{v}}^{-z} \right) G = 0 \quad (2.130)$$

If these two equations are added, they yield the same equations as obtained from (2.124). (2.129) and (2.130) are of course a stronger condition than the one obtained from (2.124). This is an effect of the strong restrictions of the generalised Bargmann superselection rule, which led to the ansatz (2.116). In addition to (2.129) and (2.130) we have the equation coming from (2.125)

$$\begin{aligned} & \left((w_2^2 - w_2)\partial_{w_2} + (w_3^2 - w_3)\partial_{w_3} - (w_4^2 + w_4)\partial_{w_4} + \right. \\ & \left. \frac{1}{z} \mathbf{u} \cdot \partial_{\mathbf{u}} + \frac{1}{z} (2w_3 - 1) \mathbf{v} \cdot \partial_{\mathbf{v}} + \mu_1 \mathbf{u}^2 \nabla_{\mathbf{u}}^{2-z} + \mu_3 \mathbf{v}^2 \nabla_{\mathbf{v}}^{2-z} + \right. \\ & \left. \tilde{\gamma}_1 \mathbf{u} \partial_{\mathbf{u}} \nabla_{\mathbf{u}}^{-z} + \tilde{\gamma}_3 \mathbf{v} \partial_{\mathbf{v}} \nabla_{\mathbf{v}}^{-z} + (\gamma_1^* + \gamma_2^*) \nabla_{\mathbf{u}}^{-z} + (\gamma_3^* + \gamma_4^*) \nabla_{\mathbf{v}}^{-z} \right) \tilde{H} = 0 \end{aligned} \quad (2.131)$$

Adding $-\frac{\mathbf{v}}{z}$ times equation (2.129) and $-\frac{\mathbf{u}}{z}$ times equation (2.130) to (2.131) and rewriting the equation obtained and equations (2.129) and (2.130) in Fourier-space

$$\left((1 - w_2) \mathbf{k} + \tilde{a}_1 \mathbf{k} |\mathbf{k}|^{-z} + z \mu_1 i^{2-z} |\mathbf{k}|^{2-z} \partial_{\mathbf{k}} \right) \hat{\tilde{H}} = 0 \quad (2.132)$$

$$\left(w_3 \mathbf{q} + \tilde{a}_3 \mathbf{q} |\mathbf{q}|^{-z} + z \mu_3 i^{2-z} |\mathbf{q}|^{2-z} \partial_{\mathbf{q}} \right) \hat{\tilde{H}} = 0 \quad (2.133)$$

$$\begin{aligned} & \left((w_2^2 - w_2)\partial_{w_2} + (w_3^2 - w_3)\partial_{w_3} - (w_4^2 + w_4)\partial_{w_4} - \frac{d}{z} (w_2 + w_3 - 1) \right. \\ & \left. - \frac{1}{z} (w_3 - 1) \mathbf{q} \cdot \partial_{\mathbf{q}} - \frac{w_2}{z} \mathbf{k} \cdot \partial_{\mathbf{k}} - b_1 i^{-z} \mathbf{k} |\mathbf{k}|^{-z} \partial_{\mathbf{k}} - b_2 i^{-z} \mathbf{q} |\mathbf{q}|^{-z} \partial_{\mathbf{q}} \right) \hat{\tilde{H}} = 0 \end{aligned} \quad (2.134)$$

where we have defined

$$\begin{aligned} \tilde{a}_1 &= (\gamma_1^\dagger - \gamma_2^\dagger) i^{-z} + \mu_1 z i^{2-z} (2 - z), & \tilde{a}_3 &= (\gamma_3^\dagger - \gamma_4^\dagger) i^{-z} + \mu_3 z i^{2-z} (2 - z) \\ b_1 &= \frac{1}{2} (\tilde{\gamma}_1 + \tilde{\gamma}_2), & b_3 &= \frac{1}{2} (\tilde{\gamma}_3 + \tilde{\gamma}_4) \end{aligned} \quad (2.135)$$

Equation (2.132) and (2.133) do not involve w_2, w_3, w_4 and are solved to yield

$$\hat{\tilde{H}} = |\mathbf{k}|^{-z\alpha_1 \hat{a}_1} |\mathbf{q}|^{-z\alpha_3 \hat{a}_3} \exp(-\alpha_1 (1 - w_2) |\mathbf{k}|^z - \alpha_3 w_3 |\mathbf{q}|^z) \chi(w_2, w_3, w_4) \quad (2.136)$$

where we have already substituted some of the shorthands. The remaining undetermined function $\chi(w_2, w_3, w_4)$ satisfies the following equation

$$\begin{aligned} & \left((w_2^2 - w_2)\partial_{w_2} + (w_3^2 - w_3)\partial_{w_3} - (w_4^2 + w_4)\partial_{w_4} \right) \chi = \\ & - \left(-\frac{d}{z} (w_2 + w_3 - 1) + \alpha_1 w_2 + \alpha_3 (w_3 - 1) \right. \\ & \left. + b_1 \tilde{a}_1 z \alpha_1 |\mathbf{k}|^{-z} + b_2 \tilde{a}_3 z \alpha_3 |\mathbf{q}|^{-z} + b_1 z \alpha_1 i^{-z} (1 - w_2) + b_2 z \alpha_3 i^{-z} w_3 \right) \chi \end{aligned} \quad (2.137)$$

The terms involving \mathbf{k} and \mathbf{q} on the righthand side of (2.137) have to vanish. For this reason the conditions

$$b_1 \tilde{a}_1 = 0, \quad b_2 \tilde{a}_3 = 0 \quad (2.138)$$

have to hold. There are four possibilities so solve condition (2.138). For each possibility, equation (2.137) takes a slightly different form, but it can be solved for each case by standard methods. We only list the result

1. $b_1 = 0$ and $b_2 = 0 \Leftrightarrow \gamma_1 = -\gamma_2$ and $\gamma_3 = -\gamma_4$ In this case χ is given by

$$\chi(w_2, w_3, w_4) = (w_2 - 1)^{d/z+\beta_1/z} w_3^{d/z+\beta_3/z} f\left(\frac{w_2(w_3 - 1)}{w_3(w_2 - 1)}, \frac{w_4(w_2 - 1)}{w_2(w_4 + 1)}\right) \quad (2.139)$$

where f is a remaining, undetermined function. Remember the shorthand introduced above $\beta_i = -(2 - z)(1 - 2\gamma_i/\mu_i)$.

2. $\tilde{a}_1 = 0$ and $b_2 = 0 \Leftrightarrow \mu_1 = \gamma_1 - \gamma_2$ and $\gamma_3 = -\gamma_4$ In this case χ is given by

$$\begin{aligned} \chi(w_2, w_3, w_4) &= (1 - 1/w_2)^{d/z} w_2^{d/z-\beta_1/z} w_3^{d/z+\beta_3/z} \\ &\times f\left(\frac{w_2(w_3 - 1)}{w_3(w_2 - 1)}, \frac{w_4(w_2 - 1)}{w_2(w_4 + 1)}\right) \end{aligned} \quad (2.140)$$

3. $\tilde{a}_3 = 0$ and $b_1 = 0 \Leftrightarrow \gamma_1 = -\gamma_2$ and $\mu_3 = \gamma_3 - \gamma_4$ In this case, χ is given by

$$\begin{aligned} \chi(w_2, w_3, w_4) &= (1 - 1/w_2)^{-d/z} (1 - w_2)^{d/z+\beta_1/z} (1 - w_3)^{d/z-\beta_3/z} \\ &\times f\left(\frac{w_2(w_3 - 1)}{w_3(w_2 - 1)}, \frac{w_4(w_2 - 1)}{w_2(w_4 + 1)}\right) \end{aligned} \quad (2.141)$$

4. $\tilde{a}_1 = 0$ and $\tilde{a}_3 = 0 \Leftrightarrow \mu_1 = \gamma_1 - \gamma_2$ and $\mu_3 = \gamma_3 - \gamma_4$ In this case, χ is given by

$$\chi(w_2, w_3, w_4) = (w_3 - 1)^{d/z+\beta_3/z} w_2^{-d/z+\beta_1/z} f\left(\frac{w_2(w_3 - 1)}{w_3(w_2 - 1)}, \frac{w_4(w_2 - 1)}{w_2(w_4 + 1)}\right) \quad (2.142)$$

At this point let us remark, that if we had implemented also invariance under X_{-1} , the results would be the same except for the replacements $f(x, y) \rightarrow f(x)$ in the above four cases.

Before proceeding let us comment on these results. First, one realises when substituting all shorthands that the space-time behaviour (2.136) is essentially given by two functions of the type (2.110). Furthermore, for applications, one usually encounters the case when $\gamma := \gamma_1 = \gamma_3 = -\gamma_2 = -\gamma_4$, and $\mu := \mu_1 = \mu_3 = -\mu_2 = -\mu_4$. This has the following consequences for the four different cases

1. $\beta := \beta_1 = \beta_3$ and β is a free parameter
2. $\mu_1 = 2\gamma_1$ and $\beta_1 = \beta_3$ and therefore $\beta_1 = \beta_3 = 0$. Thus the space-time behaviour is comparatively trivial, as it corresponds essentially to a free field theory.
3. $\mu_3 = 2\gamma_3$ and $\beta_1 = \beta_3$ and therefore $\beta_1 = \beta_3 = 0$. Also in this case the space-time behaviour is trivial.

4. $\mu_1 = 2\gamma_1$ and $\mu_3 = 2\gamma_3$ and therefore $\beta_1 = \beta_3 = 0$. This case also yields a trivial space-time behaviour.

From this consideration we see that only the first of the above cases is suitable for further application. Therefore we only list the complete result for the first case. The other three cases can easily be obtained from the above expression by substituting all shorthands. The complete result for the four-point function in the first case is

$$\begin{aligned}
F(\{t_i\}, \{\mathbf{r}_i\}) &= \prod_{i<j} (t_i - t_j)^{-\rho_{ij}} \prod_{i=1}^4 t_i^{-\sigma_i} f_1 \left(\frac{(t_2 - t_4)(t_1 - t_3)}{(t_1 - t_2)(t_3 - t_4)}, \frac{t_4(t_2 - t_1)}{t_1(t_2 - t_4)} \right) \\
&\times \delta_{\alpha_1, -\alpha_2} \delta_{\beta_1, \beta_2} \mathcal{F}^{(\alpha_1, \beta_1)} \left(\frac{\mathbf{r}_1 - \mathbf{r}_2}{(t_1 - t_2)^{1/z}} \right) \delta_{\alpha_3, -\alpha_4} \delta_{\beta_3, \beta_4} \mathcal{F}^{(\alpha_3, \beta_3)} \left(\frac{\mathbf{r}_3 - \mathbf{r}_4}{(t_3 - t_4)^{1/z}} \right) \quad (2.143) \\
&+ \prod_{i<j} (t_i - t_j)^{-\rho'_{ij}} \prod_{i=1}^4 t_i^{-\sigma'_i} f_2 \left(\frac{(t_3 - t_4)(t_1 - t_2)}{(t_1 - t_3)(t_2 - t_4)}, \frac{t_4(t_3 - t_1)}{t_1(t_3 - t_4)} \right) \\
&\times \delta_{\alpha_1, -\alpha_3} \delta_{\beta_1, \beta_3} \mathcal{F}^{(\alpha_1, \beta_1)} \left(\frac{\mathbf{r}_1 - \mathbf{r}_3}{(t_1 - t_3)^{1/z}} \right) \delta_{\alpha_2, -\alpha_4} \delta_{\beta_2, \beta_4} \mathcal{F}^{(\alpha_2, \beta_2)} \left(\frac{\mathbf{r}_2 - \mathbf{r}_4}{(t_2 - t_4)^{1/z}} \right) \\
&+ \prod_{i<j} (t_i - t_j)^{-\rho''_{ij}} \prod_{i=1}^4 t_i^{-\sigma''_i} f_3 \left(\frac{(t_4 - t_2)(t_1 - t_3)}{(t_1 - t_4)(t_3 - t_2)}, \frac{t_2(t_4 - t_1)}{t_1(t_4 - t_2)} \right) \\
&\times \delta_{\alpha_1, -\alpha_4} \delta_{\beta_1, \beta_4} \mathcal{F}^{(\alpha_1, \beta_1)} \left(\frac{\mathbf{r}_1 - \mathbf{r}_4}{(t_1 - t_4)^{1/z}} \right) \delta_{\alpha_3, -\alpha_2} \delta_{\beta_3, \beta_2} \mathcal{F}^{(-\alpha_3, \beta_3)} \left(\frac{\mathbf{r}_3 - \mathbf{r}_2}{(t_3 - t_2)^{1/z}} \right)
\end{aligned}$$

Here the functions f_i are arbitrary functions undetermined by the symmetries. The sets of parameters $\{\rho_{ij}, \sigma_i\}$, $\{\rho'_{ij}, \sigma'_i\}$ and $\{\rho''_{ij}, \sigma''_i\}$ has each to satisfy the conditions (2.121) and (2.122). We could have implemented as well invariance under X_{-1} . The computations are quite analogous and the result can be obtained from formula (2.143) by setting $\xi = 0$ and $\sigma_i = 0$ and by dropping the last argument of the scaling functions f_i , i.e. by making the replacements

$$f_i(x, y) \longrightarrow \tilde{f}_i(x) \quad (2.144)$$

It is worthwhile to give a short look to this latter case. The form of the solution is then not dissimilar to what is known from the conformal fourpoint function [72, 107]: Prefactors of the type $\prod_{i<j}^4 (t_i - t_j)^{-\rho_{ij}}$ are present (just like for the conformal case) and the dependence on the invariant ratios of the type $(t_4 - t_2)(t_1 - t_3)/((t_1 - t_4)(t_3 - t_2))$ can not be fixed. For the case when invariance under X_1 is not implemented, there is a dependence on additional terms like t_2/t_1 which break time-translation invariance. The space-time behaviour is completely fixed and essentially described by products of the function $\mathcal{F}^{(\alpha, \beta)}$.

For later use, we specialise this formula to the case when we consider an expression like $\langle \phi(t_1, \mathbf{r}_1) \phi(t_2, \mathbf{r}_2) \tilde{\phi}(t_3, \mathbf{r}_3) \phi(t_4, \mathbf{r}_4) \rangle$ that is the case $\mu := \mu_1 = \mu_2 = -\mu_3 = -\mu_4$ and $\gamma := \gamma_1 = \gamma_2 = -\gamma_3 = -\gamma_4$. Then the first term in (2.143) vanishes and for the parameters ρ'_{ij} and ρ''_{ij} we make a choice similar to (2.126). The four-point function then reads

$$\begin{aligned}
F(\{t_i\}, \{\mathbf{r}_i\}) &= (t_1 t_2)^{2\xi/z} (t_3 t_4)^{2\tilde{\xi}/z} \\
&(t_1 - t_2)^{-2(2\xi+x)/z+2(2\tilde{\xi}+\tilde{x})/z} (t_1 - t_3)^{-(2\tilde{\xi}+\tilde{x})/z} (t_1 - t_4)^{-(2\tilde{\xi}+\tilde{x})/z} (t_2 - t_3)^{-(2\tilde{\xi}+\tilde{x})/z} (t_2 - t_4)^{-(2\tilde{\xi}+\tilde{x})/z} \\
&\times \left[f_2 \left(\frac{(t_3 - t_4)(t_1 - t_2)}{(t_1 - t_3)(t_2 - t_4)}, \frac{t_4(t_3 - t_1)}{t_1(t_3 - t_4)} \right) \mathcal{F}^{(\mu, \gamma)} \left(\frac{\mathbf{r}_1 - \mathbf{r}_3}{(t_1 - t_3)^{1/z}} \right) \mathcal{F}^{(\mu, \gamma)} \left(\frac{\mathbf{r}_2 - \mathbf{r}_4}{(t_2 - t_4)^{1/z}} \right) \right. \\
&+ \left. f_3 \left(\frac{(t_4 - t_2)(t_1 - t_3)}{(t_1 - t_4)(t_3 - t_2)}, \frac{t_2(t_4 - t_1)}{t_1(t_4 - t_2)} \right) \mathcal{F}^{(\mu, \gamma)} \left(\frac{\mathbf{r}_1 - \mathbf{r}_4}{(t_1 - t_4)^{1/z}} \right) \mathcal{F}^{(\mu, \gamma)} \left(\frac{\mathbf{r}_3 - \mathbf{r}_2}{(t_3 - t_2)^{1/z}} \right) \right] \quad (2.145)
\end{aligned}$$

with two undetermined functions f_2 and f_3 .

2.5 Results for the response and the correlation function

At long last, we can return to our original task of the computation of response and correlation functions. We recall that for the case $z = 2$, the following procedure for the calculation of n -point functions was developed [192, 114, 126]

1. we break time-translation-invariance *explicitly* by considering a Langevin equation of the form (2.78) with a time-dependent potential $v(t)$. We can reduce this to the standard form via the gauge transformation (2.80) and set

$$g_\mu(t) = \exp \left(-\frac{1}{\mu} \int_0^t du v(u) \right) \sim t^F \quad \text{or equivalently} \quad v(t) = -\frac{\mu F}{t} \quad (2.146)$$

which defines a new parameter F ,

2. recall that for ageing-invariance the scaling operators ϕ (with scaling dimension x) do not transform as conventional quasi-primary scaling operators, but are related via (2.56) to *bona fide* quasiprimary scaling operators Φ , with scaling dimension $x + 2\xi$,
3. We then use full local scale-invariance for the calculation of the required two- and four-point functions.

For the case of general z , we will leave out the generator X_{-1} for the computation of the two- and four-point functions. This does not change the result for the two-point function, but for the fourpoint function it entails more flexibility in the case of critical dynamics (which will be needed). Recall the formulæ (2.91), (2.93) and (2.94) for the response and correlation functions. Using the results of the last section and the gauge transformation (2.80), the two- and four-point functions are then given by

$$\langle \phi(t, \mathbf{x}) \tilde{\phi}(s, \mathbf{y}) \rangle = \frac{g_\mu(t)}{g_\mu(s)} F^{(2)}(t, s; \mathbf{x} - \mathbf{y}) \quad (2.147)$$

and

$$\langle \phi(t, \mathbf{x}) \phi(s, \mathbf{y}) \tilde{\phi}(u, \mathbf{R}) \tilde{\phi}(u', \mathbf{R}') \rangle = \frac{g_\mu(t) g_\mu(s)}{g_\mu(u) g_\mu(u')} F^{(4)}(t, s, u, u'; \mathbf{x}, \mathbf{y}, \mathbf{R}, \mathbf{R}') \quad (2.148)$$

2.5.1 Response function

We start with the response function, which is given by, according to (2.91)

$$R(t, s, \mathbf{r}) = r_0 s^{-2(x+\tilde{x})/z} \left(\frac{t}{s}\right)^{(2\tilde{\xi}+\tilde{x}-x)/z+F} \left(\frac{t}{s}-1\right)^{-((2\xi+x)+(2\tilde{\xi}+\tilde{x}))/z} \\ \times \mathcal{F}^{(\alpha,\beta)}\left(\frac{\mathbf{r}}{(t-s)^{1/z}}\right) \quad (2.149)$$

with a normalisation constant r_0 . Here we have taken equation (2.109) and the gauge transform (2.80) into account.

Although our approach is in general more restrictive than simple Galilei- or Schrödinger-invariance which apply for $z = 2$, our result for the two-point function also includes the $z = 2$ case, since for the two-point functions, the generalised Bargmann rule (2.77) and the Bargmann rule for $z = 2$ coincide.⁹ We define the ageing exponents

$$a := \frac{1}{z}(x + \tilde{x}) - 1, \quad a' := \frac{1}{z}\left((2\xi + x) + (2\tilde{\xi} + \tilde{x})\right) - 1, \quad \lambda_R/z := -F + \frac{2}{z}(\xi + x) \quad (2.150)$$

and then find the autoresponse function ($\mathbf{r} = 0$)

$$R(t, s) = r_0 s^{-a-1} \left(\frac{t}{s}\right)^{1+a'-\lambda_R/z} \left(\frac{t}{s}-1\right)^{-1-a'}. \quad (2.151)$$

The form of $R(t, s)$ has not changed compared to the old version of LSI [109, 192, 121]. Therefore all tests of LSI which have been performed for the autoresponse function remain valid. We refer the reader to recent reviews and articles [122, 125, 121], where these results and tables with the corresponding ageing exponents can be found. The full space-time response functions reads

$$R(t, s; \mathbf{r}) = R(t, s) \mathcal{F}^{(\alpha,\beta)}\left(\frac{\mathbf{r}}{(t-s)^{1/z}}\right) \quad (2.152) \\ = r_0 s^{-a-1} \left(\frac{t}{s}\right)^{1+a'-\lambda_R/z} \left(\frac{t}{s}-1\right)^{-1-a'} \int_{\mathbb{R}^d} \frac{d\mathbf{k}}{(2\pi)^d} |\mathbf{k}|^\beta \exp\left(\frac{i\mathbf{r} \cdot \mathbf{k}}{(t-s)^{1/z}} - \alpha|\mathbf{k}|^z\right)$$

For a plot of the space-time behaviour of this function, see appendix C of [21].

2.5.2 Correlation function

Here, we must distinguish the cases of (i) phase-ordering kinetics [37], when the preparation part $C_{init}(t, s; \mathbf{r})$ dominates, and (ii) the case of non-equilibrium critical dynamics [45], when the thermal part $C_{th}(t, s; \mathbf{r})$ is the leading one.

We start with the former case. Here we have to evaluate expression $C_{init}(t, s; \mathbf{r})$ further. By assigning the masses μ and $\tilde{\mu} = -\mu$ to the fields ϕ and $\tilde{\phi}$ respectively, we obtain from (2.143), (2.126) and (2.148)

$$C_{init}(t, s; \mathbf{x} - \mathbf{y}) = c_0 s^{2F-2(x+\tilde{x})/z-4\tilde{\xi}/z} y^{F-2(\tilde{x}+2\tilde{\xi}-\xi)/z} (y-1)^{-2(x+2\xi-\tilde{x}-2\tilde{\xi})/z} \quad (2.153) \\ \int_{\mathbb{R}^d} d\mathbf{u} d\mathbf{v} \mathcal{F}^{(\alpha_1,\beta_1)}\left(\frac{\mathbf{x}}{t^{1/z}} - \frac{\mathbf{u}}{t^{1/z}}\right) \mathcal{F}^{(\alpha_3,\beta_3)}\left(\frac{\mathbf{y}}{s^{1/z}} - \frac{\mathbf{v}}{s^{1/z}}\right) a(\mathbf{u}, \mathbf{v})$$

⁹This is not true any more for the four-point function and in consequence for the correlation functions discussed below.

with $a(\mathbf{R}, \mathbf{R}') = \langle \phi(0, \mathbf{R}) \phi(0, \mathbf{R}') \rangle$ for the initial correlations. We also admit that this term does not break translation invariance, that is $a(\mathbf{R}, \mathbf{R}')$ depends only on $\mathbf{R} - \mathbf{R}'$ and its Fourier transform can be written as $(2\pi)^d \delta(\mathbf{k} + \mathbf{q}) \widehat{a}(\mathbf{k})$. Before proceeding it is useful to note the following property of the function $\mathcal{F}^{(\alpha, \beta)}(\mathbf{u})$, which is easily verified. For an arbitrary function $g(\mathbf{u}, \mathbf{k})$ and constants $c, \mathbf{a}, d, \mathbf{b}$ we have

$$\begin{aligned} & \int_{\mathbb{R}^d} d\mathbf{u} d\mathbf{v} \mathcal{F}^{(\alpha_1, \beta_1)}(c\mathbf{u} + \mathbf{a}) \mathcal{F}^{(\alpha_3, \beta_3)}(d\mathbf{v} + \mathbf{b}) g(\mathbf{u}, \mathbf{v}) \\ &= \int_{\mathbb{R}^d} \frac{d\mathbf{k}}{(2\pi)^d} \int_{\mathbb{R}^d} \frac{d\mathbf{q}}{(2\pi)^d} e^{i\mathbf{a} \cdot \mathbf{k}} e^{i\mathbf{b} \cdot \mathbf{q}} \widehat{g}(c\mathbf{k}, d\mathbf{q}) |\mathbf{k}|^{\beta_1} |\mathbf{q}|^{\beta_3} \exp(-\alpha_1 |\mathbf{k}|^z) \exp(-\alpha_3 |\mathbf{q}|^z) \end{aligned} \quad (2.154)$$

where $\widehat{g}(\mathbf{k}, \mathbf{q})$ is the Fourier Transform of the function $g(\mathbf{u}, \mathbf{v})$. With this we obtain

$$\begin{aligned} C_{init}(t, s; \mathbf{r}) &= c_0 s^{2F - 2(2\tilde{\xi} + x + \tilde{x})/z + 2\beta/z + 2d/z} y^{F - 2(\tilde{x} + 2\tilde{\xi} - \xi)/z + \beta/z + d/z} \\ &\times (y - 1)^{-2(x - \tilde{x})/z - 4(\xi - \tilde{\xi})/z} \int_{\mathbb{R}^d} \frac{d\mathbf{k}}{(2\pi)^d} |\mathbf{k}|^{2\beta} \exp(-\alpha |\mathbf{k}|^z (t + s)) e^{i\mathbf{r} \cdot \mathbf{k}} \widehat{a}(\mathbf{k}) \end{aligned} \quad (2.155)$$

We are ultimately interested in the case of decorrelated initial conditions, which means $\widehat{a}(\mathbf{k}) = a_0 = \text{const.}$ At this point, we need to take into account the following: For computational reasons, we had to find the three-point function via the four-point function. We now have to pull two points together for the case of decorrelated initial conditions. But it is known from the case $z = 2$ that in this case, the scaling dimensions of the field $\widetilde{\phi}^2$ acquires an additional contribution and only in the free-field case the scaling dimension of $\widetilde{\phi}^2$ is equal to two times the scaling dimension of $\widetilde{\phi}$. In order to get a prediction for this case also we should therefore replace $(\tilde{x}, \tilde{\xi}) \rightarrow (\tilde{x}_2, \tilde{\xi}_2)$ where these new parameters denote the scaling dimension of the composite field $\widetilde{\phi}^2$. This then gives us the final result for the preparation part of the correlation function for decorrelated initial conditions.

$$\begin{aligned} C_{init}(t, s; \mathbf{r}) &= c_0 a_0 s^{-b_{init} + 2\beta/z + d/z} y^{-b_{init} + \lambda_C/z} (y - 1)^{b_{init} + d/z - 2\lambda_C/z + 2\beta/z} \\ &\times \int_{\mathbb{R}^d} \frac{d\mathbf{k}}{(2\pi)^d} |\mathbf{k}|^{2\beta} \exp(-\alpha |\mathbf{k}|^z (t + s)) e^{i\mathbf{r} \cdot \mathbf{k}} \end{aligned} \quad (2.156)$$

where the following identifications were used

$$b_{init} := -2F + \frac{2}{z}(x + \tilde{x}_2) + \frac{4}{z}\tilde{\xi}_2 - \frac{d}{z}, \quad \frac{\lambda_C}{z} := -F + \frac{2}{z}(x + \xi) + \frac{\beta}{z} = \frac{\lambda_R}{z} + \frac{\beta}{z} \quad (2.157)$$

and the scaling function $f_C(y)$ is given by

$$f_C(y) = c_0 y^{-b_{init} + \lambda_C/z} (y - 1)^{b_{init} + d/z - 2\lambda_C/z + 2\beta/z} (y + 1)^{-d/z - 2\beta/z} \quad (2.158)$$

Notice that we have $\lambda_R \neq \lambda_C$ unless $z = 2$ or $\gamma/\mu = 1/2$ (as $\beta = -(2 - z)(1 - \frac{2\gamma}{\mu})$), see (2.101). This is different from the case $z = 2$, where the equality $\lambda_R = \lambda_C$ holds [37, 192]. For the exactly solvable models treated in section 3 this fact can not be verified as for these models $\gamma/\mu = 1/2$. But numerical studies of the disordered Ising model are indeed consistent with distinct autocorrelation and autoresponse exponents $\lambda_R \neq \lambda_C$ [121, 125, 20].

We could also imagine a long-range initial correlator, which decreases for large distances as

$$\langle \phi(0, \mathbf{R}) \phi(0, \mathbf{R}') \rangle = |\mathbf{R} - \mathbf{R}'|^{-\kappa - d} \Leftrightarrow a(\mathbf{k}) = |\mathbf{k}|^\kappa \quad (2.159)$$

For a parameter κ . In this case formula (2.155) evaluates to

$$C_{init}(t, s; \mathbf{r}) = c_0 a_0 s^{-b_{init}+2\beta/z+\kappa/z+d/z} y^{-b_{init}+\lambda_C/z} (y-1)^{b_{init}+d/z-2\lambda_C/z+2\beta/z+\kappa/z} \\ \times \int_{\mathbb{R}^d} \frac{d\mathbf{k}}{(2\pi)^d} |\mathbf{k}|^{2\beta+\kappa} \exp\left(-\frac{|\mathbf{k}|^z}{z^2 \mu i^{2-z}}(t+s)\right) e^{i\mathbf{r}\cdot\mathbf{k}}$$

where this time

$$b_{init} = -2F + \frac{2}{z}(x + \tilde{x}_2) + \frac{4}{z}\tilde{\xi}_2 + \frac{\kappa}{z} - \frac{d}{z}, \quad \lambda_C/z = -F + \frac{2}{z}(x + \xi) + \frac{\beta}{z} + \frac{\kappa}{z} = \frac{\lambda_R}{z} + \frac{\beta}{z} + \frac{\kappa}{z}. \quad (2.160)$$

The scaling function $f_C(y)$ then reads

$$f_C(y) = c_0 y^{-b_{init}+\lambda_C/z} (y-1)^{b_{init}+d/z-2\lambda_C/z+2\beta/z+\kappa/z} (y+1)^{-d/z-2\beta/z-\kappa/z} \quad (2.161)$$

We also want to look here at a slightly more general situation, namely when the initial condition is imposed at an arbitrary time $u \leq s$ and not necessarily at time 0. The computations for this case follow the same lines as for the simpler case we have just seen. The four-point function in this case reads ($t_1 = t, t_2 = s, t_3 = t_4 = u$)

$$F(t, s, u, u; \{\mathbf{r}_i\}) = (t \cdot s)^{2\xi/z} u^{4\tilde{\xi}/z} (t-s)^{-2(2\xi+x)/z+2(2\tilde{\xi}+\tilde{x})/z} (t-u)^{-2(2\tilde{\xi}+\tilde{x})/z} (s-u)^{-2(2\tilde{x}+\tilde{x})/z} \\ \times \left[\mathcal{F}^{(\mu,\gamma)}\left(\frac{\mathbf{r}_1 - \mathbf{r}_3}{(t-u)^{1/z}}\right) \mathcal{F}^{(\mu,\gamma)}\left(\frac{\mathbf{r}_2 - \mathbf{r}_4}{(s-u)^{1/z}}\right) \right. \\ \left. + f_3\left(\frac{s}{t} \frac{u-t}{u-s}\right) \mathcal{F}^{(\mu,\gamma)}\left(\frac{\mathbf{r}_1 - \mathbf{r}_4}{(t-u)^{1/z}}\right) \mathcal{F}^{(\mu,\gamma)}\left(\frac{\mathbf{r}_2 - \mathbf{r}_3}{(u-s)^{1/z}}\right) \right] \quad (2.162)$$

Then the correlation function is given by

$$C_{init}(t, s; \mathbf{x}, \mathbf{y}) = \int d\mathbf{R} d\mathbf{R}' F(t, s, u, u; \mathbf{x}, \mathbf{y}, \mathbf{R}, \mathbf{R}') a(u, \mathbf{R}, \mathbf{R}') \quad (2.163)$$

where $a(u, \mathbf{R}, \mathbf{R}')$ is the equal-time correlator at time u . Using property (2.154), one obtains as general result

$$C_{init}(t, s; \mathbf{r}) = c_0 (t \cdot s)^{2\xi/z+F} u^{4\tilde{x}/z-2F} (t-s)^{-2(2\xi+x)/z+2(2\tilde{\xi}+\tilde{x})/z} (t-u)^{-2(2\tilde{\xi}+\tilde{x})/z} \\ (s-u)^{-2(2\tilde{x}+\tilde{x})/z} \tilde{f}\left(\frac{s}{t} \frac{u-t}{u-s}\right) \int \frac{d\mathbf{k}}{(2\pi)^d} \exp(i\mathbf{r}\cdot\mathbf{k}) |\mathbf{k}|^{2\beta} \exp\left(-\alpha |\mathbf{k}|^z (t+s-2u)\right) \hat{a}(u, \mathbf{k}) \quad (2.164)$$

where \tilde{f} is an undetermined function. For $u = 0$ we recover the result (2.155) whereas for example for $u = s$ and $a(s, \mathbf{R}, \mathbf{R}') = \exp(-\nu(\mathbf{R} - \mathbf{R}')^2/s^{2/z})$ (with a new parameter ν), we get

$$C_{init}(t, s; \mathbf{r}) = c_0 s^{-b_{init}+d/z+2\beta/z} y^\rho (y-1)^{-\rho-\lambda_C/z+d/z+2\beta/z} \\ \int \frac{d\mathbf{k}}{(2\pi)^d} \exp(i\mathbf{r}\cdot\mathbf{k}) |\mathbf{k}|^{2\beta} \exp\left(-\alpha |\mathbf{k}|^z s(y-1) - \frac{|\mathbf{k}|^2 s^{2/z}}{4\nu}\right) \quad (2.165)$$

where we have identified

$$b_{init} = -\frac{4}{z}\tilde{\xi} + \frac{2}{z}x + \frac{\beta}{z} + \frac{d}{z}, \quad \frac{\lambda_C}{z} = -F + \frac{2}{z}(\xi + x) + \frac{\beta}{z} = \frac{\lambda_R}{z} + \frac{\beta}{z}, \quad \rho = \frac{2}{z}\xi + F \quad (2.166)$$

This means for the function $f_C(y)$, that

$$f_C(y) = c_0 y^\rho (y-1)^{-\rho-\lambda_C/z+2\beta/z+d/z} \int \frac{d\mathbf{k}}{(2\pi)^d} |\mathbf{k}|^{2\beta} \exp\left(-\alpha|\mathbf{k}|^z (y-1) - \frac{|\mathbf{k}|^2}{4\nu}\right) \quad (2.167)$$

The parameter ρ could in principle still be fixed by the requirement that for $y \rightarrow 1$ the autocorrelator should have a finite and nonvanishing value. This leads to

$$\rho = \frac{2\beta}{z} + \frac{d}{z} - \frac{\lambda_C}{z} \quad (2.168)$$

For the second case of non-equilibrium critical dynamics, the thermal part $C_{th}(t, s; \mathbf{r})$ is the dominant contribution. Let $b(\mathbf{R}, \mathbf{R}')$ denote the spatial part of the noise-correlator, that is

$$\langle \eta(t, \mathbf{R}) \eta(t', \mathbf{R}') \rangle = 2T \delta(t-t') b(\mathbf{R}, \mathbf{R}'). \quad (2.169)$$

Also here, we admit translation-invariance of $b(\mathbf{R}, \mathbf{R}')$ and denote with $\widehat{b}(\mathbf{k})$ its Fourier transform. With the help of (2.145), (2.126) and (2.148) one finds

$$\begin{aligned} C_{th}(t, s; \mathbf{r}) &= 2T c_0 s^{1-2(x+\tilde{x})/z+4\tilde{\xi}/z+2\beta/z+2d/z} y^{F+2\xi/z} (y-1)^{-2(2\xi+x-2\tilde{\xi}-\tilde{x})/z} \\ &\times \int_0^1 d\theta (y-\theta)^{-2(2\tilde{\xi}+\tilde{x})/z+\beta/z+d/z} (1-\theta)^{-2(2\tilde{\xi}+\tilde{x})/z+\beta/z+d/z} \theta^{-2F+4\tilde{\xi}/z} \\ &\times g\left(\frac{1}{y} \cdot \frac{y-\theta}{1-\theta}\right) \int_{\mathbb{R}^d} \frac{d\mathbf{k}}{(2\pi)^d} |\mathbf{k}|^{2\beta} e^{-i\mathbf{r}\cdot\mathbf{k}} \widehat{b}(\mathbf{k}) \exp(-\alpha|\mathbf{k}|^z s(y+1-2\theta)) \end{aligned} \quad (2.170)$$

where $g(u)$ is a remaining undetermined function, which is related to f_2 and f_3 from formula (2.145) via $g(u) = f_2(0, \infty) + f_3(1, u)$. For the case of white noise ($\widehat{b}(\mathbf{k}) = b_0 = \text{const}$), we face the same problem as before and introduce the new scaling dimensions \tilde{x}_2 and $\tilde{\xi}_2$. This then yields for the case of white noise the result

$$\begin{aligned} C_{th}(t, s; \mathbf{r}) &= 2T c_0 s^{-b_{th}+2\beta/z+d/z} y^{F+2\xi/z} (y-1)^{2(1+a')-2(F+\lambda_R/z)+b'_{th}-4\xi/z} \\ &\times \int_0^1 d\theta \theta^{-2F+4\tilde{\xi}_2/z} (y-\theta)^{2\xi/z+\lambda_R/z+F-2(1+a')+\beta/z+d/z-b'_{th}} \\ &\times (1-\theta)^{2\xi/z+\lambda_R/z+F-2(1+a')+\beta/z+d/z-b'_{th}} g\left(\frac{1}{y} \frac{\theta-y}{1-\theta}\right) \\ &\times \int_{\mathbb{R}^d} \frac{d\mathbf{k}}{(2\pi)^d} e^{-i\mathbf{k}\cdot\mathbf{r}} |\mathbf{k}|^{2\beta} \exp(-\alpha|\mathbf{k}|^z s(y+1-2\theta)) \end{aligned} \quad (2.171)$$

where we have defined the exponents

$$b_{th} := \frac{2}{z}(x + \tilde{x}_2) - 1 - \frac{d}{z}, \quad b'_{th} := \frac{2}{z}(\tilde{x}_2 - \tilde{x}) \quad (2.172)$$

The scaling function $f_C(y)$ reads (up to a constant prefactor).

$$\begin{aligned} f_C(y) &= y^{F+\frac{2}{z}\xi} (y-1)^{2(1+a')-2(F+\lambda_R/z)-4\xi/z} \\ &\times \int_0^1 d\theta \theta^{-2F+4\tilde{\xi}_2/z} (y-\theta)^{2\xi/z+\lambda_R/z+F-2(1-a')+\beta/z+d/z} \\ &\times (1-\theta)^{2\xi/z+\lambda_R/z+F-2(1-a')+\beta/z+d/z} (y+1-2\theta)^{-2\beta-d/z} g\left(\frac{1}{y} \frac{\theta-y}{1-\theta}\right) \end{aligned} \quad (2.173)$$

The value of λ_C can not be inferred from this expression, as we do not know the behaviour of $g(u)$. As an illustration we will show, how we can derive an upper bound for λ_C , if we suppose that $g(u)$ satisfies a Hölder condition

$$|g(x) - g(y)| \leq C|x - y|^\aleph \quad \text{for all } x, y \quad (2.174)$$

with a Hölder exponent $0 \leq \aleph \leq 1$ and some constant C . If we identify in (2.174)

$$x = \frac{1 - \theta - y}{y(1 - \theta)} = -\frac{1}{1 - \theta} + \frac{\theta/y}{1 - \theta} < 0, \quad \text{and} \quad y = -\frac{1}{1 - \theta} < x \quad (2.175)$$

and suppose further that $g(u)$ is monotonously increasing, we get that

$$g\left(\frac{1 - \theta - y}{y(1 - \theta)}\right) \leq C\left(\frac{\theta/y}{1 - \theta}\right)^\aleph + g\left(-\frac{1}{1 - \theta}\right) \quad (2.176)$$

When we introduce this into (2.173) we have to distinguish different scenarios, according to whether the term involving $g(-1/(1 - \theta))$ under the integral vanishes for $y \rightarrow \infty$ or not. If it does not vanish, one finds the upper bound

$$\frac{\lambda_C}{z} \geq \frac{\lambda_R}{z} + \frac{\beta}{z}. \quad (2.177)$$

If it does vanish, the subleading term has to be taken into account and one gets

$$\frac{\lambda_C}{z} \geq \frac{\lambda_R}{z} + \frac{\beta}{z} + \aleph. \quad (2.178)$$

We see that for the case of critical dynamics $\lambda_R = \lambda_C$ is still possible, also for $\beta \neq 0$. As there were several assumptions about $g(u)$ involved, these bounds might not apply to all models. They should rather be considered as an illustration pointing out the remaining difficulties caused by the undetermined scaling function $g\left(\frac{1 - \theta - y}{y(1 - \theta)}\right)$.

Let us finish this section with a general remark concerning the correlation function. As it is already known from the case $z = 2$, the above expressions strictly apply only in the dynamical scaling regime, i.e. for large y . In order to fix equally the behaviour for y close to 1, one would have to construct a similar extension of the symmetry algebra as proposed in [111] and use these higher symmetries to fix the behaviour of $f_C(y)$ also for small y [114]. This work is left for the future.

2.6 Conclusions of this chapter

In this chapter, we have presented a reformulation of the principles of a theory of local scale-invariance (LSI). This reformulation was motivated on one hand by several exact results [20] (which have here been deferred to section 3.3 of chapter 3), which are in disagreement with an earlier formulation of LSI [109] and on the other hand by several conceptual weaknesses of the older formulation which in particular did not allow to treat explicitly the dynamical symmetries of stochastic Langevin equations. While the main principles of LSI have been kept unchanged, our reformulation concerns the precise definition of the infinitesimal generators of local scale-invariance and this implies in particular

a thorough reconsideration of the fractional derivatives which appear in these generators and in the invariant equations for the order-parameter. Implicit in the current formulation of LSI is an algebraic growth law of a single physically relevant length scale $L(t) \sim t^{1/z}$ and the assumption of the validity of an extension of Galilei-invariance to $z \neq 2$.

The following results have been obtained:

1. Non-trivial dynamical symmetries are not a property of the entire Langevin equation but only of a related system, called the ‘deterministic part’ and which is in the most simple cases obtained by simply suppressing the noisy parts in the Langevin equation.
2. Besides on the scaling dimensions, the quasi-primary scaling operators of the ‘deterministic part’ also depend on several non-universal ‘mass parameters’, denoted here as γ and μ . For a dynamical exponent $z = 2$, only μ is relevant and only the relatively weak constraint (the Bargman superselection rule (2.90)) fixes the sum $\sum_{i=1}^n \mu_i$ of the mass parameters of the scaling operators ϕ_i in an LSI-covariant n -point function. We have shown here that for $z \neq 2$, there exists, beside the usual conservation of momentum, at least a further conservation law which roughly speaking states that certain powers of the momentum are also conserved. Being quite analogous to instances of factorisable scattering seen before in relationship with $2D$ conformal invariance and integrable systems [235, 236], this has led to a considerable strengthening eq. (2.77) of the Bargman superselection rule.
3. If the noise is gaussian and centred and furthermore the noise correlator satisfies certain structural requirements (which are always met for a thermal or an initial noise [137]) then, given only spatial translation-invariance and generalised Galilei-invariance, the Bargman superselection rules permit to express any average in terms of an average within the ‘deterministic part’ only. In particular, we have derived for any given value z the exact reduction formulæ eq. (2.91) for the two-time response function and eqs. (2.93,2.94) for the two-time correlation function.

Clearly, response and correlation functions have quite a different origin, despite a similarly scaling behaviour under global dilatations. Response functions do not depend explicitly of the noise, while correlations functions are derived from either thermal or initial noises.

4. The required ‘deterministic’ or ‘noiseless’ two- and four-point functions can now be calculated from the requirement of local dynamical scaling (leaving of course out time-translation invariance). In particular, we have derived the following scaling form for the two-time response function

$$\begin{aligned}
 R(t, s; \mathbf{r}) &= \langle \phi_1(t, \mathbf{r}) \phi_2(s, \mathbf{0}) \rangle = R(t, s) \mathcal{F}^{(\mu_1, \gamma_1)}(|\mathbf{r}|(t-s)^{-1/z}) \\
 R(t, s) &= r_0 s^{-1-a} \left(\frac{t}{s}\right)^{1+a'-\lambda_R/z} \left(\frac{t}{s} - 1\right)^{-1-a'}
 \end{aligned} \tag{2.179}$$

of the two quasi-primary scaling operators $\phi_{1,2}$ and such that $\mu_1 + \mu_2 = \gamma_1 + \gamma_2 = 0$ and where $a, a', \lambda_R/z$ are ageing exponents and r_0 a normalisation constant. The spatio-temporal scaling function is the solution of a certain fractional differential equation and is given by eq. (2.110). By formally letting $z \rightarrow 2$, we recover the previously treated special case of Schrödinger/ageing invariance [192, 126].

The response field $\tilde{\phi}$ of non-equilibrium field-theory, conjugate to the order-parameter field ϕ , formally plays the rôle of a ‘complex conjugate’ which is needed in order to have non-trivial n -point functions.

The above factorisation, as well as the autoresponse function $R(t, s)$, was already obtained in the ‘old’ formulation of LSI [109]. However, since in that formulation no generalised Bargman rule could be derived, stochastic equations could not be treated and a result such as (2.179) remained a conjecture without a clear conceptual foundation. For the first time we are able, for arbitrary z , to formulate sufficient conditions from which (2.179) follows.

The above form for $R(t, s)$ has by now been observed in numerous ageing systems, both quenched to $T < T_c$ and to $T = T_c$, and for a wide range of values of z , going from ≈ 1.7 to ≈ 5 for systems with a non-linear Langevin equation, as reviewed in [125, 124, 126].

5. The derivation of generalised Bargman superselection rules has also permitted, for the first time, to derive explicit predictions for the correlation functions for any given dynamical exponent $z \neq 2$. In contrast to the autoresponse function, for which one might have guessed the final result eq. (2.179), that would not have been possible for the two-time correlation function.

We recall that already for $z = 2$, the theoretical calculation of two-time correlators which are in agreement with simulational data is still a very difficult problem, see [126] and references therein.

At the same time, a number of important questions remains open and we now mention a few of them.

1. What is the meaning of a fractional derivative in the infinitesimal generators of LSI ? How to find the finite transformations corresponding to the infinitesimal generators ?
2. Presently, the choice of a certain kind of fractional derivatives is simply dictated by the empirical *a posteriori* comparison with explicit models. Is there a physical criterion which kind of fractional derivative should be used ?
3. For $z \neq 1, 2$, the generators of local scale-transformations do no longer close into an ordinary Lie algebra. On the other hand, if one applies the generators of LSI to n -point functions built from quasi-primary scaling operators, we have derived generalised Bargman superselection rules which guarantee that one has a finite set of self-consistent conditions. What type of algebraic structure is underlying LSI ?
4. Generalised Galilei-invariance of the ‘deterministic part’ is an essential ingredient of LSI. Already for $z = 2$, the analysis of the Ward-identities of Schrödinger/ageing invariance shows that Galilei-invariance must be seen as a further requirement independent of dynamical scaling [111]. That analysis remains to be extended to $z \neq 2$.

The physical origin of generalised Galilei-invariance (GGI) is not yet understood. On the other hand, it is already clear that the requirement of GGI of the equations of motion or equivalently of the field-theoretical action for *all* times is too strong

and it would be sufficient to have GGI valid inside the scaling regime.¹⁰ How could one formulate such a slightly weaker form of GGI ?

5. Our present treatment of LSI is exact for Langevin equations of the form eq. (2.78) with a linear ‘deterministic part’.¹¹ Is there a way to extend LSI to non-linear equations, possibly following the routes explored in [222] for $z = 2$?
6. For the non-equilibrium critical dynamics of $O(n)$ models, where $z \gtrsim 2$, the results of the second-order ε -expansion are not in agreement with the LSI-prediction eq. (2.179), in particular if in addition $a = a'$ is assumed [42, 43, 198]. On the other hand, a convenient choice for the exponent $a' \neq a$ restores the compatibility of the simulational data of [198] and eq. (2.179) [122] while the results of the ε -expansion deviate from the simulational data, especially in $d = 2$ dimensions.

What is the correct interpretation of these findings ? Should one first re-sum the ε -expansion series before performing any numerical comparisons with simulational data or symmetry arguments as LSI ? Is it preferable to use other numerical estimates for the scaling functions than the simple [2,0] Padé approximant employed in [42, 43] ? Is the introduction of the new exponent $a' \neq a$ which has an algebraic meaning and is physically possible because of the breaking of time-translation invariance,¹² the correct interpretation ?

7. The present formulation of LSI only considers explicitly Langevin equations. It remains to be seen how master equations could be included into the formalism which would allow a more direct comparison with simulational results which are all obtained from a master equation.

All in all, we arrived at a more profound understanding on the foundations of a theory of local scale-invariance. The existing exact confirmations in many exactly solvable systems and the good or excellent agreement with the results of many non-perturbative simulational studies (see also chapter 3) provides strong evidence that the basic principles of LSI, as stated in our axiomatic formulation in section 2.2.1, should reflect the physical reality and certainly give a good overall description of the scaling of the two-time quantities on which LSI was tested. At the same time, we can now better appreciate the many subtleties which arise when making precise quantitative comparisons. Finding answers to the questions thus raised will require progress both in the physical understanding as well as in the mathematical background. We hope that in this way a new systematic approach for the description of strongly interacting many-body systems far from equilibrium can be constructed. In the next chapter the new LSI predictions will be compared with the results from several concrete model computations.

¹⁰Alternatively, one might think that one should require GGI not on the equations of motion, but rather for the averages. We thank C. Maes for interesting discussions on this point.

¹¹Certain non-linearities in the action \mathcal{J} which may arise from the different forms of the noise correlators which occur e.g. for reaction-diffusion models, can be treated by a straightforward generalisation of the methods used in [17].

¹²For example, in the 1D Glauber-Ising model, comparison of the exact solution for $R(t, s)$ with eq. (2.179) gives $0 = a \neq a' = -\frac{1}{2}$.

Chapter 3

Application of LSI to space-time scaling functions

In chapter 2 we have formulated a general theory, which gives predictions for the form of the response and correlation functions for $z \neq 2$ extending the existing theory of LSI for the case $z = 2$. As already done in the past for the case $z = 2$ [192, 114, 117, 106, 112], we want to test these predictions in concrete models. This will also offer a possibility to decide, which definition for the fractional derivative we should use. Notice that on the level of the response function, one has to look at the space-time behaviour, as the autoresponse function is the same for both kinds of fractional derivatives.

The first examples in section 3.1 will be two surface growth models, namely the Edward-Wilkinson (EW) model and the Mullins-Herring (MH) model. Although a lot of papers have appeared on surface growth models, it is relatively new to consider them in the context of ageing phenomena and the computation of two-time quantities is only at its very beginning. For the future, we hope that LSI might offer here a new approach to attack some problems in this field.

In section 3.2 the kinetic spherical model with conserved order parameter will be considered. For this model, as for some of the surface growth models, the dynamical exponent is $z = 4$. For these cases the comparison with LSI is discussed both for the 'old' kind of fractional derivatives and for the 'new' kind, and both versions of LSI are found to give the right predictions.

This is different for the case of the long-range spherical model, which is treated in section 3.3. In this model the dynamical exponent can take a value between 0 and 2. Here we find, that only the version of LSI presented in chapter 2 gives the right predictions.

Finally numerical results from the diluted Ising model will provide the possibility to test the LSI-predictions also in a nonlinear model. This will be presented in section 3.4 of this chapter.

The content of this chapter can be found in the following publications and preprints:

- A. Röthlein, F. Baumann and M. Pleimling, Phys. Rev. **E 74**, 061604 (2006);
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- F. Baumann and M. Henkel, J. Stat. Mech., P01012 (2007)
- F. Baumann, S.B. Dutta and M. Henkel, J. Phys. A: Math. Theor. **40**, 7389 (2007)
- F. Baumann and M. Henkel, submitted to Nucl. Phys. B
- F. Baumann, M. Henkel and M. Pleimling, submitted to Europhys. Lett.

3.1 Surface growth processes

3.1.1 Introduction

Fluctuations are omnipresent when analyzing surfaces and interfaces. These fluctuations can be equilibrium fluctuations, as encountered for example when looking at steps on surfaces, or they can be of nonequilibrium origin as it is the case in various growth processes. Well known examples of nonequilibrium surface fluctuations are found in kinetic roughening or nonequilibrium growth processes [172, 100, 7] as for example in thin film growth due to vapour deposition. Interestingly, both equilibrium and nonequilibrium interface and surface fluctuations can be described on a mesoscopic level through rather simple Langevin equations [150]. In this approach the fast degrees of freedom are modelled by a noise term, thus yielding stochastic equations of motion for the slow degrees of freedom. In many instances the physics of dynamical processes is to a large extent captured by linearised Langevin equations [151] where one distinguishes whether the dynamics is purely diffusive or whether mass conservation has to be implemented.

For purely diffusive dynamics (called model A dynamics in critical dynamics [128, 226]) the linear Langevin equation can be written in the following way:

$$\frac{\partial h(\mathbf{x}, t)}{\partial t} = \nu_2 \nabla^2 h(\mathbf{x}, t) + \lambda + \eta(\mathbf{x}, t) \quad (3.1)$$

where $h(\mathbf{x}, t)$ is the value of the macroscopic field h at site \mathbf{x} at time t . In the physical context of fluctuating interfaces and growth processes in $d + 1$ spatial dimensions h is the height field whereas \mathbf{x} is the lateral position in the underlying d dimensional substrate lattice. In addition, $\nu_2 > 0$ is the diffusion constant whereas λ is the mean growth velocity (which may of course be zero). Finally, the random variable η models the noise due to the fast degrees of freedom. Depending on the physical problem at hand, either Gaussian white noise or spatially and/or temporally correlated noise is usually considered [234].

In the context of kinetic roughening and nonequilibrium growth processes Eq. (3.1) is called the Edwards-Wilkinson (EW) equation [79]. This equation has been used for the description of many dynamical processes, as for example equilibrium step fluctuations with random attachment/detachment events at the step edge [91, 74, 75]. This equation also describes the dynamics of a growing surface with a normal incidence of the incoming particles. An obliquely incident particle beam, however, generates anisotropies which can only be described by a more complex non-linear Langevin equation [215].

In growth processes with mass conservation the following linear Langevin equation (with $\nu_4 > 0$)

$$\frac{\partial h(\mathbf{x}, t)}{\partial t} = -\nu_4 \nabla^4 h(\mathbf{x}, t) + \lambda + \eta(\mathbf{x}, t) \quad (3.2)$$

has been proposed [175, 231]. This equation is sometimes called the noisy Mullins-Herring (MH) equation. The noise term again reflects the physics of the investigated system. In the case of equilibrium fluctuations conserved noise must be considered, leading to the so-called model B dynamics [128, 226]. On the other hand, when studying out-of-equilibrium processes one can again focus on Gaussian white noise or on noise which is correlated in space and/or time [155].

The Langevin equation (3.2) is used for example to describe film growth via molecular beam epitaxy [231, 96, 63], equilibrium fluctuations limited by step edge diffusion [75, 30] or even tumor growth [40, 82].

An important notion in nonequilibrium growth processes is that of dynamical scaling. Dynamical scaling is nicely illustrated through the behaviour of the mean-square width of the surface or interface which for a substrate of linear size L scales as [83]

$$W^2(L, t) = L^{2\zeta} F(t/L^z) \quad (3.3)$$

where ζ is the roughness exponent and z is the dynamical exponent. For EW we have $z = 2$ whereas for MH $z = 4$. The value of ζ depends on whether correlated or uncorrelated noise is considered.

Langevin equations have the drawback that they do not really mirror the atomistic processes underlying the fluctuations of the interfaces and surfaces. In order to capture the physics on the microscopic level one commonly designs simple atomistic models (characterised by some specific deposition and/or diffusion rules) which are then often studied numerically. However, it is not always clear what the corresponding Langevin equation is. Usually, numerical simulations are used in order to extract the exponents ζ and z (see Eq. (3.3)) which generally permit to relate the microscopic model to one of the Langevin equations (universality classes). These exponents, however, encode only partly the information given by a scaling behaviour, as the scaling functions, like $F(y)$ in Eq. (3.3), are themselves different for different universality classes.

In this section we focus on two-point quantities as for example the space-time response and the space-time correlation functions which also display a dynamical scaling behaviour. On a more fundamental level we show, using arguments first given in [192], that in systems described by the equations (3.1) and (3.2) the scaling functions of these two-point quantities can be derived by exclusively exploiting the symmetry properties of the underlying *noiseless*, i.e. deterministic, equations. This approach, which is based on generalised, space and time dependent, symmetries of the dynamical system [108, 109], has in the past already been applied successfully in the special case $z = 2$ to systems undergoing phase ordering [110, 114, 192, 16] and to nonequilibrium phase transitions [17]. Here we show that local space-time symmetries also permit to fix (up to some numerical factors) the scaling functions of space-time response and correlation functions in cases where $z = 4$. On a more practical level we demonstrate the usefulness of the scaling functions of these two-point quantities (which depend on two different space-time points (\mathbf{x}, t) and (\mathbf{y}, s)) in the characterisation of the universality classes of nonequilibrium growth processes. Whereas in the study of critical systems scaling functions, which are universal and characterise the different universality classes, are routinely investigated (and this both at equilibrium [190] and far from equilibrium [162, 45]), in nonequilibrium growth processes the focus usually lies on simple quantities like for example the exponents ζ and z . There are some notable exceptions where scaling functions have been discussed (see, for example, [155, 234]), but these studies were in general restricted to one-time quantities. However, also in nonequilibrium growth processes scaling functions of two-point functions are universal and should therefore be very valuable in the determination of the universality class of a given microscopic model or experimental system. We illustrate this by computing through Monte Carlo simulations the two-point space-time correlation function for two microscopic models which have been proposed to belong to the same universality class as the Edwards-Wilkinson equation (3.1) with Gaussian white noise [84, 173, 159, 182, 183]. The section is organised in the following way. In the next subsection we discuss the EW and the MH equations in more detail and introduce the two-point functions. subsection 3.1.3 is devoted to the computation of the exact expressions of the space-time correlation

and response functions by Fourier transformation. These exact results show *inter alia* that the response of the system to the noise does not depend explicitly on the specific choice of the noise itself. In subsection 3.1.4 we discuss the space-time symmetries of the noiseless equations, whereas in subsection 3.1.5 we show how these symmetries can be used for the derivation of the scaling functions of two-point functions, using the old version of LSI. In subsection 3.1.6 we demonstrate, that the new version of LSI presented in the last chapter also leads to the correct result. In subsection 3.1.7 we numerically study two microscopic growth models which have been proposed to belong to the Edwards-Wilkinson universality class. There has been a recent debate on the universality class of these models which we resolve by studying the scaling function of the space-time correlation function. Finally, in subsection 3.1.8 we give our conclusions. Some technical points can be found in the Appendices of [207].

3.1.2 Noise modelization and space-time quantities

Our main interest in this section is the investigation of space-time quantities in systems described by the quite general linear stochastic equations (3.1) and (3.2). Setting the mean growth velocity λ to zero (which can always be achieved by transforming into the co-moving frame) both cases can be captured by the single equation

$$\frac{\partial h(\mathbf{x}, t)}{\partial t} = -\nu_{2l}(-\nabla^2)^l h(\mathbf{x}, t) + \eta(\mathbf{x}, t) \quad (3.4)$$

with $l = 1$ (EW) or $l = 2$ (MH). As it is well known, these equations of motion can be derived from a free field theory [226].

Depending on the physical context, different types of noise may be considered. For the EW case we shall discuss both Gaussian white noise (EW1)

$$\langle \eta(\mathbf{x}, t) \rangle = 0, \quad \langle \eta(\mathbf{x}, t) \eta(\mathbf{y}, s) \rangle = 2D \delta^d(\mathbf{x} - \mathbf{y}) \delta(t - s) \quad (3.5)$$

and spatially correlated noise (EW2)

$$\langle \eta(\mathbf{x}, t) \rangle = 0, \quad \langle \eta(\mathbf{x}, t) \eta(\mathbf{y}, s) \rangle = 2D |\mathbf{x} - \mathbf{y}|^{2\rho-d} \delta(t - s) \quad (3.6)$$

with $0 < \rho < d/2$. In the past, these two types of noise have been used in the modelling of nonequilibrium growth processes [150, 151]. If, however, one wishes to model thermal equilibrium interface fluctuations, as for example step fluctuations rate-limited by evaporation-condensation, one has to consider white noise with the Einstein relation $D = \nu_2 k_B T$ where T is the temperature and k_B the Boltzmann constant. For the MH case we also consider the noises (3.5) and (3.6), called MH1 and MH2 in the following. In this case, however, white noise can only be used in nonequilibrium situations as it breaks the conservation of mass encoded in the Langevin equation (3.2). We shall not consider here the noisy Mullins-Herring equation with conserved noise which assures the relaxation towards equilibrium of a system with conserved dynamics, as this is covered in [19] and section 3.2.

Two-time quantities have been shown in many circumstances to yield useful insights into the dynamical behaviour of systems far from equilibrium [45]. Of special interest are space and time dependent functions as for example the space-time response $R(\mathbf{x}, \mathbf{y}, t, s)$ or the

height-height space-time correlation $C(\mathbf{x}, \mathbf{y}, t, s)$, which are both defined in the same way as for the magnetic systems considered before:

$$C(\mathbf{x}, \mathbf{y}, t, s) = \langle h(\mathbf{x}, t)h(\mathbf{y}, s) \rangle \quad (3.7)$$

where the brackets indicate an average over the realization of the noise. The space-time response, defined by

$$R(\mathbf{x}, \mathbf{y}, t, s) = \left. \frac{\delta \langle h(\mathbf{x}, t) \rangle}{\delta j(\mathbf{y}, s)} \right|_{j=0}, \quad (3.8)$$

measures the response of the interface at time t and position \mathbf{x} to a small perturbation $j(\mathbf{y}, s)$ at an earlier time s and at a different position \mathbf{y} ¹. For reasons of causality we have $t > s$. At the level of the Langevin equation the perturbation enters through the addition of j to the right hand side. Assuming spatial translation invariance in the directions parallel to the interface, we have

$$C(\mathbf{x}, \mathbf{y}, t, s) = C(\mathbf{x} - \mathbf{y}, t, s), \quad R(\mathbf{x}, \mathbf{y}, t, s) = R(\mathbf{x} - \mathbf{y}, t, s). \quad (3.9)$$

The autocorrelation and autoresponse functions are then defined by

$$C(t, s) := C(\mathbf{0}, t, s), \quad R(t, s) := R(\mathbf{0}, t, s). \quad (3.10)$$

It is well known that the systems discussed here present a simple dynamical scaling behaviour (see eq. (3.3)). For the two-time quantities one expects the same scaling behaviour as it was introduced in chapter 1 for the magnetic systems. For the autoresponse and the autocorrelation functions we expect the scaling forms (1.11) which defines the nonequilibrium exponents a and b . Combining equations (3.3), (3.7) and (1.11), one ends up with the scaling relation $b = -2\zeta/z$, which relates b to the known exponents ζ and z . In addition the scaling functions f_R and f_C define two additional exponents λ_R and λ_C by their asymptotic behaviour, see equation (1.12). Similarly, one obtains for the space-time quantities the following scaling forms:

$$R(\mathbf{x} - \mathbf{y}, t, s) \sim s^{-a-1} F_R(|\mathbf{x} - \mathbf{y}|^z / s, t/s), \quad (3.11)$$

$$C(\mathbf{x} - \mathbf{y}, t, s) \sim s^{-b} F_C(|\mathbf{x} - \mathbf{y}|^z / s, t/s). \quad (3.12)$$

3.1.3 Response and correlation functions: exact results

This subsection is devoted to the computation of space-time quantities by directly solving the Langevin equations (3.1) and (3.2) in the physically relevant cases $d = 1$ and $d = 2$. These exact results will be used in the following in two different ways. In subsection 3.1.5 we use these expressions in order to check whether our approach, which exploits exclusively the generalised space-time symmetries of the deterministic part of the equation of motion, yields the correct results. In addition, in subsection 3.1.7 we compare these expressions with the numerically determined scaling functions obtained for two different atomistic models in order to decide on the universality class of these models.

¹The response function (3.8), which results from a perturbation in the flux, can be viewed as the response of the system to the noise itself.

$z = 2$: The Edwards-Wilkinson case

In order to compute the response of the surface/interface to a small perturbation we add the term $j(\mathbf{x}, t)$ to the right-hand side of the Langevin equation and then go to reciprocal space. In the EW case the solution of the resulting equation is (with $d = 1, 2$)

$$\widehat{h}(\mathbf{k}, t) = e^{-\nu_2 \mathbf{k}^2 t} \int_0^t dt' e^{\nu_2 \mathbf{k}^2 t'} (\widehat{\eta}(\mathbf{k}, t') + \widehat{j}(\mathbf{k}, t')) \quad (3.13)$$

where we denote by $\widehat{h}(\mathbf{k}, t)$, $\widehat{\eta}(\mathbf{k}, t)$ resp. $\widehat{j}(\mathbf{k}, t)$ the Fourier transform of $h(\mathbf{x}, t)$, $\eta(\mathbf{x}, t)$ resp. $j(\mathbf{x}, t)$. We prepare the system at time $t = 0$ in an out-of-equilibrium state. For simplicity we assume flat initial conditions, i.e. $h(\mathbf{x}, 0) = 0$, but our results are the same for any initial state with $\langle h(\mathbf{x}, 0) \rangle = 0$ ². This preparation enables us to study the approach to equilibrium for the EW1 case with a valid Einstein relation. For the corresponding study of equilibrium dynamical properties (as encountered in the recent experiments on step fluctuations [91, 74, 75]) we have to prepare the system at $t = -\infty$ and replace in (3.13) the lower integration boundary 0 by $-\infty$. We shall in the following concentrate on the out-of-equilibrium situation.

Taking the functional derivative of (3.13) and transforming back to real space yields the result

$$R(\mathbf{x} - \mathbf{y}, t, s) = \widehat{r}_0 \int \frac{d\mathbf{k}}{(2\pi)^d} e^{i\mathbf{k}(\mathbf{x}-\mathbf{y})} e^{-\nu_2 \mathbf{k}^2 (t-s)} \quad (3.14)$$

$$= \widehat{r}_0 (t-s)^{-\frac{d}{2}} \exp\left(-\frac{(\mathbf{x}-\mathbf{y})^2}{4\nu_2(t-s)}\right) \quad (3.15)$$

with $r_0 = \frac{1}{(2\sqrt{\pi\nu_2})^d}$ and $t > s$. The exponents a and λ_R as well as the scaling function f_R can readily be obtained from the expression of the autoresponse function (see Equations (1.11) and (1.12))

$$R(t, s) = r_0 (t-s)^{-\frac{d}{2}}, \quad (3.16)$$

yielding $a = \frac{d}{2} - 1$, $\lambda_R = d$ and $f_R(y) \sim (y-1)^{\frac{d}{2}-1}$.

The expression for the space-time response is completely independent from choice of the noise term as long as $\langle \widehat{\eta}(\mathbf{k}, t) \rangle = 0$. This also holds for the MH case, as discussed in the next subsection. In subsection 3.1.7 we shall discuss an alternative way of looking at this fact.

A similar straightforward calculation yields for the space-time correlation the expression

$$C(\mathbf{x} - \mathbf{y}, t, s) = \int_0^t dt' \int_0^s dt'' \int \frac{d\mathbf{k}}{(2\pi)^d} e^{i\mathbf{k}(\mathbf{x}-\mathbf{y})} e^{-\nu_2 \mathbf{k}^2 (t+s-t'-t'')} \langle \widehat{\eta}(\mathbf{k}, t') \widehat{\eta}(-\mathbf{k}, t'') \rangle \quad (3.17)$$

where we have exploited the spatial translation invariance of the noise correlator. For *Gaussian white noise* we then obtain for the space-time correlation

$$C(\mathbf{x} - \mathbf{y}, t, s) = c_0 |\mathbf{x} - \mathbf{y}|^{2-d} \left[\Gamma\left(\frac{d}{2} - 1, \frac{(\mathbf{x} - \mathbf{y})^2}{4\nu_2(t+s)}\right) - \Gamma\left(\frac{d}{2} - 1, \frac{(\mathbf{x} - \mathbf{y})^2}{4\nu_2(t-s)}\right) \right] \quad (3.18)$$

²This assumption is also important in connection with the symmetry based approach presented in this work. A nonvanishing initial average of $h(\mathbf{x}, 0)$ would lead to modifications.

with $c_0 = \frac{D}{2^{d+3}\pi^{3d/2}\nu_2}$. The autocorrelation function for $d \neq 2$ [152] is obtained by using the known series expansion of the incomplete Gamma-functions Γ :

$$C(t, s) = \frac{2c_0(4\nu_2)^{1-\frac{d}{2}}}{2-d} s^{1-\frac{d}{2}} \left[\left(\frac{t}{s} + 1 \right)^{1-\frac{d}{2}} - \left(\frac{t}{s} - 1 \right)^{1-\frac{d}{2}} \right] \quad (3.19)$$

from which we find $b = \frac{d}{2} - 1$, $\lambda_C = d$ and $f_C(y) \sim (y+1)^{1-\frac{d}{2}} - (y-1)^{1-\frac{d}{2}}$. For the special case $d = 2$ one has to take the logarithmic behaviour of the Gamma-functions into account which yields

$$C(t, s) = c_0 \ln \frac{t+s}{t-s}. \quad (3.20)$$

For *spatially correlated noise* the space-time correlator can only be written as a series expansion:

$$C(\mathbf{x} - \mathbf{y}, t, s) = \sum_{n=0}^{\infty} (-1)^n a_n^{(d)}(\rho) |\mathbf{x} - \mathbf{y}|^{2n} \times \left[(t+s)^{-(2n-2\rho+d-2)/2} - (t-s)^{-(2n-2\rho+d-2)/2} \right] \quad (3.21)$$

with $a_n^{(d)}(\rho) = b_n^{(d)} \frac{2^{2\rho} D \Gamma(\rho) \Gamma(n-\rho+d/2)}{(2\rho-2n-d+2)\pi^{2-3d/2} \Gamma(d/2-\rho) \nu_2^{n-\rho+d/2}}$ and $b_n^{(1)} = \frac{1}{(2n)!}$, $b_n^{(2)} = \frac{1}{((2n)!!)^2}$, whereas for the autocorrelator one gets

$$C(t, s) = a_0^{(d)}(\rho) s^{1-\frac{d}{2}+\rho} \left[\left(\frac{t}{s} + 1 \right)^{1-\frac{d}{2}+\rho} - \left(\frac{t}{s} - 1 \right)^{1-\frac{d}{2}+\rho} \right], \quad (3.22)$$

yielding $b = \frac{d}{2} - 1 + \rho$, $\lambda_C = d - 2\rho$ and $f_C(y) \sim (y+1)^{1-\frac{d}{2}+\rho} - (y-1)^{1-\frac{d}{2}+\rho}$.

Looking at the expressions (3.18) and (3.21), we see that in both cases the space-time correlation has the following scaling form:

$$C(\mathbf{x} - \mathbf{y}, t, s) = |\mathbf{x} - \mathbf{y}|^\alpha F \left(\frac{(\mathbf{x} - \mathbf{y})^2}{t+s}, \frac{(\mathbf{x} - \mathbf{y})^2}{t-s} \right) \quad (3.23)$$

with $\alpha = 2 - d$ resp. $2 - d + 2\rho$ for EW1 resp. EW2. The scaling function F is then a function of the two scaling variables $\frac{(\mathbf{x}-\mathbf{y})^2}{t+s}$ and $\frac{(\mathbf{x}-\mathbf{y})^2}{t-s}$. In the non-equilibrium situation we discuss here the space-time correlation function is therefore not time translation invariant. For equilibrium systems which are prepared at $t = -\infty$ time translation invariance is of course recovered. It is worth noting that the scaling form (3.23) corrects the scaling forms given in [7] where only a dependence on $\frac{(\mathbf{x}-\mathbf{y})^2}{t-s}$ was predicted far from equilibrium.

$z = 4$: The Mullins-Herring case

For the Mullins-Herring case we proceed along the same line as for the Edwards-Wilkinson case. We here only give the results for one-dimensional interfaces and refer the reader to the Appendix A of [207] for the two-dimensional case. The solution of the Langevin equation in Fourier space reads in the MH case

$$\widehat{h}(\mathbf{k}, t) = e^{\nu_4 \mathbf{k}^4 t} \int_0^t dt' e^{-\nu_4 \mathbf{k}^4 t'} (\widehat{\eta}(\mathbf{k}, t') + \widehat{j}(\mathbf{k}, t')) \quad (3.24)$$

which gives as a result the integral expression

$$R(\mathbf{x} - \mathbf{y}, t, s) = \int_{\mathbb{R}^d} \frac{d\mathbf{k}}{(2\pi)^d} e^{i\mathbf{k}\cdot\mathbf{r}} e^{-\nu_4|\mathbf{k}|^4(t-s)}. \quad (3.25)$$

This yields after some algebra for one-dimensional interfaces the expression

$$\begin{aligned} R(\mathbf{x} - \mathbf{y}, t, s) &= \frac{1}{\pi\nu_4^{1/4}} ((t-s))^{-1/4} \left[\Gamma\left(\frac{5}{4}\right) {}_0F_2\left(\frac{1}{2}, \frac{3}{4}; \frac{(\mathbf{x}-\mathbf{y})^4}{256\nu_4(t-s)}\right) \right. \\ &\quad \left. - 2\Gamma\left(\frac{3}{4}\right) \left(\frac{(\mathbf{x}-\mathbf{y})^4}{256(\nu_4(t-s))}\right)^{1/2} {}_0F_2\left(\frac{5}{4}, \frac{3}{2}; \frac{(\mathbf{x}-\mathbf{y})^4}{256\nu_4(t-s)}\right) \right] \end{aligned} \quad (3.26)$$

for the space-time response. Here the ${}_0F_2$ functions are generalised hypergeometric functions. It is worth noting that exponentially growing contributions to the functions ${}_0F_2$ just cancel each other, yielding a response function which decreases for $(\mathbf{x}-\mathbf{y})^4/(t-s) \rightarrow \infty$, as it should.

The autoresponse function is straightforwardly found (with $t > s$):

$$R(t, s) = \frac{\Gamma\left(\frac{5}{4}\right)}{\pi\nu_4^{1/4}} (t-s)^{-\frac{1}{4}} \quad (3.27)$$

which gives us the quantities $a = -\frac{3}{4}$, $\lambda_R = 1$ and $f_R(y) \sim (y-1)^{-\frac{1}{4}}$. One straightforwardly verifies that in any space dimension d one has the relations $a = \frac{d}{4} - 1$, $\lambda_R = d$ and $f_R(y) \sim (y-1)^{-\frac{d}{4}}$.

As for the EW case we remark that the exact expressions (3.26) and (3.27) are independent of the noise: we obtain the same results for Gaussian white noise and for spatially correlated noise. Let us add that we have here only considered perturbations which are not mass conserving. Whereas this is physically sound for the cases we have in mind here, one usually considers mass conserving perturbations in the context of critical dynamics [226, 19].

Turning to the correlation function, we proceed as for the EW case and obtain

$$C(\mathbf{x} - \mathbf{y}, t, s) = \int_0^t dt' \int_0^s dt'' \int \frac{d\mathbf{k}}{(2\pi)^d} e^{i\mathbf{k}\cdot(\mathbf{x}-\mathbf{y})} e^{-\nu_4\mathbf{k}^4(t+s-t'-t'')} \langle \hat{\eta}(\mathbf{k}, t') \hat{\eta}(-\mathbf{k}, t'') \rangle. \quad (3.28)$$

For Gaussian white noise this then yields in 1 + 1 dimensions the expressions

$$\begin{aligned} C(\mathbf{x} - \mathbf{y}, t, s) &= \frac{D}{(2\pi)^2} \sum_{n=0}^{\infty} \frac{(-1)^n |\mathbf{x} - \mathbf{y}|^{2n}}{(2n)! \nu_4^{(2n+1)/4} (3-2n)} \\ &\quad \times \Gamma\left(\frac{2n+1}{4}\right) [(t+s)^{(3-2n)/4} - (t-s)^{(3-2n)/4}] \end{aligned} \quad (3.29)$$

and

$$C(t, s) = \frac{D \Gamma(5/4)}{3\pi 2\nu_4^{1/4}} [(t+s)^{3/4} - (t-s)^{3/4}] \quad (3.30)$$

for the space-time correlation and the autocorrelation functions. Similarly, for spatial correlated noise we have

$$C(\mathbf{x}-\mathbf{y}, t, s) = \sum_{n=0}^{\infty} (-1)^n \tilde{a}_n^{(1)}(\rho) |\mathbf{x}-\mathbf{y}|^{2n} [(t+s)^{-(2n-2\rho+d-4)/4} - (t-s)^{-(2n-2\rho+d-4)/4}] \quad (3.31)$$

with $\tilde{a}_n^{(1)}(\rho) = \frac{2^{2\rho} D \Gamma(\rho) \Gamma((1+2n-2\rho)/4)}{(2n)!(2\rho-2n+3)\pi^{1/2} \Gamma((1-2\rho)/2) \nu_4^{(1+2n-2\rho)/4}}$, the autocorrelation being given by the term with $n = 0$.

3.1.4 Space-time symmetries of the noiseless equations

We have presented in chapter 2 generators, which act as dynamical symmetries on the equation

$$\left[-\mu \partial_t + \frac{1}{z^2} \nabla_r^z \right] \Psi = 0. \quad (3.32)$$

where $z > 0$ is a real number. Here, we will first consider the *old* version of LSI (for $d = 1$) and consider the symmetries of

$$\left[-\mu \partial_t + \frac{1}{z^2} \partial_r^z \right] \Psi = 0. \quad (3.33)$$

We will see, that both the old and the new version of LSI agree with the results from subsection 3.1.3. It is easy to see that equation (3.33) is equivalent to (3.1) for $z = 2$ resp. to (3.2) for $z = 4$ when setting $\nu_2 = (4\mu)^{-1}$ resp. $\nu_4 = -(16\mu)^{-1}$. The generators of the corresponding Lie algebra were explicitly given (for $d = 1$) in (2.37) and the scaling dimension x is related to γ and μ via

$$x = \frac{z-1}{2} + \frac{\gamma}{\mu} (2-z). \quad (3.34)$$

As shown in [109] these space-time symmetries (2.37) can be used to fix the form of the two-time response function completely. Using all generators and writing $\mathbf{r} = \mathbf{x} - \mathbf{y}$, one obtains

$$R_0(\mathbf{r}, t, s) = (t-s)^{-2x/z} \phi\left(\frac{|\mathbf{r}|}{(t-s)^{1/z}}\right) \quad (3.35)$$

where the index 0 indicates that this is the result for the noise-free theory. The scaling function $\phi(\rho)$ satisfies the fractional differential equation (2.43). We have to stress that the scaling function given in [109] is not the most general solution of this equation. In appendix C of [207] we derive this most general solution for any rational z . As shown in the next subsection it is this solution which permits us to derive the exact expressions for the space-time response and correlation functions in the MH case by exploiting exclusively the space-time symmetries of the deterministic equation (3.2). For $z = 2$ we recover the known result [109]

$$\phi(u) = \phi_0 \exp(-\mu u^2) \quad (3.36)$$

where the numerical factor ϕ_0 is not fixed by the theory. For the case $z = 4$ and $d = 1$ our new result is (see the appendices of [207] for the expression obtained in two space

dimensions)

$$\begin{aligned} \phi(u) &= \tilde{c}_0 \left(-\frac{\mu}{16}u^4\right)^{1/4} {}_0F_2\left(\frac{3}{4}, \frac{5}{4}, -\frac{\mu}{16}u^4\right) \\ &+ \tilde{c}_1 \left(-\frac{\mu}{16}u^4\right)^{1/2} {}_0F_2\left(\frac{5}{4}, \frac{3}{2}, -\frac{\mu}{16}u^4\right) + \tilde{c}_2 {}_0F_2\left(\frac{1}{2}, \frac{3}{4}, -\frac{\mu}{16}u^4\right) \end{aligned} \quad (3.37)$$

with some constants \tilde{c}_0 , \tilde{c}_1 and \tilde{c}_2 . Here we have used the fact that $x = \frac{d}{2}$ in a free field theory as is easily obtained from a dimensional analysis (see also the next subsection). The coefficients \tilde{c}_0 , \tilde{c}_1 and \tilde{c}_2 have to be arranged in such a way that $\phi(u)$ vanishes for $u \rightarrow \infty$. Analysing the leading terms [232, 233] one realizes that the condition

$$\Gamma\left(\frac{5}{4}\right)\Gamma\left(\frac{3}{4}\right)\tilde{c}_0 + \Gamma\left(\frac{5}{4}\right)\Gamma\left(\frac{3}{2}\right)\tilde{c}_1 + \Gamma\left(\frac{3}{4}\right)\Gamma\left(\frac{1}{2}\right)\tilde{c}_2 = 0 \quad (3.38)$$

provides exactly this, as it cancels all exponentially growing terms.

Let us close this subsection by noting that in the derivation of expression (3.35) we exploited the fact that the exact responses of both the EW and MH case are time translation invariant. Often when discussing out-of-equilibrium systems this is not the case and one has to consider the sub-algebra where the generator X_{-1} , responsible for time translation invariance, is omitted [108, 109, 110, 123, 192]. This then yields for the autoresponse the expression $R_0(t, s) = r_0 s^{-1-a} \left(\frac{t}{s}\right)^{1+a'} - \lambda_R/z \left(\frac{t}{s} - 1\right)^{-1-a'}$, where the parameters a and a' have to be determined by comparing with known results. When setting $a = a' = \lambda_R/z - 1$, one recovers our result.

3.1.5 Determination of response and correlation functions from space-time symmetries (old version of LSI)

In order to use the symmetry considerations of the last subsection, we have to adopt the standard field theoretical setup for the description of Langevin equations [165, 134, 192]. This has already been introduced in chapters 1 and 2, but we briefly recall it in order to establish notations. Apart from the field $h(\mathbf{x}, t)$ we consider the so-called response field $\tilde{h}(\mathbf{x}, t)$ which leads to the action

$$\begin{aligned} S[h, \tilde{h}] &= \int du d\mathbf{R} \left[\tilde{h} (\partial_u + \nu_{2l}(-\nabla^2)^l) h \right] \\ &+ \frac{1}{2} \int du d\mathbf{R} du' d\mathbf{R}' \tilde{h}(\mathbf{R}, u) \langle \eta(\mathbf{R}, u) \eta(\mathbf{R}', u') \rangle \tilde{h}(\mathbf{R}', u') \end{aligned} \quad (3.39)$$

where $l = 1$ for the EW case and $l = 2$ for the MH case. The temporal integration is from 0 to ∞ whereas the spatial integration is over the whole space.

Varying the action yields the equation of motion for the fields h and \tilde{h}

$$\frac{\partial h(\mathbf{x}, t)}{\partial t} = -\nu_{2l}(-\nabla^2)^l h(\mathbf{x}, t) - \int du d\mathbf{R} \tilde{h}(\mathbf{R}, u) \langle \eta(\mathbf{R}, u) \eta(\mathbf{x}, t) \rangle \quad (3.40)$$

$$\frac{\partial \tilde{h}(\mathbf{x}, t)}{\partial t} = \nu_{2l}(-\nabla^2)^l \tilde{h}(\mathbf{x}, t) \quad (3.41)$$

As expected, one recovers for the height $h(\mathbf{x}, t)$ the Equations (3.1) and (3.2) by identifying the noise with the term $-\int du d\mathbf{R} \tilde{h}(\mathbf{R}, u) \langle \eta(\mathbf{R}, u) \eta(\mathbf{x}, t) \rangle$.

One can now proceed by looking at the multi-point functions which are defined in the usual way via functional integrals:

$$\left\langle \prod_{i=1}^n h(\mathbf{x}_i, t_i) \prod_{j=n+1}^m \tilde{h}(\mathbf{x}_j, t_j) \right\rangle := \int \mathcal{D}[h] \mathcal{D}[\tilde{h}] \prod_{i=1}^n h(\mathbf{x}_i, t_i) \prod_{j=n+1}^m \tilde{h}(\mathbf{x}_j, t_j) \exp(-S[h, \tilde{h}]). \quad (3.42)$$

Within this formalism the space-time response (3.8) is given by

$$R(\mathbf{x}, \mathbf{y}, t, s) = \langle h(\mathbf{x}, t) \tilde{h}(\mathbf{y}, s) \rangle. \quad (3.43)$$

In order to proceed one splits up the action in the same way as done in [192], that is as

$$S[h, \tilde{h}] = S_0[h, \tilde{h}] + S_{th}[h, \tilde{h}] \quad (3.44)$$

with the deterministic part

$$S_0[h, \tilde{h}] = \int du d\mathbf{R} \left[\tilde{h}(\mathbf{R}, u) (\partial_u + \nu_{2l}(-\nabla^2)^l) h(\mathbf{R}, u) \right] \quad (3.45)$$

and the noise part

$$S_{th}[h, \tilde{h}] = \frac{1}{2} \int du d\mathbf{R} du' d\mathbf{R}' \tilde{h}(\mathbf{R}, u) \langle \eta(\mathbf{R}, u) \eta(\mathbf{R}', u') \rangle \tilde{h}(\mathbf{R}', u') \quad (3.46)$$

We call the theory exclusively described by S_0 noise-free and denote averages with respect to this theory with $\langle \dots \rangle_0$. The n -point functions of the full theory can then be written as

$$\left\langle \prod_{i=1}^n h(\mathbf{x}_i, t_i) \prod_{j=n+1}^m \tilde{h}(\mathbf{x}_j, t_j) \right\rangle = \left\langle \prod_{i=1}^n h(\mathbf{x}_i, t_i) \prod_{j=n+1}^m \tilde{h}(\mathbf{x}_j, t_j) \exp(-S_{th}[h, \tilde{h}]) \right\rangle_0. \quad (3.47)$$

It is easy to see that the noise-free theory has a Gaussian structure both for the EW and the MH model. Introducing the two-component field $\Psi = \begin{pmatrix} h \\ \tilde{h} \end{pmatrix}$ one can write the exponential $\exp(-S_0[h, \tilde{h}])$ as $\exp(-\int du d\mathbf{r} du' d\mathbf{r}' \Psi^t \mathbf{A} \Psi)$ with

$$\mathbf{A} = \frac{1}{2} \begin{pmatrix} 0 & \delta(u-u')\delta(\mathbf{r}-\mathbf{r}')((-\nabla^2)^l - \partial_u) \\ \delta(u-u')\delta(\mathbf{r}-\mathbf{r}')((-\nabla^2)^l + \partial_u) & 0 \end{pmatrix}. \quad (3.48)$$

From this one deduces two important facts which we will need in the sequel. Firstly, one has

$$\underbrace{\langle h \dots h \rangle}_n \underbrace{\langle \tilde{h} \dots \tilde{h} \rangle}_m = 0 \quad (3.49)$$

unless $n = m$, which is due to the antidiagonal structure of \mathbf{A} (see for instance [226], chapter 4). As explained in chapter 2, for the new version of LSI, another justification for this fact, which does not rely on the structure of \mathbf{A} , is the Bargmann superselection

rule and its generalisation (2.77). Secondly, Wick's theorem holds. With this it follows that one can write the four-point function as

$$\begin{aligned} \langle h(\mathbf{x}, t)h(\mathbf{y}, s)\tilde{h}(\mathbf{R}, u)\tilde{h}(\mathbf{R}', u') \rangle_0 &= \langle h(\mathbf{x}, t)\tilde{h}(\mathbf{R}, u) \rangle_0 \langle h(\mathbf{y}, s)\tilde{h}(\mathbf{R}', u') \rangle_0 \\ &+ \langle h(\mathbf{y}, s)\tilde{h}(\mathbf{R}, u) \rangle_0 \langle h(\mathbf{x}, t)\tilde{h}(\mathbf{R}', u') \rangle_0 \end{aligned} \quad (3.50)$$

where we have used eq. (3.49).

Now one can calculate the quantities of interest, namely the space-time response and correlation functions. For this one develops the exponential in (3.47) in a power series. One remarks immediately that due to the selection rule (3.49) one has

$$R(\mathbf{x}, \mathbf{y}, t, s) = R_0(\mathbf{x}, \mathbf{y}, t, s) := \langle h(\mathbf{x}, t)\tilde{h}(\mathbf{y}, s) \rangle_0, \quad (3.51)$$

i.e. the linear response function of the full theory is *equal* to the noise-less linear response function. It follows that for any realization of the noise one gets the same expression for the response function, in agreement with the exact results derived in subsection 3.1.3. It is also worth noting that within a free field theory non-linear responses vanish due to the same superselection rule. Things are of course more tricky for a field theory which is not free as here the noise can contribute to the response. Whether this is the case depends on the concrete form of the interaction.

By expanding the exponential in (3.47) we obtain in a similar way that the space-time correlation function is given by the expression

$$C(\mathbf{x}, \mathbf{y}, t, s) = \int du d\mathbf{R} du' d\mathbf{R}' \langle h(\mathbf{x}, t)h(\mathbf{y}, s)\tilde{h}(\mathbf{R}, u)\tilde{h}(\mathbf{R}', u') \rangle_0 \langle \eta(\mathbf{R}, u)\eta(\mathbf{R}', u') \rangle. \quad (3.52)$$

Using Wick's theorem we can replace the four-point function by two-point functions (see Eq. (3.50)) and obtain

$$\begin{aligned} C(\mathbf{x}, \mathbf{y}, t, s) &= 2 \int du d\mathbf{R} du' d\mathbf{R}' \langle \eta(\mathbf{R}, u)\eta(\mathbf{R}', u') \rangle \\ &\times \langle h(\mathbf{x}, t)\tilde{h}(\mathbf{R}, u) \rangle_0 \langle h(\mathbf{y}, s)\tilde{h}(\mathbf{R}', u') \rangle_0. \end{aligned} \quad (3.53)$$

Inspection of eqs. (3.51) and (3.53) reveals that the only remaining undetermined quantity is the two-point function $\langle h(\mathbf{x}, t)\tilde{h}(\mathbf{y}, s) \rangle_0$. However, as discussed in the previous subsection, this two-point function is fully determined by the space-time symmetries of the deterministic equation of motion. It remains to show that the insertion of this two-point function into Eqs. (3.51) and (3.53) indeed yields the exact expressions for the space-time quantities both for the EW and for the MH case.

$z = 2$: The Edwards-Wilkinson case

This case with Gaussian white noise has already been discussed in [192] in the context of phase ordering kinetics and of critical dynamics. The response function can be read off from the Equation (3.35) after inserting the scaling function (3.36). Recalling that for the EW case we have $z = 2$, $x = \frac{d}{2}$, and $\nu_2 = (4\mu)^{-1}$ we readily obtain the exact result (3.15). The only quantity left free by the theory is the numerical prefactor ϕ_0 .

The space-time correlation function is obtained by inserting the same two-point function into Eq. (3.53). This is most easily seen by using the integral representation (3.14) of the two-point function which yields after interchanging the order of integration:

$$C(\mathbf{x}, \mathbf{y}, t, s) = c_0 \int_0^t dt' \int_0^s dt'' \int \frac{d\mathbf{k}}{(2\pi)^d} e^{i\mathbf{k}\cdot(\mathbf{x}-\mathbf{y})} e^{-\nu_2 \mathbf{k}^2(t-t')} e^{-\nu_2 \mathbf{k}^2(s-t'')} \times \langle \hat{\eta}(\mathbf{k}, t') \hat{\eta}(-\mathbf{k}, t'') \rangle \quad (3.54)$$

which is exactly the same expression (up to the undetermined constant c_0) as (3.17), and this for any choice of the noise correlator $\langle \hat{\eta}(\mathbf{k}, t') \hat{\eta}(-\mathbf{k}, t'') \rangle$. It then immediately follows that we recover the exact results for C given in subsection 3.1.3.

$z = 4$: The Mullins-Herring case

For the MH case we proceed along the same lines as for the EW case. Let us start with the one-dimensional case $d = 1$. As already seen for the EW model, the response function is just the response function of the noise-free theory whose scaling function is given by (3.37) together with the condition (3.38) needed for a response which vanishes for $u \rightarrow \infty$. In order to proceed further we remark that in a powers series expansion of (3.37) odd powers of the scaling variable u only enter through the term with coefficient \tilde{c}_0 . However, odd powers of the scaling variable are absent in the exact result (3.26), so we have to set $\tilde{c}_0 = 0$. From Eq. (3.38) it then follows that

$$\Gamma\left(\frac{5}{4}\right) \tilde{c}_1 = -2 \Gamma\left(\frac{3}{4}\right) \tilde{c}_2. \quad (3.55)$$

Recalling that for the MH case $z = 4$, $x = \frac{d}{2}$, and $\nu_4 = -(16\mu)^{-1}$, it is now easy to check that the proposed scaling function together with (3.55) indeed yields the exact result (3.26) up to the normalisation constant \tilde{c}_2 . This so determined two-point function can then be inserted into the correlation function (3.53), yielding the exact result (3.28). This is again most easily seen by using the integral representation

$$R(\mathbf{x} - \mathbf{y}, t, s) = \hat{r}_0 \int \frac{d\mathbf{k}}{(2\pi)^d} e^{i\mathbf{k}\cdot(\mathbf{x}-\mathbf{y})} e^{-\nu_4 \mathbf{k}^4(t-s)} \quad (3.56)$$

of the response function (3.26).

In two dimensions we have to replace the expression (3.37) by (see the appendix of [207])

$$\phi(u) = \tilde{c}_1 \left(-\frac{\mu}{16} u^4\right)^{1/2} {}_0F_2\left(\frac{3}{2}, \frac{3}{2}, -\frac{\mu}{16} u^4\right) + \tilde{c}_2 {}_0F_2\left(\frac{1}{2}, 1, -\frac{\mu}{16} u^4\right) \quad (3.57)$$

It follows that in $d = 2$ the scaling function obtained from LSI only contains two parameters which are furthermore related through the condition [207]

$$\tilde{c}_1 = -\frac{4}{\sqrt{\pi}} \tilde{c}_2. \quad (3.58)$$

We are therefore left with a single undetermined parameter which only appears as a numerical prefactor, similar to the EW case. Inserting the resulting scaling function into the expressions (3.51) and (3.53) readily yields the exact results for the space-time quantities in two dimensions.

3.1.6 Determination of response and correlation functions from space-time symmetries (new version of LSI)

We finally show, that the new version of LSI also gives the right predictions for the models treated in this section. For the Edward-Wilkinson case, where $z = 2$, the old and the new version of LSI agree, as there are no fractional derivatives in this case. Therefore it is enough to check the Mullins-Herring model.

The easiest way to show agreement is to use expressions (3.25) and (3.28) for the response function and the correlation function respectively. Expression (3.25) clearly agrees with equation (2.152) from chapter 2 if we identify

$$z = 4, \quad a = a' = \frac{d}{4} - 1, \quad \lambda_R = d, \quad \beta = 0, \quad \alpha = \nu_4 \quad (3.59)$$

Turning to the correlation function, we first state, that we suppose that the Fourier transform of the noise correlator in (3.28) always has the form

$$\langle \eta(\mathbf{k}, t) \eta(-\mathbf{k}, t') \rangle = 2D\delta(t - t') \widehat{b}(\mathbf{k}) \quad (3.60)$$

where the function $\widehat{b}(\mathbf{k})$ is a constant for non-conserving noise and $\widehat{b}(\mathbf{k}) = \mathbf{k}^2$ for conserving noise. Now it is straightforward to see that the expression (2.170) reproduces correctly the result (3.28) with the choices (3.59) and

$$x = \tilde{x} = \frac{d}{2}, \quad \xi = \tilde{\xi} = 0, \quad F = 0, \quad c_0 = D/T \quad (3.61)$$

and by setting the function $g(u) = 1$. This agreement is independent for the kind of noise used, as long as the second moment of the noise has the form (3.60).

There is a final point we should mention. When deriving the value of the ageing exponent b_{th} from equation (2.170) in chapter 2, we have only done this for white noise, i.e. for $\widehat{b}(\mathbf{k}) = const$. One could in principle also consider different second moments for the noise, just as for the Edward-Wilkinson model (which we have *not* done up until here). For instance, one would have $\widehat{b}(\mathbf{k}) = \mathbf{k}^2$ for conserving noise and $\widehat{b}(\mathbf{k}) = |\mathbf{k}|^{-2\rho}$ (up to a prefactor) for coloured noise as given by (3.6). It is a straightforward but somewhat tedious task to repeat the steps performed in chapter 2 to find the relation between b_{th} and the scaling dimensions of the field. The results are as follows. For nonconserving noise (MH1), we have the relation (2.172)

$$b_{th} = \frac{2}{z}(x + \tilde{x}_2) - 1 - \frac{d}{z}. \quad (3.62)$$

For conserving noise (MHc), where $\widehat{b} = \mathbf{k}^2$, this gets modified to

$$b_{th} = \frac{2}{z}(x + \tilde{x}_2) - 1 - \frac{d}{z} + \frac{2}{z} \quad (3.63)$$

and for coloured noise (MH2), in which case $\widehat{b} = \mathbf{k}^{-2\rho}$ up to a constant prefactor, one has

$$b_{th} = \frac{2}{z}(x + \tilde{x}_2) - 1 - \frac{d}{z} - \frac{2\rho}{z} \quad (3.64)$$

This then yields the values given in table (3.5) at the end of this chapter.

3.1.7 Microscopic growth models and space-time correlations

Many theoretical studies of growth processes focus on atomistic models where particles are deposited on a surface and are then incorporated into the growing surface following some specific rules which might include local diffusion processes. Of special interest is the determination of the universality class to which these models belong. This is usually achieved by computing some universal quantities through numerical simulations and comparing them to the corresponding quantities obtained from continuum growth equations like the EW and the MH equations discussed in this section. In a commonly used approach one focuses on the estimation of the exponents z and ζ , which govern the behaviour of the surface width (3.3), through the best data collapse.

In order to show that it is useful to look at two-time quantities in nonequilibrium growth processes we discuss in the following the space-time correlation function in the Family model [84] and in a variant of this model [182]. Even so these are very simple models, there is still some debate on the universality class to which these models belong, especially in 2+1 dimensions. Whereas earlier numerical studies yielded the value $z = 2$ for the dynamical exponent in the 2+1-dimensional Family model [84, 173, 159, 1], in agreement with the EW universality class with Gaussian white noise, Pal et al. [182, 183] in their study obtained a value $z \approx 1.65$, pointing to a different universality class. In addition they studied a variant of this model (which we call restricted Family model in the following) for which they recovered $z = 2$. These results of Pal et al. are surprising, especially so as Vvedensky succeeded [230] in deriving in 1+1 dimensions the EW equation with Gaussian white noise from both the Family and the restricted Family model through a coarse-graining procedure.

	D	ν_2
$d = 1$	6.26(1)	0.794(1)
$d = 1$ restricted	6.27(1)	0.770(1)
$d = 2$	38.9(2)	0.686(2)
$d = 2$ restricted	38.5(2)	0.372(2)

Table 3.1: Estimates for the nonuniversal constants D and ν_2 .

The Family model is a ballistic deposition model with surface diffusion where a particle is dropped at a randomly chosen surface site. Instead of fixing itself at this site, the particle first explores the local environment (usually one restricts this exploration to the nearest neighbors) and fixes itself at the lattice site with the lowest height. When two or more lattice sites other than the originally selected site have the same lowest height, one of these sites is selected randomly. In case the originally chosen lattice site is among the sites with the lowest height, the particle remains at this site. In the restricted version of this model, introduced in [182], the particle only moves to a site of lowest height when it is unique. This change has the effect that the moving of the particle only contributes deterministically to the surface shape.

We have simulated these two models both in 1+1 and 2+1 dimensions. For the 1+1 dimensional models all previous studies agree that $z = 2$ and that both models belong to the one-dimensional EW universality class with Gaussian white noise. Our main interest here is the height-height space-time correlation function $C(\mathbf{x} - \mathbf{y}, t, s)$. From the exact

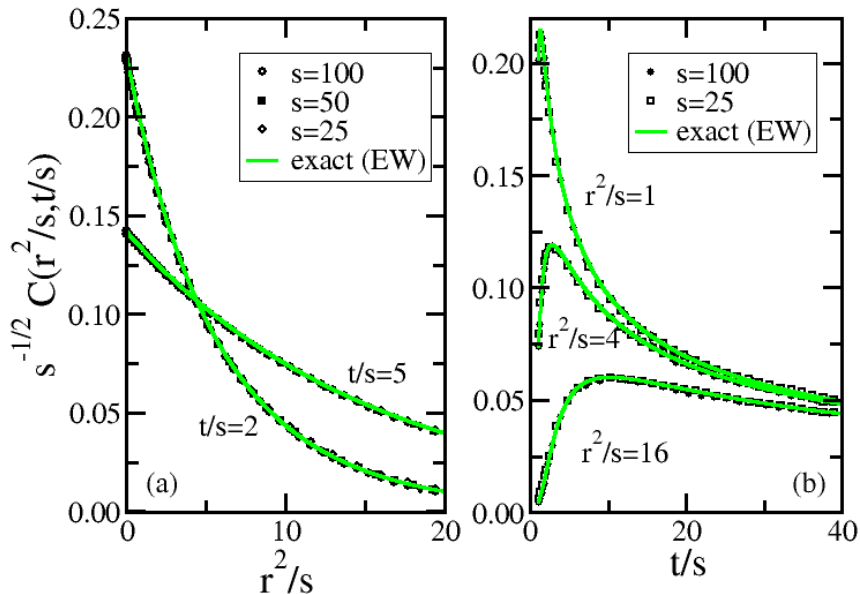


Figure 3.1: (Color online) Dynamical scaling of the space-time correlation function $C(r^2/s, t/s)$ for Family model in 1+1 dimensions with different values of the waiting time s : (a) C vs r^2/s for some fixed values of t/s , (b) C vs t/s for some fixed values of r^2/s . The green curves (full lines) are obtained from the exact result (3.18) derived from the continuum EW equations with uncorrelated Gaussian white noise. Numerical error bars are smaller than the sizes of the symbols.

results presented in the first part of the section we conclude that this two-time quantity should only depend on the two scaling variables t/s and r^2/s where $r = |\mathbf{x} - \mathbf{y}|$. In Figure 3.1 we test this expected scaling behaviour in the 1+1 dimensional Family model. In Figure 3.1a we fix t/s and plot the correlation function as a function of r^2/s , whereas in Figure 3.1b r^2/s is fixed and C is plotted vs t/s . Lattices with 12800 sites have been simulated and the data shown result from averaging over 1000 runs with different random numbers. The curves obtained for different values of the waiting time s collapse on a common master curve when multiplying C with $s^{-1/2}$. In addition, these master curves nicely agree with the expression (3.18) obtained from the EW equation with uncorrelated white noise, once the nonuniversal constants D and ν_2 have been determined³. A similar good agreement is obtained for the restricted Family model. We list our estimates for D and ν_2 for both one-dimensional models in Table 3.1. It follows from this table that the two models seem to have the same value of D , whereas the value of ν_2 is distinct. In addition, D/ν_2 is slightly larger for the restricted model, even so the error bars are overlapping. One might expect that the continuum description may not completely describe the lattice models for small values of r^2/s because of the discrete nature of the lattice, but one can see that the agreement is perfect. After having verified that the computed scaling functions in both versions of the 1+1 dimensional Family model agree with the solution of the EW continuum equation, let us now proceed to the more controversial 2+1 dimensional case.

³We follow here the procedure used in [110] in the context of phase ordering kinetics.

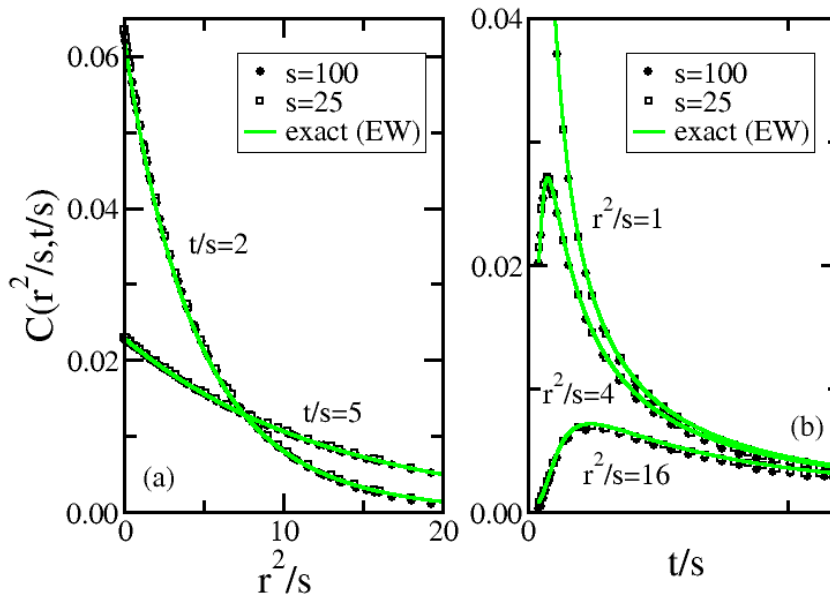


Figure 3.2: (Color online) The same as in Figure 3.1, but now for the Family model in 2+1 dimensions. Numerical error bars are comparable to the sizes of the symbols.

In Figure 2 we display the space-time correlation computed for the original Family model in 2+1 dimensions. Again, in the left panel we fix t/s , whereas in the right panel r^2/s is kept constant. The data shown here have been obtained for lattices with 300×300 sites with 5000 runs for every waiting time. We carefully checked that our nonequilibrium data are not affected by finite-size effects. Furthermore, we ran different simulations with different random number generators and obtained the same results within error bars. We obtain as the main result of these simulations that the scaling function of the space-time correlation function is in excellent agreement (once the values of the nonuniversal constants have been determined, see Table 3.1) with the exact result obtained from solving the two-dimensional EW equation with uncorrelated white noise. Our results are in accordance with the results of [84, 173, 159, 1, 230] but strongly disagree with those of Pal et al. [182, 183]. Indeed, a noninteger value of z in a continuum description can not be realized in a linear stochastic differential equation and leads to completely different scaling functions as those obtained from the EW equation.

In Figure 3.3 (see also Table 3.1) we show our results for the restricted family model in 2+1 dimensions. Again, dynamical scaling is observed, and again the data are perfectly described by the EW scaling functions in the scaling limit. The determined value for the nonuniversal quantity D is again equal to the value obtained for the original model but the value for ν_2 is markedly different. Specifically, the ratio D/ν_2 (which is of the dimension $k_B T$) is much larger for the restricted model. Identifying D/ν_2 with a (nonequilibrium) temperature, we can view the processes in the restricted model to take place at a higher temperature than in the original model. This is in agreement with the observation from Pal et al. [183] that the surface is locally rougher in the restricted model, as evidenced by the larger value of the interface width. In addition, the change in the diffusion rule

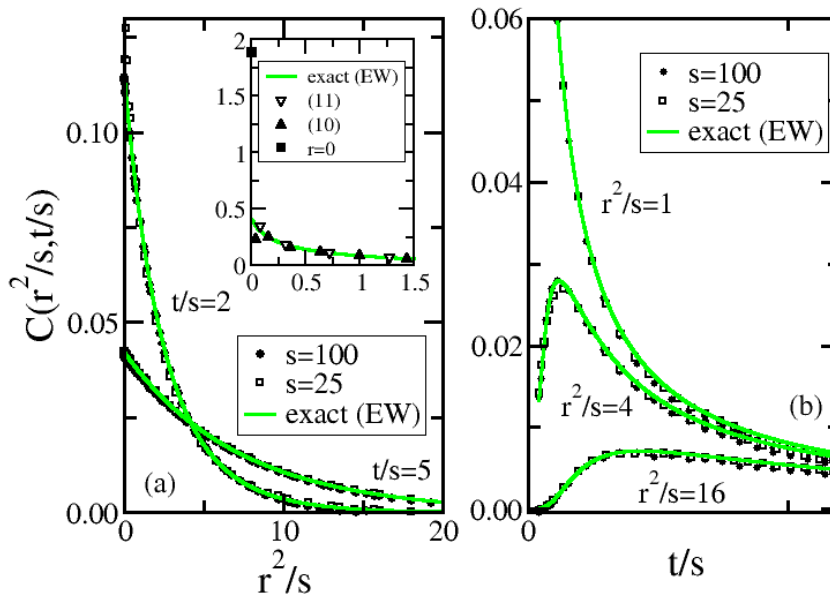


Figure 3.3: (Color online) The same as in Figure 3.2, but now for the restricted Family model in 2+1 dimensions. The inset in (a) shows the correlation function in the (10) and (11) directions for the case $s = 25$ and $t/s = 1.04$. The change of the diffusion rule has a strong impact on the autocorrelation with $r = 0$ and on the nearest neighbour correlations. Numerical error bars are comparable to the sizes of the symbols.

leads to a nonmonotonous behaviour of the correlation function for small r^2/s , as shown in the inset of Figure 3.3a for $s = 25$ and $t/s = 1.04$. Plotting the correlation function in both the (10) and the (11) direction, we see that correlations between nearest neighbours are suppressed, whereas the autocorrelation, i.e. the correlation with $r = 0$, is strongly enhanced. This behaviour can be understood by recalling that in the restricted model a particle only diffuses to a lower nearest neighbour site when this site is unique, but otherwise remains on the original site. If we increase s and r , this effect weakens, and it completely vanishes in the scaling limit of large waiting times and large values of r^2/s .

From our observation that the numerically computed space-time correlation functions of both microscopic models coincide in the scaling limit with the exact expression from the EW model we conclude that both the Family model and the restricted Family model belong to the EW universality class with uncorrelated noise, and this not only in 1+1 dimensions but also in 2+1 dimensions.

3.1.8 Conclusions of this section

The aim of the present section is twofold: on the one hand we discuss the usefulness of universal scaling functions of space-time quantities in characterising the universality class of nonequilibrium growth models, on the other hand we demonstrate how the general symmetry principles allow to derive scaling functions of two-point quantities for equilibrium and nonequilibrium processes described by linear stochastic Langevin equations.

In the context of nonequilibrium growth processes it is rather uncommon to study universal scaling functions of two-point quantities in the dynamical scaling limit in order to determine the universality class to which a given microscopic model belongs. We have illustrated the usefulness of this approach by comparing the numerically obtained space-time correlation functions for two atomistic growth models with the exact expressions obtained from the corresponding continuum stochastic Langevin equation. This approach has allowed us to show that both models belong to the same universality class, thus correcting conclusions obtained in earlier numerical studies.

The study of universal scaling functions of space-time quantities should also be of value in more complex growth processes which are no more described by linear stochastic differential equations. Examples include ballistic deposition with an oblique incident particle beam [215] or growth processes of the KPZ [141] and related [154] universality classes where nonlinear effects can no more be neglected. In addition, the scaling functions studied here can also be measured in experiments involving nonequilibrium or equilibrium interface fluctuations. A promising system is given by equilibrium step fluctuations [91, 74, 75, 30], as these are again described by linear Langevin equations.

In addition we have shown that in nonequilibrium growth processes scaling functions of out-of-equilibrium quantities can be derived by using the theory presented in chapter 2. We have also shown, that for the cases at hand (where $z = 2$ and $z = 4$) also the old version of LSI yields the correct expressions for response and correlation functions. We have also computed the most general form of the two-point function implied by the old version of LSI in the case of a rational dynamical exponent z , following the general ideas formulated by Henkel a few years ago [109]. The case $z = 2$ has already been studied extensively in the past. For the case $z = 4$, however, we present to our knowledge for the first time the derivation of nonequilibrium scaling functions by exploiting the mentioned symmetry principles. As these scaling functions are found to agree with the exact expressions derived from the MH equation for both versions of LSI, we conclude that the postulated space-time symmetries and the proposed way for constructing the scaling functions can also be valid for other cases than merely the case $z = 2$.

3.2 Spherical model with conserved order parameter

3.2.1 Introduction

In this section, we are interested in carrying out another case-study on the ageing and its local scale-invariance when the order-parameter is conserved. Physically, this may describe the phase-separation of binary alloys, where the order-parameter is given by the concentration difference of the two kinds of atoms. Another example are kinetic growth-processes at surfaces when mass conservation holds. One of the most simple models of this kind is the Mullins-Herring model [175, 231], which leads to a dynamical exponent $z = 4$ and has been discussed in detail in section 3.1.

Presently, there exist very few studies on ageing with a conserved order-parameter. In a numerical study of the $2D$ Ising model quenched to $T < T_c$, where $z = 3$, Godrèche, Krzakala and Ricci-Tersenghi [95] calculated the scaling function $f_C(y)$ which remarkably shows a cross-over between a first power-law decay $f_C(y) \sim y^{-\lambda'_C/z}$ for intermediate values of y to the final asymptotic behaviour (1.12) for $y \gg 1$. They find a value of $\lambda'_C = 2.5$,

whereas the value for λ_C is much smaller with $\lambda_C = 1$. On the other hand, Sire [220] calculated $f_C(y)$ exactly in the critical spherical model ($T = T_c$), where $z = 4$, and found a single power-law regime.⁴ For a review, see [45].

In this section, we shall revisit the spherical model with a conserved order-parameter, quenched to $T = T_c$. Besides reviewing the calculation of the two-time correlation function we shall also provide the exact solution for the two-time response function. This will be described in subsection 3.2.2. Our main focus will be to show that these exact results can be understood by both versions of LSI with $z = 4$. In subsection 3.2.3, we recall the main results of the old version of LSI for that case and in particular write down a linear partial differential equation of which this LSI is a dynamical symmetry. In subsection 3.2.4, we consider the Langevin equation which describes the kinetics with a conserved order-parameter (model B in the Halperin-Hohenberg classification) and show that the treatment presented in chapter 2 can be carried over to this case: The Langevin-equation can be split into a ‘deterministic’ and a ‘noise’ part, so that all averages to be calculated can be exactly reduced to quantities to be found in a noise-less theory. Local scale-invariance directly determines the latter, as we have already seen. In 3.2.5 we can compare the predictions of the old version of LSI with the exact spherical model results of subsection 3.2.2. Finally we do the same for the new version of LSI in subsection 3.2.6. This is, together with the earlier study of the Mullins-Herring model in [207], the first example where local scale-invariance can be confirmed for an exactly solvable model with dynamical exponent $z \neq 2$. Our conclusions are formulated in subsection 3.2.7. Some technical points are reported in the appendices of [19].

3.2.2 The spherical model with a conserved order-parameter

The spherical model was conceived in 1953 by Berlin and Kac as a mathematical model for strongly interacting spins which is yet easily solvable and it has indeed served a useful rôle in providing exact results in a large variety of interesting physical situations. It may be defined in terms of a real spin variable $S(t, \mathbf{x})$ attached to each site \mathbf{x} of a hypercubic lattice $\Lambda \subset \mathbb{Z}^d$ and depending on time t , subject to the (mean) spherical constraint

$$\left\langle \sum_{\mathbf{x} \in \Lambda} S(t, \mathbf{x})^2 \right\rangle = \mathcal{N} \quad (3.65)$$

where \mathcal{N} is the number of sites of the lattice. The Hamiltonian is $\mathcal{H} = - \sum_{(\mathbf{x}, \mathbf{y})} S_{\mathbf{x}} S_{\mathbf{y}}$ where the sum is over pairs of nearest neighbours. The kinetics is assumed to be given by a Langevin equation of model B type

$$\partial_t S(t, \mathbf{x}) = - \nabla_{\mathbf{x}}^2 \left[\nabla_{\mathbf{x}}^2 S(t, \mathbf{x}) + \mathfrak{z}(t) S(t, \mathbf{x}) + h(t, \mathbf{x}) \right] + \eta(t, \mathbf{x}) \quad (3.66)$$

where $\mathfrak{z}(t)$ is the Lagrange multiplier fixed by the mean spherical constraint⁵ and the coupling to the heat bath with the *critical* temperature T_c is described by a Gaussian

⁴It is well-known that the spherical model with conserved order-parameter quenched to below T_c shows a multiscaling which is not captured by the simple scaling form (1.12) [55]. It is understood that this is a peculiarity of the $n \rightarrow \infty$ limit of the conserved $O(n)$ vector-model [168].

⁵Considering the spherical constraint in the mean simplifies the calculations and should not affect the scaling behaviour. See [86] for a careful study of this point in the non-conserved case.

noise η of vanishing average and variance

$$\langle \eta(t, \mathbf{x}) \eta(t', \mathbf{x}') \rangle = -2T_c \nabla_{\mathbf{x}}^2 \delta(t - t') \delta(\mathbf{x} - \mathbf{x}'). \quad (3.67)$$

and $h(t, \mathbf{x})$ is a small external magnetic field.⁶ Here the derivative on the right-hand side of (3.67) expresses the fact that the noise is chosen in such a way that it does not break the conservation law. On the other hand, there are physical situations such as surface growth with mass conservation, where this is not the case. The non-conserved Mullins-Herring model [175, 231] is given by equation (3.66) with $\mathfrak{z} = 0$ and the noise correlator $\langle \eta(t, \mathbf{x}) \eta(t', \mathbf{x}') \rangle = 2T_c \delta(t - t') \delta(\mathbf{x} - \mathbf{x}')$, see [207] for details. Here we shall study the conserved Mullins-Herring model, that is equation (3.66) with $\mathfrak{z}(t) = 0$ and the noise correlator (3.67). A similar remark applies on the way we included the perturbation $h(t, \mathbf{x})$. Here we study the case, where the perturbation does not break the conservation law.

The spherical constraint is taken into account through the Lagrange multiplier $\mathfrak{z}(t)$ which has to be computed self-consistently. These equations have already been considered several times in the literature [145, 166, 220].

The correlation function

We repeat here the main steps of the calculation of the correlation function [145, 166, 220]. Equation (3.66) with $h(t, \mathbf{x}) = 0$ is readily solved in Fourier-space, yielding

$$\widehat{S}(t, \mathbf{k}) = \left[\widehat{S}(0, \mathbf{k}) + \int_0^t d\tau \exp(\omega(\tau, \mathbf{k})) \eta(\tau, \mathbf{k}) \right] \exp(-\omega(t, \mathbf{k})) \quad (3.68)$$

where $\widehat{S}(t, \mathbf{k})$ denotes the spatial Fourier transformation of $S(t, \mathbf{r})$ and

$$\omega(t, \mathbf{k}) = k^4 t - k^2 \int_0^t d\tau \mathfrak{z}(\tau), \quad \text{with} \quad k := |\mathbf{k}| \quad (3.69)$$

Next, $\omega(t, \mathbf{k})$ is determined from the spherical constraint. This is easiest in the continuum limit where spatial translation-invariance leads to

$$\langle S^2(t, \mathbf{x}) \rangle = (2\pi)^{-d} \int^\Lambda d\mathbf{k} \langle \widehat{S}(t, -\mathbf{k}) \widehat{S}(t, \mathbf{k}) \rangle = 1 \quad (3.70)$$

where Λ is the inverse of a lattice cutoff. This has already been analysed in the literature [145, 166, 220], with the result

$$\omega(t, \mathbf{k}) = k^4 t - \mathfrak{g}_d k^2 t^{1/2} \quad (3.71)$$

where the constant \mathfrak{g}_d is determined by the condition [145]

$$\int_0^\infty dx x^{d-1} \left\{ 2x^2 \int_0^1 dy \exp[-2x^4(1-y) + 2\mathfrak{g}_d x^4(1-\sqrt{y})] - \frac{1}{x^2} \right\} = 0 \quad (3.72)$$

⁶Since we are only interested in averages of local quantities and the initial magnetisation is assumed to vanish, this description is sufficient and we need not consider the analogue of the more elaborate equations studied by Annibale and Sollich [5] for the non-conserved case.

In particular, $\mathbf{g}_d = 0$ for $d > 4$ and asymptotic forms for $d \rightarrow 2$ and $d \rightarrow 4$ are listed in [145]. Then from (3.68) the two-time correlator $\widehat{C}(t, s, \mathbf{k}) := \langle \widehat{S}(t, -\mathbf{k}) \widehat{S}(s, \mathbf{k}) \rangle$ is straightforwardly derived

$$\begin{aligned} \widehat{C}(t, s, \mathbf{k}) &= s_0(\mathbf{k})^2 \exp\left(-\omega(t, \mathbf{k}) - \omega(s, \mathbf{k})\right) \\ &+ 2T_c \int_0^s du k^2 \exp\left(-\omega(t, \mathbf{k}) - \omega(s, \mathbf{k}) + 2\omega(u, \mathbf{k})\right) \end{aligned} \quad (3.73)$$

where $s_0(\mathbf{k})^2 := \langle \widehat{S}(0, -\mathbf{k}) \widehat{S}(0, \mathbf{k}) \rangle$. Transforming back to direct space, one obtains

$$C(t, s; \mathbf{r}) = A_1(t, s; \mathbf{r}) + A_2(t, s; \mathbf{r}) \quad (3.74)$$

where $A_1(t, s; \mathbf{r})$ and $A_2(t, s; \mathbf{r})$ are the inverse Fourier transforms of the first and the second line of the right-hand side of equation (3.73), respectively. They are explicitly given by the following expressions, where we use the shorthand $y := t/s$

$$\begin{aligned} A_1(t, s; \mathbf{r}) &= (t+s)^{-d/4} \int_{\mathbb{R}^d} \frac{d\mathbf{k}}{(2\pi)^d} s_0(\mathbf{k})^2 \exp\left(-\frac{\mathbf{i}\mathbf{k} \cdot \mathbf{r}}{(t+s)^{1/4}}\right) \\ &\times \exp\left(-k^4 + \mathbf{g}_d k^2 \frac{y^{1/2} + 1}{(y+1)^{1/2}}\right) \end{aligned} \quad (3.75)$$

and

$$\begin{aligned} A_2(t, s; \mathbf{r}) &= 2T_c s^{-(d-2)/4} \int_0^1 d\theta (y+1-2\theta)^{-(d+2)/4} \int_{\mathbb{R}^d} \frac{d\mathbf{k}}{(2\pi)^d} k^2 \\ &\times \exp\left(-\frac{\mathbf{i}\mathbf{k} \cdot \mathbf{r}}{(s(y+1-2\theta))^{1/4}}\right) \exp\left(-k^4 + \mathbf{g}_d k^2 \left(\frac{y^{1/2} + 1 - 2\theta^{1/2}}{(y+1-2\theta)^{1/2}}\right)\right) \end{aligned} \quad (3.76)$$

The term $A_2(t, s; \mathbf{r})$ is the dominating one in the scaling regime where $t, s \rightarrow \infty$ and $y = t/s$ is kept fixed. There we recover the scaling form (1.11) with $b = (d-2)/4$. The explicit expression for the scaling function $f_C(y)$ is quite cumbersome but, if the last term in the second exponential in eq. (5.138) can be treated as a constant, one has, up to normalisation

$$f_C(y) \sim \begin{cases} \frac{8T_c}{2-d} [(y-1)^{(2-d)/4} - (y+1)^{(2-d)/4}] & ; \quad d > 2 \\ 2T_c \ln\left(\frac{y-1}{y+1}\right) & ; \quad d = 2 \end{cases} \quad (3.77)$$

This is exact for the spherical model for $d > 4$, since then $\mathbf{g}_d = 0$. Equation (3.77) also applies to the Mullins-Herring equation for any $d \geq 1$ (since here $\mathbf{z} = 0$, in this case $\mathbf{g}_d = 0$ exactly). For y sufficiently large, the above condition is also approximately satisfied. In any case, in the limit $y \rightarrow \infty$ we can read off the autocorrelation exponent $\lambda_C = d + 2$. The scaling behaviour of the spatio-temporal two-time correlator is illustrated in figure 3.4. We see that for relatively small values of $y = t/s$, the correlation function does not decay monotonously towards zero, but rather displays oscillations whose amplitude decays with $|\mathbf{r}|s^{-1/4}$. This behaviour is quite close to the well-known one for the equal-time correlation function. As y increases, these oscillations become less pronounced. There is no apparent qualitative difference between the cases $d < 4$ and $d > 4$.

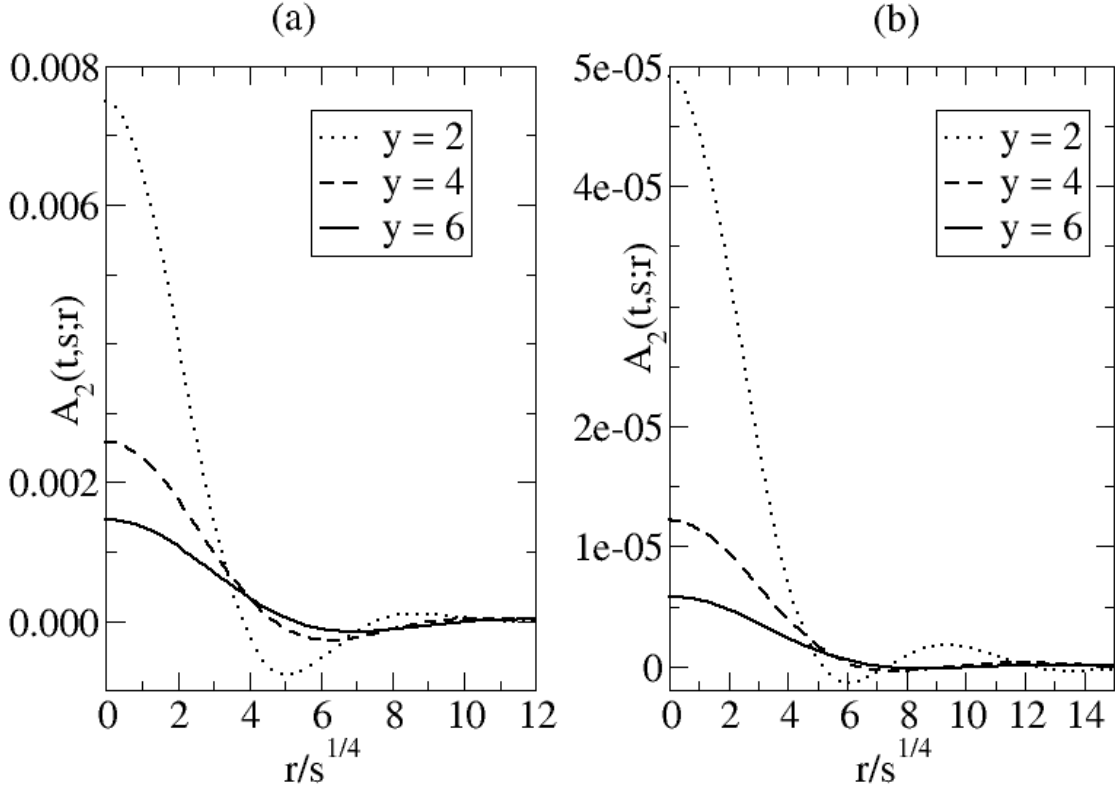


Figure 3.4: Scaling of the spatio-temporal correlation function $C(t, s; \mathbf{r}) \simeq A_2(t, s; \mathbf{r})$ with $s = 20$ and for several values of $y = t/s$ for (a) $d = 3$ (left panel) and (b) $d = 5$ (right panel).

The response function

The response function can be computed in a way similar to the non-conserved case [93]. Equation (3.66) is solved in Fourier space yielding an equation similar to (3.68)

$$\begin{aligned} \widehat{S}(t, \mathbf{k}) &= \left[\widehat{S}(0, \mathbf{k}) + \int_0^t d\tau \exp(\omega(\tau, \mathbf{k})) \right. \\ &\quad \left. \times (\widehat{\eta}(\tau, \mathbf{k}) + k^2 \widehat{h}(\tau, \mathbf{k})) \right] \exp(-\omega(t, \mathbf{k})) \end{aligned} \quad (3.78)$$

From this the Fourier transform of the response function is computed as $\widehat{R}(t, s, \mathbf{k}) = \delta \langle \widehat{S}(t, \mathbf{k}) \rangle / \delta h(s, -\mathbf{k})$. Transforming the result back to direct space, we obtain for $t > s$

$$\begin{aligned} R(t, s; \mathbf{r}) &= (t-s)^{-(d+2)/4} \int_{\mathbb{R}^d} \frac{d\mathbf{k}}{(2\pi)^d} k^2 \exp\left(-\frac{\mathbf{i}\mathbf{k} \cdot \mathbf{r}}{(t-s)^{1/4}}\right) \\ &\quad \times \exp\left(-k^4 + \mathfrak{g}_d k^2 \frac{y^{1/2} - 1}{(y-1)^{1/2}}\right) \end{aligned} \quad (3.79)$$

It is easy to see that the scaling form (1.11) holds with $a = (d-2)/4 = b$. For large values of y the scaling function $f_R(y)$ is given by

$$f_R(y) \sim (y-1)^{-(d+2)/4}. \quad (3.80)$$

Again, for $d > 4$ this expression is exact up to a prefactor. The value of the autoresponse exponent therefore is, for $d > 2$

$$\lambda_R = d + 2 = \lambda_C \quad (3.81)$$

in agreement with field-theoretical expectations for the $O(n)$ model [45].

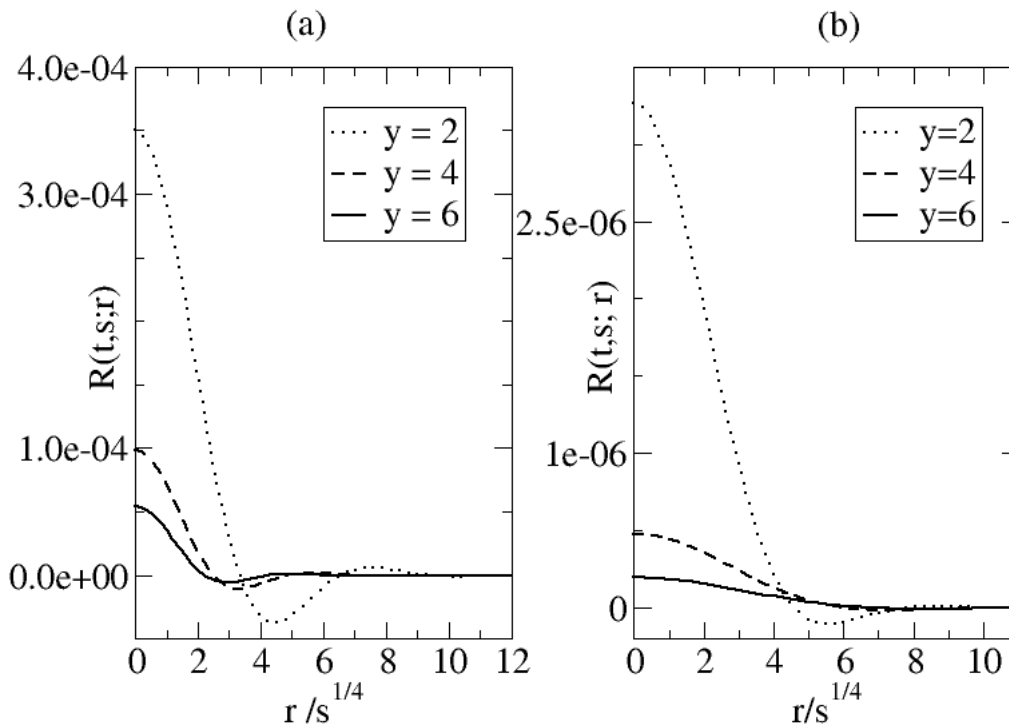


Figure 3.5: Scaling of the spatio-temporal response function $R(t,s;\mathbf{r})$ for $s=20$ and several values of $y=t/s$ for $d=3$ (left panel) and $d=5$ (right panel).

It is instructive to consider the full space-time response function explicitly for the case that $\mathbf{g}_d = 0$, that is for $d > 4$ in the spherical model and for any d in the Mullins-Herring equation. The integral in (3.79) is done in appendix B of [19] and we find

$$R(t,s;\mathbf{r}) = \frac{\sqrt{\pi}}{2^{3d/2}\pi^{d/2}\Gamma(d/4)} (t-s)^{-(d+2)/4} \left[{}_0F_2 \left(\frac{1}{2}, \frac{d}{4}; \frac{r^4}{256(t-s)} \right) - \frac{8}{d} \frac{\Gamma(\frac{d}{4}+1)}{\Gamma(\frac{d}{4}+\frac{1}{2})} \left(\frac{r^2}{16\sqrt{t-s}} \right) {}_0F_2 \left(\frac{3}{2}, \frac{d}{4} + \frac{1}{2}; \frac{r^4}{256(t-s)} \right) \right] \quad (3.82)$$

This expression will be useful later for direct comparison with the results obtained from the theory of local scale-invariance. For $\mathbf{g}_d \neq 0$ it is more convenient to use the integral

representation (3.79). In figure 3.5 we display the spatio-temporal response function. In contrast to the non-conserved case for a fixed value of $y = t/s$ there are decaying oscillations with the scaling variable $|\mathbf{r}|s^{-1/4}$. These oscillations disappear rapidly when y is increased. This qualitative behaviour also arises, as we show in appendix D of [19], for the simple random walk with a conserved noise.

Having found both correlation and response functions, we can also calculate the fluctuation-dissipation ratio $X(t, s) = TR(t, s)(\partial C(t, s)/\partial s)^{-1}$ which measures the distance from equilibrium [58]. In particular, we find for the fluctuation-dissipation limit

$$X_\infty = \lim_{s \rightarrow \infty} \left(\lim_{t \rightarrow \infty} X(t, s) \right) = \frac{1}{2} \quad (3.83)$$

in agreement with the known result [45] of the conserved $n \rightarrow \infty$ limit of the $O(n)$ model.

3.2.3 Symmetries of the deterministic equation

We recall briefly some facts about the dynamical symmetries in Langevin equations and show, how the old version of LSI can be adapted to the case at hand. Consider the ‘Schrödinger operator’

$$\widehat{S} := -\mu \partial_t + \frac{1}{16} (\nabla_{\mathbf{r}}^2)^2. \quad (3.84)$$

which we shall encounter in the context of the conserved spherical model and where obviously $z = 4$. Using the shorthands $\mathbf{r} \cdot \partial_{\mathbf{r}} := \sum_{k=1}^d r_k \partial_{r_k}$, $\nabla_{\mathbf{r}}^2 := \sum_{k=1}^d \partial_{r_k}^2$ and $\mathbf{r}^2 := \sum_{k=1}^d r_k^2$, the infinitesimal generators of local scale-transformations read (using a notation analogous to [109])

$$\begin{aligned} X_{-1} &:= -\partial_t \\ X_0 &:= -t \partial_t - \frac{1}{4} \mathbf{r} \cdot \partial_{\mathbf{r}} - \frac{x}{4} \\ X_1 &:= -t^2 \partial_t - \frac{x}{2} t - \mu \mathbf{r}^2 (\nabla_{\mathbf{r}}^2)^{-1} - \frac{1}{2} t \mathbf{r} \cdot \partial_{\mathbf{r}} \\ &\quad + 4\gamma (\mathbf{r} \cdot \partial_{\mathbf{r}}) (\nabla_{\mathbf{r}}^2)^{-2} + 2\gamma (d-4) (\nabla_{\mathbf{r}}^2)^{-2} \\ R^{(i,j)} &:= r_i \partial_{r_j} - r_j \partial_{r_i} \quad ; \quad \text{where } 1 \leq i < j \leq d \\ Y_{-1/4}^{(i)} &= -\partial_{r_i} \\ Y_{3/4}^{(i)} &= -t \partial_{r_i} - 4\mu r_i (\nabla_{\mathbf{r}}^2)^{-1} + 8\gamma \partial_{r_i} (\nabla_{\mathbf{r}}^2)^{-2} \end{aligned} \quad (3.85)$$

where x is the scaling dimension of the fields on which these generators act and γ, μ are further field-dependent parameters. Here, the generators $X_{\pm 1, 0}$ correspond to projective changes in the time t , the generators $Y_{n-1/4}^{(i)}$ are space-translations, generalised Galilei-transformations and so on and $R^{(i,j)}$ are spatial rotations. In writing these generators, we have used the ‘old’ kind of fractional derivative. The following properties of the derivative ∂_r^α are assumed

$$\partial_r^\alpha \partial_r^\beta = \partial_r^{\alpha+\beta} \quad , \quad [\partial_r^\alpha, r] = \alpha \partial_r^{\alpha-1} \quad (3.86)$$

and which can be justified in terms of fractional derivatives as shown in detail in appendix A of [109]. The operator $(\nabla_{\mathbf{r}}^2)^{-1}$ can then be defined formally as follows. For

example, in $d = 2$ dimensions, we have

$$(\nabla_{\mathbf{r}}^2)^{-1} := (\partial_{r_x}^2 + \partial_{r_y}^2)^{-1} := \sum_{n=0}^{\infty} (-1)^n \partial_{r_x}^{-2-2n} \partial_{r_y}^{2n} \quad (3.87)$$

The remaining negative powers of $\nabla_{\mathbf{r}}$ are then defined by concatenation, e.g. $(\nabla_{\mathbf{r}}^2)^{-2} = (\nabla_{\mathbf{r}}^2)^{-1} \cdot (\nabla_{\mathbf{r}}^2)^{-1}$. We easily verify the following commutation relations for $n \in \mathbb{Z}$

$$[(\nabla_{\mathbf{r}}^2)^n, r_i] = n \partial_{r_i} (\nabla_{\mathbf{r}}^2)^{n-1} \quad (3.88)$$

$$[(\nabla_{\mathbf{r}}^2)^n, \mathbf{r}^2] = 2n (\mathbf{r} \cdot \partial_{\mathbf{r}}) (\nabla_{\mathbf{r}}^2)^{n-1} + n(n-2+d) (\nabla_{\mathbf{r}}^2)^{n-1} \quad (3.89)$$

The generators eq. (3.85) describe dynamical symmetries of the ‘Schrödinger operator’ (3.84). This can be seen from the commutators of \widehat{S} and the generators \mathcal{X} from eq. (3.85). Straightforward, but a little tedious calculations give, analogously to [109]

$$\begin{aligned} [\widehat{S}, X_{-1}] &= 0, \quad [\widehat{S}, Y_{-1/4}^{(i)}] = 0, \quad [\widehat{S}, Y_{3/4}^{(i)}] = 0 \\ [\widehat{S}, X_0] &= -\widehat{S}, \quad [\widehat{S}, R^{(i,j)}] = 0 \end{aligned} \quad (3.90)$$

This means that for a solution of the ‘Schrödinger equation’ $\widehat{S}\phi = 0$ the transformed function $\mathcal{X}\phi$ is again solution of the ‘Schrödinger equation’. For the commutator with X_1 we find

$$[\widehat{S}, X_1] = -2t\widehat{S} + \frac{\mu}{2} \left(x - \frac{d}{2} - 1 + \frac{2\gamma}{\mu} \right) \quad (3.91)$$

hence a dynamical symmetry is found if the field ϕ has the scaling dimension

$$x = \frac{d}{2} + 1 - \frac{2\gamma}{\mu} \quad (3.92)$$

which for $d = 1$ reproduces the result of [109].⁷ Generalising from conformal or Schrödinger-invariance, quasiprimary fields transform covariantly and their n -point functions will again satisfy eq. (1.37). A quasiprimary field is now characterised by its scaling dimension x_i and the further parameters γ_i, μ_i . For example, any two-point function $F^{(2)} = \langle \phi_1 \phi_2 \rangle$ built from two quasiprimary fields $\phi_{1,2}$ is completely fixed by solving the conditions (1.37) for the generators in (3.85). We quote the result and refer to appendix A of [19] for the details of the calculation.

$$\begin{aligned} F^{(2)}(t-s, \mathbf{x}-\mathbf{y}) &:= \langle \phi_1(t, \mathbf{x}) \phi_2(s, \mathbf{y}) \rangle \\ &= \delta_{x_1, x_2} \delta_{\mu_1, -\mu_2} \delta_{\gamma_1, -\gamma_2} (t-s)^{-x/2} \sum_{s \in \mathcal{E}'} c_s \phi^{(s)}(|\mathbf{x}-\mathbf{y}|(t-s)^{-1/4}) \end{aligned} \quad (3.93)$$

Here $\phi^{(s)}(u)$ are scaling functions, the c_s are free parameters and the set \mathcal{E}' is defined as follows

$$\mathcal{E}' := \begin{cases} \{2, 4\} & \text{if } d > 4 \\ \{2, 4, 4-d\} & \text{if } 2 < d \leq 4 \\ \{2, 4, 2-d, 4-d\} & \text{if } d \leq 2 \end{cases} \quad (3.94)$$

⁷For a free field-theory, where $x = d/2$, this implies $\gamma/\mu = \frac{1}{2}$.

We shall see later that boundary conditions may impose further conditions on the c_s . The functions $\phi^{(s)}(u)$ are given by the series, convergent for all $|u| < \infty$

$$\phi^{(s)}(u) = \sum_{\ell=0}^{\infty} b_{\ell}^{(s)} u^{4\ell+s-4}. \quad (3.95)$$

with the coefficients $b_{\ell}^{(s)}$

$$b_{\ell}^{(s)} = 2^4 \frac{\Gamma(\frac{s}{2} + 1)\Gamma(\frac{s}{2} + \frac{d}{2})}{\Gamma(\frac{s+d}{4} - \frac{1}{2} - \frac{\gamma}{\mu})} \cdot \frac{\Gamma(\ell + \frac{s+d}{4} - \frac{1}{2} - \frac{\gamma}{\mu})}{\Gamma(2\ell + \frac{s}{2} - 1)\Gamma(2\ell + \frac{s}{2} + \frac{d}{2} - 2)} (-\mu)^{\ell} \quad (3.96)$$

3.2.4 Local scale-invariance

General remarks

The following procedure is similar to what we have already presented in chapter 2. There are however some subtle differences, for instance in the way the potential $v(t)$ is included. Therefore we repeat the main steps, which will also allow us to establish the notations of this section.

Consider the following stochastic Langevin equation

$$\partial_t \phi = -\frac{1}{16\mu} \nabla_{\mathbf{r}}^2 \left(-\nabla_{\mathbf{r}}^2 \phi + v(t)\phi \right) + \eta \quad (3.97)$$

where the noise correlator respects the global conservation law

$$\langle \eta(\mathbf{r}, t) \eta(\mathbf{r}', t') \rangle = -\frac{T}{8\mu} \nabla_{\mathbf{r}}^2 \delta(\mathbf{r} - \mathbf{r}') \delta(t - t') \quad (3.98)$$

Here and in what follows, we shall often suppress the arguments of the fields for the sake of simplicity, if no ambiguity arises. We shall adopt the standard field-theoretical setup for the description of Langevin equations, see e.g. [227, 228, 226] for introductions. The Janssen- de Dominicis action can be written in terms of the order-parameter field ϕ and its conjugate response field $\tilde{\phi}$ and reads

$$\begin{aligned} \mathcal{J}[\phi, \tilde{\phi}] &= \int du d\mathbf{R} \left[\tilde{\phi} \left(\partial_u - \frac{1}{16\mu} \nabla_{\mathbf{R}}^2 (\nabla_{\mathbf{R}}^2 - v(u)) \right) \phi \right] \\ &+ \frac{T}{16\mu} \int du d\mathbf{R} \tilde{\phi}(u, \mathbf{R}) (\nabla_{\mathbf{R}}^2 \tilde{\phi})(u, \mathbf{R}) \end{aligned} \quad (3.99)$$

to which an extra term describing the initial noise must be added, by analogy with the non-conserved case [171, 192]⁸

$$\mathcal{J}_{init}[\phi, \tilde{\phi}] = \frac{1}{2} \int d\mathbf{R} d\mathbf{R}' \tilde{\phi}(0, \mathbf{R}) \langle \phi(0, \mathbf{R}) \phi(0, \mathbf{R}') \rangle \tilde{\phi}(0, \mathbf{R}') \quad (3.100)$$

⁸It has been shown by Janssen that at the initial time $t = 0$, the order-parameter field $\phi(0, \mathbf{r})$ and the response field $\tilde{\phi}(0, \mathbf{r})$ are proportional [137].

Averages of an observable \mathcal{O} are defined as usual by functional integrals with weight $\exp(-\mathcal{J}[\phi, \tilde{\phi}])$, viz.

$$\langle \mathcal{O} \rangle := \int \mathcal{D}[\phi] \mathcal{D}[\tilde{\phi}] \mathcal{O} \exp(-\mathcal{J}[\phi, \tilde{\phi}]) \quad (3.101)$$

We decompose the action, in the same way as done in [192] for the non-conserved case, into a deterministic and a noise part, that is

$$\mathcal{J}[\phi, \tilde{\phi}] = \mathcal{J}_0[\phi, \tilde{\phi}] + \mathcal{J}_b[\tilde{\phi}] \quad (3.102)$$

with

$$\mathcal{J}_0[\phi, \tilde{\phi}] = \int du d\mathbf{R} \left[\tilde{\phi} \left(\partial_u - \frac{1}{16\mu} \nabla_{\mathbf{R}}^2 (\nabla_{\mathbf{R}}^2 - v(u)) \right) \phi \right] \quad (3.103)$$

and $\mathcal{J}_b = \mathcal{J}_{\text{th}} + \mathcal{J}_{\text{init}}$ where

$$\mathcal{J}_{\text{th}}[\tilde{\phi}] = \frac{T}{16\mu} \int du d\mathbf{R} \tilde{\phi}(u, \mathbf{R}) (\nabla_{\mathbf{R}}^2 \tilde{\phi})(u, \mathbf{R}) \quad (3.104)$$

The point of this split-up is, as we shall show, that the action $\mathcal{J}_0[\phi, \tilde{\phi}]$ has nontrivial symmetry properties, in contrast to the full action $\mathcal{J}[\phi, \tilde{\phi}]$, where these symmetries are destroyed by the noise. We call the theory with respect to $\mathcal{J}_0[\phi, \tilde{\phi}]$ *noise-free* and denote averages taken with respect to $\mathcal{J}_0[\phi, \tilde{\phi}]$ only by $\langle \dots \rangle_0$. Averages of the full theory can then be computed by formally expanding around the noise-free theory

$$\langle \mathcal{O} \rangle = \langle \mathcal{O} \exp(-\mathcal{J}_b[\tilde{\phi}]) \rangle_0 \quad (3.105)$$

The noise-free theory has a Gaussian structure, if we consider the two-component field $\Psi = \begin{pmatrix} \phi \\ \tilde{\phi} \end{pmatrix}$. Then the factor $\exp(-\mathcal{J}_0[\phi, \tilde{\phi}])$ can be written as $\exp(-\int du d\mathbf{R} du' d\mathbf{R}' \Psi^t \mathbf{A} \Psi)$ with an antidiagonal matrix \mathbf{A} . From this, two important facts can be deduced:

1. Wick's Theorem holds [238]. That is, we can write the $2n$ -point function as

$$\begin{aligned} \langle \phi(t_1, \mathbf{r}_1) \dots \phi_{2n}(t_{2n}, \mathbf{r}_{2n}) \rangle_0 &= \sum_{\substack{\text{all possible pairings} \\ \text{P of } 1, 2, \dots, 2n}} \quad (3.106) \\ &\langle \phi_{P_1}(t_{P_1}, \mathbf{r}_{P_1}) \phi_{P_2}(t_{P_2}, \mathbf{r}_{P_2}) \rangle_0 \dots \langle \phi_{P_{2n-1}}(t_{P_{2n-1}}, \mathbf{r}_{P_{2n-1}}) \phi_{P_{2n}}(t_{P_{2n}}, \mathbf{r}_{P_{2n}}) \rangle_0 \end{aligned}$$

2. We have the statement

$$\left\langle \underbrace{\phi \dots \phi}_n \underbrace{\tilde{\phi} \dots \tilde{\phi}}_m \right\rangle_0 = 0 \quad (3.107)$$

unless $n = m$. This is due to the antidiagonal structure of \mathbf{A} and can be seen by performing the Gaussian integral (see for instance [226], chapter 4) explicitly and taking care of the fact, that the inverse matrix \mathbf{A}^{-1} is antidiagonal again. For the new version of LSI, this can be justified in a more satisfying way by using the generalisation of the Bargmann superselection rule.

With these tools at hand we can demonstrate, quite analogous to the non-conserved case [192] an exact reduction of any average to an average computed only with the noiseless theory. For example, for the two-time response function, we have

$$R(t, s) = \langle \phi(t) \tilde{\phi}(s) \rangle = \langle \phi(t) \tilde{\phi}(s) e^{-\mathcal{J}_b[\tilde{\phi}]} \rangle_0 = \langle \phi(t) \tilde{\phi}(s) \rangle_0 \quad (3.108)$$

In going to the last line, we have expanded the exponential and use that because of Wick's theorem any $2n$ -point function can be rewritten as a sum over a product of n two-time functions which in turn are determined by the Bargman rules. From the special structure of $J_b[\tilde{\phi}]$ it follows that only a single term of the entire series remains. As a consequence, the two-time response function does not depend explicitly on the noise. A similar result holds for the correlation function, see subsection 3.2.5. We shall now first consider the noise-free theory and find the two-point function from the dynamical symmetry. Afterwards, we shall show that the two-point functions of the full noisy theory can be reconstructed from this case.

The response function of the noise-free theory

First, we consider the linear response function of the order-parameter with respect to an external magnetic field h

$$R(t, s; \mathbf{x} - \mathbf{y}) := \left. \frac{\delta \langle \phi(t, \mathbf{x}) \rangle}{\delta h(s, \mathbf{y})} \right|_{h=0} \quad (3.109)$$

As already mentioned in the previous section, we choose here, and in contrast to [207], a perturbation respecting the conservation law, which means that we have to add the term $\nabla_{\mathbf{R}}^2 h$ to the Langevin equation (3.97) or the term $-\int d\mathbf{R} du h \nabla_{\mathbf{R}}^2 \tilde{\phi}$ to the action (3.99). Then it is easy to see that the response function (3.109) is given by

$$R(t, s; \mathbf{x} - \mathbf{y}) = \langle \phi(t, \mathbf{x}) \nabla_{\mathbf{y}}^2 \tilde{\phi}(s, \mathbf{y}) \rangle \quad (3.110)$$

We make the important assumption that the field $\phi(t, \mathbf{r})$, characterised by the parameters μ and γ and the scaling dimension x , is quasiprimary. As suggested in [109, 192] we consider also the response field $\tilde{\phi}(t, \mathbf{r})$ to be quasiprimary, with parameters $\tilde{\mu} = -\mu$ and $\tilde{\gamma} = -\gamma$ but the same scaling dimension $\tilde{x} = x$.

We can concentrate on the model with $v = 0$ for the following reason: Suppose $\phi(\mathbf{r}, t)$ is a solution of equation (3.97) with $\eta = 0$. Then we define

$$\Psi(t, \mathbf{r}) := \exp\left(\frac{1}{16\mu} \int_0^t d\tau v(\tau) \nabla_{\mathbf{r}}^2\right) \phi(t, \mathbf{r}). \quad (3.111)$$

$\Psi(t, \mathbf{r})$ fulfils the following dynamical equation

$$\partial_t \Psi(t, \mathbf{r}) = \frac{1}{16\mu} \nabla_{\mathbf{r}}^4 \Psi(t, \mathbf{r}), \quad (3.112)$$

which is the same equation with $v = 0$. It suffices thus to consider the problem with $v = 0$ and then to apply the inverse of the gauge transformation (3.111) for treating the case $v \neq 0$. In this way, the breaking of time-translation invariance is implemented.

The case $v = 0$

This case is relevant for $d > 4$ in the spherical model and for any d in the Mullins-Herring model. We compute (3.110) for the noise-free theory, taking translation-invariance into account. Then the response function is given by

$$R_0(t, s; \mathbf{r}) = \nabla_{\mathbf{r}}^2 F^{(2)}(t, s, \mathbf{r}) \quad (3.113)$$

where the two-point function $F^{(2)}(t, s, \mathbf{r})$ has been computed in the last subsection. We obtain, with the scaling variable $u = |\mathbf{r}|(t - s)^{-1/4}$

$$\begin{aligned} R_0(t, s; \mathbf{r}) &= (t - s)^{-(x+1)/2} (u^{1-d} \partial_u (u^{d-1} \partial_u)) \sum_{s \in \mathcal{E}'} c_s \phi^{(s)}(u) \\ &= (t - s)^{-(x+1)/2} \sum_{s \in \mathcal{E}''} \widehat{c}_s \widehat{\phi}^{(s)}(u) \end{aligned} \quad (3.114)$$

where \widehat{c}_s are constants, \mathcal{E}'' the set of admissible values for s given below, and the solutions $\widehat{\phi}^{(s)}$ are given by

$$\widehat{\phi}^{(s)}(u) = u^{s-6} \sum_{\ell=0}^{\infty} \widehat{b}_{\ell}^{(s)} u^{4\ell} \quad (3.115)$$

with the coefficients

$$\widehat{b}_{\ell}^{(s)} = (-\mu)^{\ell} \frac{\Gamma(\frac{s}{2} + 1) \Gamma(\frac{s}{2} + \frac{d}{2})}{\Gamma(\frac{s+d}{4} - \frac{1}{2} - \frac{\gamma}{\mu})} \cdot \frac{\Gamma(\ell + \frac{s+d}{4} - \frac{1}{2} - \frac{\gamma}{\mu})}{\Gamma(2\ell + \frac{s}{2} - 2) \Gamma(2\ell + \frac{s}{2} + \frac{d}{2} - 3)} \quad (3.116)$$

A priori, s could take the values $s \in \{2, 4, 2 - d, 4 - d\} \setminus \{-2, -4, \dots\}$ as derived in appendix B of [19]. However, certain values of s have to be excluded, since the solution has to be regular for $u \rightarrow 0$ and has to vanish for $u \rightarrow \infty$. By inspection of the coefficients $\widehat{b}_{\ell}^{(s)}$ one finds, in a similar way as done at the end of appendix B of [19]:

$$\mathcal{E}'' := \begin{cases} \{2, 4\} & \text{if } d \geq 4 \\ \{2, 4, 2 - d\} & \text{if } 2 < d < 4 \\ \{2, 4, 2 - d, 4 - d\} & \text{if } d \leq 2 \end{cases} \quad (3.117)$$

In the specific example of the spherical model it turns out that $\frac{\gamma}{\mu} = \frac{1}{2}$. Then the solution with $s = 4 - d \in \mathcal{E}''$ disappears and is no longer admissible for $d \leq 2$.

For completeness, we rewrite the solutions $\phi^{(s)}(u)$ as hypergeometric functions for the admissible s , suppressing some constant prefactors which can be absorbed into the constants \widehat{c}_s .

$$\widehat{\phi}^{(2)}(u) = {}_1F_3 \left(1 + \frac{d}{4} - \frac{\gamma}{\mu}; \frac{1}{2}, \frac{d}{4}, \frac{1}{2} + \frac{d}{4}; -\frac{\mu u^4}{16} \right) \quad (3.118)$$

$$\widehat{\phi}^{(4)}(u) = \left(-\frac{\mu u^4}{16} \right)^{1/2} {}_1F_3 \left(\frac{3}{2} + \frac{d}{4} - \frac{\gamma}{\mu}; \frac{3}{2}, \frac{1}{2} + \frac{d}{4}, 1 + \frac{d}{4}; -\frac{\mu u^4}{16} \right) \quad (3.119)$$

$$\widehat{\phi}^{(2-d)}(u) = \left(-\frac{\mu u^4}{16} \right)^{1-d/4} {}_1F_3 \left(2 - \frac{\gamma}{\mu}; \frac{3}{2} - \frac{d}{4}, 2 - \frac{d}{4}, \frac{3}{2}; -\frac{\mu u^4}{16} \right) \quad (3.120)$$

$$\widehat{\phi}^{(4-d)}(u) = \left(-\frac{\mu u^4}{16} \right)^{(2-d)/4} {}_1F_3 \left(\frac{3}{2} - \frac{\gamma}{\mu}; 1 - \frac{d}{4}, \frac{3}{2} - \frac{d}{4}, \frac{1}{2}; -\frac{\mu u^4}{16} \right) \quad (3.121)$$

The constants \widehat{c}_s are not completely arbitrary for the case $\mu < 0$, but have to be arranged so that $\widehat{\phi}(u) \rightarrow 0$ for $u \rightarrow \infty$. From [232, 233], one knows the asymptotic behaviour of the hypergeometric functions. In general, there is an infinite series of terms growing exponentially with u , together with terms falling off algebraically. The leading term of the exponentially growing series can be eliminated by imposing the following condition on the coefficients

$$\begin{aligned} & c_2 \frac{\Gamma(\frac{1}{2})\Gamma(\frac{d}{4})\Gamma(\frac{1}{2} + \frac{d}{4})}{\Gamma(1 + \frac{d}{4} - \frac{\gamma}{\mu})} + c_4 \frac{\Gamma(\frac{3}{2})\Gamma(\frac{1}{2} + \frac{d}{4})\Gamma(1 + \frac{d}{4})}{\Gamma(\frac{3}{2} + \frac{d}{4} - \frac{\gamma}{\mu})} \\ & + c_{2-d} \frac{\Gamma(\frac{3}{2} - \frac{d}{4})\Gamma(2 - \frac{d}{4})\Gamma(\frac{3}{2})}{\Gamma(2 - \frac{\gamma}{\mu})} + c_{4-d} \frac{\Gamma(1 - \frac{d}{4})\Gamma(\frac{3}{2} - \frac{d}{4})\Gamma(\frac{1}{2})}{\Gamma(\frac{3}{2} - \frac{\gamma}{\mu})} = 0 \end{aligned} \quad (3.122)$$

Here, some of the constants \widehat{c}_s might have to be set to zero, if the corresponding value of s is not admissible. Indeed, the condition (3.122) is sufficient to cancel the *entire* exponentially growing series and the remaining part decreases algebraically, but we shall not prove this here. The most important case for us is $c_{2-d} = c_{4-d} = 0$. In this case (3.122) implies the relation $c_2 = -\frac{\Gamma(\frac{d}{4} + \frac{1}{2})}{\Gamma(\frac{d}{4} + \frac{3}{2} - \frac{\gamma}{\mu})} \frac{c_4}{2}$ and it is easy to show that (see appendix B of [19] for the details)

$$\begin{aligned} R_0(t, s; \mathbf{r}) &= \nabla_{\mathbf{r}}^2 F^{(2)}(t, s, \mathbf{r}) \\ &= r_0(t-s)^{-(x+1)/2} \int \frac{d\mathbf{k}}{(2\pi)^d} (k^2)^{2-\frac{2\gamma}{\mu}} \exp\left(-i\frac{\mathbf{k} \cdot \mathbf{r}}{(t-s)^{1/4}}\right) \exp(-k^4) \end{aligned} \quad (3.123)$$

This prediction of LSI with $z = 4$ is perfectly consistent with the exact results (3.79) and (3.82) of the conserved spherical model for the case $d > 4$ if we set $\frac{\gamma}{\mu} = \frac{1}{2}$ and $x = \frac{d}{2}$. The case $d < 4$ in the spherical model (where we have $v \neq 0$) will be treated next.

The case $v \neq 0$

In this case, the response function is given by

$$R(t, s; \mathbf{r}) = \exp(\xi_{t,s}) \nabla_{\mathbf{r}}^2 \nabla_{\mathbf{r}}^2 F^{(2)}(t, s, \mathbf{r}) \quad (3.124)$$

where we have defined $\xi_{t,s} := -\frac{1}{16\mu} \int_s^t d\tau v(\tau)$ using the fact that $\widetilde{\phi}$ is characterised by the parameters $-\mu$ and $-\gamma$. Therefore, remembering $u = |\mathbf{r}|(t-s)^{-1/4}$

$$R_0(t, s, \mathbf{r}) = r_0(t-s)^{-(x+1)/2} \sum_{n=0}^{\infty} \frac{(\xi_{t,s}(t-s)^{-\frac{1}{2}})^n}{n!} (\nabla_u^2)^n \sum_{s \in \mathcal{E}''} \widehat{c}_s \widehat{\phi}^{(s)}(u) \quad (3.125)$$

where $\nabla_u^2 = u^{1-d} \partial_u (u^{d-1} \partial_u)$ and the $\widehat{\phi}^{(s)}(u)$ have been given in the preceding subsection. We now make the following assumption, following the idea suggested in [192]: If we want to have scaling behaviour, we need that ⁹

$$\int_0^t d\tau v(\tau) \stackrel{t \rightarrow \infty}{\sim} \kappa_0 t^{F_2} \quad (3.126)$$

⁹Notice that the definition for F_2 differs from (2.146)

at least for long times, which implies $\xi_{t,s} \sim -\frac{1}{16\mu}\kappa_0(t^{F_2} - s^{F_2})$. Evaluating the expression (3.125), we find

$$R_0(t, s; \mathbf{r}) = r_0(t-s)^{-(x+1)/2} \sum_{s \in \mathcal{E}''} \widehat{c}_s \sum_{\ell, n=0}^{\infty} \frac{(\xi_{t,s}(t-s)^{-\frac{1}{2}})^n}{n!} 2^{2n} \widehat{b}_\ell^{(s)} \\ \times \frac{\Gamma(2\ell + \frac{s}{2} - 2)\Gamma(2\ell + \frac{s}{2} - 3 + \frac{d}{2})}{\Gamma(2\ell + \frac{s}{2} - 2 - n)\Gamma(2\ell + \frac{s}{2} - n - 3 + \frac{d}{2})} u^{4\ell + s - 2n - 6} \quad (3.127)$$

Now we introduce $u = |\mathbf{r}|(t-s)^{-1/4}$ and $\xi_{t,s} \sim -\frac{1}{16\mu}\kappa_0(t^{F_2} - s^{F_2})$ into this expression. By changing the summation variables from n and ℓ to $k := 4\ell - 2n + s - 6$ and ℓ one can then read off the dynamical exponent, which is given by

$$z = \frac{2}{F_2}. \quad (3.128)$$

The critical exponent z is therefore determined by the behaviour of the potential $v(\tau)$. However, as we shall see later when treating the correlation function, only a value of $F_2 = \frac{1}{2}$ leads to scaling behaviour of the correlation function. Nevertheless we keep F_2 arbitrary for now and proceed with the autoresponse function $R(t, s) = R(t, s; \mathbf{0})$, which can be obtained from (3.127) by setting $u = 0$. All nonvanishing terms have to satisfy the condition $4\ell + s - 2n - 6 = 0$, which excludes in particular odd values of s . Therefore only the contributions from the values $s = 2$ and $s = 4$ remain and the result for $R(t, s)$ is

$$R_0(t, s) = (t-s)^{-(x+1)/2} [\widetilde{c}_2 g^{(2)}(t, s) + \widetilde{c}_4 g^{(4)}(t, s)]. \quad (3.129)$$

\widetilde{c}_2 and \widetilde{c}_4 are parameters and the expressions $g^{(2)}(t, s)$ and $g^{(4)}(t, s)$ are given by

$$g^{(2)}(t, s) = {}_1F_1 \left(1 + \frac{d}{4} - \frac{\gamma}{\mu}; \frac{1}{2}; -4\mu \frac{\xi_{t,s}^2}{t-s} \right) \\ g^{(4)}(t, s) = (-4\mu \xi_{t,s}^2 (t-s)^{-1})^{\frac{1}{2}} {}_1F_1 \left(\frac{3}{2} + \frac{d}{4} - \frac{\gamma}{\mu}; \frac{3}{2}; -4\mu \frac{\xi_{t,s}^2}{t-s} \right) \quad (3.130)$$

Note that we can write

$$\frac{\xi_{t,s}^2}{t-s} = s^{2F_2-1} \left(\frac{(y^F - 1)^2}{y-1} \right) \quad (3.131)$$

with $y = t/s$. For future extension it is instructive to consider the different asymptotic behaviour implied by F_2 , which we carry out in appendix C of [19]. Here we check only that our theory is in line with the exact results of the conserved spherical model as derived in section 3.2.2. If we choose $c_2 = -\frac{\Gamma(\frac{d}{4} + \frac{1}{2})}{\Gamma(\frac{d}{4} + \frac{3}{2} - \frac{2}{\mu})} \frac{c_4}{2}$ and $c_{2-d} = c_{4-d} = 0$, we have seen in the last subsection that the expression $\nabla_{\mathbf{r}}^2 F^{(2)}(t, s, \mathbf{r})$ can be written as an integral (see (3.123)). On this integral representation, we apply formula (3.124). We also recall the fact that $\exp(\xi_{t,s} \nabla_{\mathbf{r}}^2) e^{ikr} = e^{ikr - \xi_{t,s} k^2}$. It then follows from a straightforward computation that the result (3.79) is reproduced correctly for $\kappa_0 = -\mathbf{g}_d$.

3.2.5 Response and correlation function in the noisy theory (old version of LSI)

The response function

We use the decomposition (3.2.4) and expand around the noise-free theory. Because of (3.107), we find that the response function is equal to the noise-free response function, derived in the last subsection

$$R(t, s; \mathbf{r}) = R_0(t, s; \mathbf{r}) \quad (3.132)$$

Therefore, we can take over the results already discussed in the last subsection. In particular, we can conclude that the form of the two-time response function in the critical spherical model with conserved order-parameter agrees with the prediction of local scale-invariance.

The correlation function

For the correlation function, the following terms remain (as usual $\mathbf{r} = \mathbf{x} - \mathbf{y}$)

$$\begin{aligned} C(t, s; \mathbf{r}) &= -\frac{T}{16\mu} \int du d\mathbf{R} \left\langle \phi(t, \mathbf{x}) \phi(s, \mathbf{y}) \tilde{\phi}(u, \mathbf{R}) \nabla_{\mathbf{R}}^2 \tilde{\phi}(u, \mathbf{R}) \right\rangle_0 \\ &\quad + \frac{a_0}{2} \int d\mathbf{R} \left\langle \phi(t, \mathbf{x}) \phi(s, \mathbf{y}) \tilde{\phi}^2(0, \mathbf{R}) \right\rangle_0 \end{aligned} \quad (3.133)$$

where we have assumed uncorrelated initial conditions, that is

$$\langle \phi(\mathbf{R}, 0) \phi(\mathbf{R}', 0) \rangle = a_0 \delta(\mathbf{R} - \mathbf{R}') \quad (3.134)$$

We denote the first term on the right-hand side of (3.133) by $C_1(t, s; \mathbf{r})$ and the second term by $C_2(t, s; \mathbf{r})$. Unfortunately, we do not have an expression for the three- and four-point functions. However, we can use Wick's theorem and the Bargmann superselection rule, which leads to

$$\begin{aligned} C_1(t, s; \mathbf{r}) &= -\frac{T}{16\mu} \int_0^s du \int d\mathbf{R} \left\langle \phi(t, \mathbf{x}) \tilde{\phi}(u, \mathbf{R}) \right\rangle_0 \nabla_{\mathbf{R}}^2 \left\langle \phi(s, \mathbf{y}) \tilde{\phi}(u, \mathbf{R}) \right\rangle_0 \\ &\quad - \frac{T}{16\mu} \int_0^s du \int d\mathbf{R} \nabla_{\mathbf{R}}^2 \left\langle \phi(t, \mathbf{x}) \tilde{\phi}(u, \mathbf{R}) \right\rangle_0 \left\langle \phi(s, \mathbf{y}) \tilde{\phi}(u, \mathbf{R}) \right\rangle_0 \end{aligned} \quad (3.135)$$

and

$$C_2(t, s; \mathbf{r}) = a_0 \int d\mathbf{R} \left\langle \phi(t, \mathbf{x}) \tilde{\phi}(0, \mathbf{R}) \right\rangle_0 \left\langle \phi(s, \mathbf{y}) \tilde{\phi}(0, \mathbf{R}) \right\rangle_0 \quad (3.136)$$

Under the integrals, we always find two sorts of factors: The two-point function $F^{(2)}(t, s; \mathbf{r}) = \langle \phi(t, \mathbf{x}) \tilde{\phi}(s, \mathbf{y}) \rangle$ was computed in appendix A of [19] and reads ($\mathbf{r} = \mathbf{x} - \mathbf{y}$ and $u = |\mathbf{r}|(t - s)^{-1/4}$)

$$F^{(2)}(t, s; \mathbf{r}) = (t - s)^{-x/2} \sum_{s \in \mathcal{E}'} c_s \phi^{(s)}(u) \quad (3.137)$$

and the response function $R_0(t, s, \mathbf{r}) = \langle \phi(t, \mathbf{x}) (\nabla_{\mathbf{y}})^2 \tilde{\phi}(s, \mathbf{y}) \rangle$ as computed in the previous subsection

$$R_0(t, s; \mathbf{r}) = (t - s)^{-(x+1)/2} \sum_{s \in \mathcal{E}''} \widehat{c}_s \widehat{\phi}^{(s)}(u) \quad (3.138)$$

When we introduce the expressions (3.137) and (3.138) with the appropriate arguments into (3.135) and (3.136) we get the most general form of the correlation function fixed by LSI with $z = 4$.

We now show, that this result is compatible with the exactly known result for $C(t, s; \mathbf{r})$ of the conserved spherical model as derived in subsection 3.2.2. From the response function, we have already seen that we need to make the choice $c_{2-d} = c_{4-d} = 0$ and $c_2 = -\frac{\Gamma(\frac{d}{4} + \frac{1}{2})}{\Gamma(\frac{d}{4} + \frac{3}{2} - \frac{\gamma}{\mu})} \frac{c_4}{2}$. Then we have the integral representation (3.123) for $R(t, s; \mathbf{r})$ to which one can still apply the gauge transform (3.111). For $F^{(2)}(t, s, \mathbf{r})$ one can find in the same way an integral representation, so that we have the following two expressions:

$$F^{(2)}(t, s; \mathbf{r}) = (t-s)^{-x/2} \int \frac{d\mathbf{k}}{(2\pi)^d} (k^2)^{1-\frac{2\gamma}{\mu}} \exp\left(-\frac{\mathbf{i}\mathbf{k} \cdot \mathbf{r}}{(t-s)^{1/4}}\right) \times \exp\left(-k^4 + \frac{k^2}{16\mu} \kappa_0 \left(\frac{t_2^F - s_2^F}{(t-s)^{1/2}}\right)\right) \quad (3.139)$$

$$R_0(t, s; \mathbf{r}) = (t-s)^{-(x+1)/2} \int \frac{d\mathbf{k}}{(2\pi)^d} (k^2)^{2-\frac{2\gamma}{\mu}} \exp\left(-\frac{\mathbf{i}\mathbf{k} \cdot \mathbf{r}}{(t-s)^{1/4}}\right) \times \exp\left(-k^4 + \frac{k^2}{16\mu} \kappa_0 \left(\frac{t_2^F - s_2^F}{(t-s)^{1/2}}\right)\right) \quad (3.140)$$

Using these representations, we obtain

$$C_1(t, s; \mathbf{r}) = -\frac{T}{8\gamma} s^{\frac{d}{4} - \frac{2\gamma}{\mu} - x + \frac{3}{2}} \int_0^1 d\theta (y - \theta)^{\frac{d}{4} + \frac{1}{2} - \frac{\gamma}{\mu} - \frac{x}{2}} (1 - \theta)^{\frac{d}{4} + \frac{1}{2} - \frac{\gamma}{\mu} - \frac{x}{2}} \times (y + 1 - 2\theta)^{-\frac{d}{4} - 2 + \frac{2\gamma}{\mu}} \int \frac{d\mathbf{k}}{(2\pi)^d} \exp\left(-\frac{\mathbf{i}\mathbf{k} \cdot \mathbf{r}}{(t+s-2s\theta)^{1/4}}\right) (k^2)^{3-\frac{4\gamma}{\mu}} \times \exp\left(-k^4 + \frac{k^2}{16\mu} \kappa_0 \frac{t_2^F + s_2^F - 2(s\theta)_2^F}{(t+s-2s\theta)^{1/2}}\right) \quad (3.141)$$

$$C_2(t, s; \mathbf{r}) = a_0 (t+s)^{-\frac{d}{4} - 1 + \frac{2\gamma}{\mu}} (ts)^{\frac{d}{4} + \frac{1}{2} - \frac{\gamma}{\mu} - \frac{x}{2}} \int \frac{d\mathbf{k}}{(2\pi)^d} \exp\left(-\frac{\mathbf{i}\mathbf{k} \cdot \mathbf{r}}{(t+s)^{1/4}}\right) (k^2)^{2-\frac{4\gamma}{\mu}} \times \exp\left(-k^4 + \frac{k^2}{16\mu} \kappa_0 \frac{t_2^F + s_2^F}{(t+s)^{1/2}}\right) \quad (3.142)$$

where we have used the fact that the integration over \mathbf{R} gives a delta function. In order to compare with the exact results eqs. (5.137,5.138), we see directly that we have the equalities $A_1(t, s; \mathbf{r}) = C_2(t, s; \mathbf{r})$ and $A_2(t, s; \mathbf{r}) = C_1(t, s; \mathbf{r})$ for $x = \frac{d}{2}$, $\mu = -\frac{1}{16}$ and $\frac{\gamma}{\mu} = \frac{1}{2}$ and $F_2 = \frac{1}{2}$. Our symmetry-based approach has thus reproduced all the results from subsection 3.2.2, up to an identification of parameters.

3.2.6 Response and correlation function in the noisy theory (new version of LSI)

In order to compare with the new version of LSI as introduced in chapter 2 we have to make a few slight adjustments to the considerations made in chapter 2. We recall that (3.66) and (3.67) differ from the dynamical equation considered in chapter 2 in the following points:

1. The Lagrangian multiplier is included in a slightly different way than in (2.78), namely with an additional $-\nabla_{\mathbf{r}}^2$ in front of it. This entails that the gauge transform takes a different form. Instead of relation (2.80), one has to use (3.111)
2. The perturbation term is included as $-\nabla_{\mathbf{r}}^2 h(t, \mathbf{r})$ into the Langevin equation, which means that the perturbation respects the conservation law (conserving perturbation).
3. For the second moment of the noise we have chosen here

$$\langle \eta(t, \mathbf{x}) \eta(t', \mathbf{x}') \rangle = -2T_c \nabla_{\mathbf{x}}^2 \delta(t - t') \delta(\mathbf{x} - \mathbf{x}'). \quad (3.143)$$

This means from a physical point of view that the noise does not destroy the conservation law (conserving noise). Taking spatial translation-invariance into account, this amounts in Fourier space to

$$\langle \eta(t, \mathbf{k}) \eta(t', -\mathbf{k}) \rangle = 2T_c \mathbf{k}^2 \delta(t - t'). \quad (3.144)$$

We have shown in the previous subsections, that points 1 and 2 entail for the response function that (3.124)

$$R(t, s; \mathbf{r}) = \exp \left(-1/(16\mu) \int_s^t d\tau v(\tau) \nabla_{\mathbf{r}}^2 \right) \nabla_{\mathbf{r}}^2 F^{(2)}(t, s; \mathbf{r}) \quad (3.145)$$

where $F^{(2)}(t, s; \mathbf{r})$ is the two-point function (2.109) determined by the new version of LSI. As outlined earlier, we suppose also that $\int_0^t d\tau v(\tau) \stackrel{t \rightarrow \infty}{\sim} \kappa_0 t^{F^2}$. Using for $F^{(2)}(t, s; \mathbf{r})$ expression (2.109) one realises first, that the factor $\exp \left(-1/(16\mu) \int_s^t d\tau v(\tau) \nabla_{\mathbf{r}}^2 \right)$ simply amounts to a factor $\exp \left(1/(16\mu) \int_s^t \tau v(\tau) k^2 \right)$ in Fourier-space and the term $\nabla_{\mathbf{r}}^2$ to an extra factor k^2 . In this way, one finds that (3.145) together with (2.109) leads to the following prediction for the response function

$$\begin{aligned} R(t, s; \mathbf{r}) &= s^{-a-1} \left(\frac{t}{s} \right)^{1+a'-\lambda_R/z} \left(\frac{t}{s} - 1 \right)^{-1-a'} \\ &\times \int_{\mathbb{R}^d} \frac{d\mathbf{k}}{(2\pi)^d} |\mathbf{k}|^{2+2\beta} \exp \left(-\frac{\mathbf{i}\mathbf{k} \cdot \mathbf{r}}{(t-s)^{1/4}} \right) \exp(-\alpha |\mathbf{k}|^z) \end{aligned} \quad (3.146)$$

where in this case, the ageing exponents are connected to the scaling dimensions via

$$\begin{aligned} a+1 &= \frac{2}{z}(x + \tilde{x}) + \frac{2}{z}, & a'+1 &= \frac{1}{z}((2\xi + x) + (2\tilde{\xi} + \tilde{x})) + \frac{2}{z} \\ \frac{\lambda_R}{z} &= \frac{2}{z}(\xi + x) + \frac{2}{z} \end{aligned} \quad (3.147)$$

This reproduces exactly (3.79) if we identify

$$\begin{aligned} z &= 4, & F_2 &= 1/2, & \gamma/\mu &= \frac{1}{2} \quad (\Leftrightarrow \beta = 0), & a = a' &= d/4 - 1/2 \\ \kappa_0 &= -\mathbf{g}_d, & \alpha &= 1 \quad (\Leftrightarrow \mu = -1/16), & \lambda_R &= d+2 \end{aligned} \quad (3.148)$$

Point 3 entails a change in correlation function predicted by LSI. We can use expression (3.133) and take into account that the four-point function for a nonvanishing potential is given by

$$\begin{aligned} \langle \phi(t, \mathbf{x}) \phi(s, \mathbf{y}) \tilde{\phi}(u, \mathbf{R}) \tilde{\phi}(u', \mathbf{R}') \rangle &= \exp \left(-1/(16\mu) \left(\int_0^t d\tau v(\tau) \nabla_{\mathbf{x}}^2 + \int_0^s d\tau v(\tau) \nabla_{\mathbf{y}}^2 \right) \right) \\ &\exp \left(1/(16\mu) \left(\int_0^u d\tau v(\tau) \nabla_{\mathbf{R}}^2 + \int_0^{u'} d\tau v(\tau) \nabla_{\mathbf{R}'}^2 \right) \right) F^{(4)}(t, s, u, u'; \mathbf{x}, \mathbf{y}, \mathbf{R}, \mathbf{R}') \end{aligned} \quad (3.149)$$

and similarly for the three-point function with nonvanishing potential. We have already taken into account that the mass of $\tilde{\phi}$ is given by

$$\tilde{\mu} = -\mu \quad (3.150)$$

$F^{(4)}(t, s, u, u'; \mathbf{x}, \mathbf{y}, \mathbf{R}, \mathbf{R}')$ is the four-point function as computed in subsection 2.4 of chapter 2. It is then straightforward but somewhat tedious to verify that formula (2.171) gets modified to

$$\begin{aligned} C_{th}(t, s; \mathbf{r}) &= 2Tc_0 s^{-b_{th} + \frac{2\beta}{z} + \frac{d}{z} + \frac{2}{z}} y^{\frac{2\xi}{z}} (y-1)^{2(1+a') - 2(\lambda_R/z) + b'_{th} - \frac{4}{z}\xi} \quad (3.151) \\ &\times \int_0^1 d\theta \theta^{\frac{4}{z}\tilde{\xi}_2} (y-\theta)^{\frac{2\xi}{z} + \frac{\lambda_R}{z} - 2(1-a') + \frac{\beta}{z} + \frac{d}{z} - b'_{th}} \times (1-\theta)^{\frac{2\xi}{z} + \frac{\lambda_R}{z} - 2(1-a') + \frac{\beta}{z} + \frac{d}{z} - b'_{th}} g \left(\frac{1-\theta-y}{y} \frac{\theta}{1-\theta} \right) \\ &\times \int_{\mathbb{R}^d} \frac{d\mathbf{k}}{(2\pi)^d} e^{-i\mathbf{k}\cdot\mathbf{r}} |\mathbf{k}|^{2\beta+2} \exp \left(-\frac{|\mathbf{k}|^z s}{z^2 \mu i^{2-z}} (y+1-2\theta) - \kappa_0 |\mathbf{k}|^2 (t^{F^2} + s^{F^2} - 2u^{F^2}) \right) \end{aligned}$$

Here b'_{th} is given by the same expression as in (2.172), whereas b_{th} is in this case related to the scaling dimensions via

$$b_{th} = \frac{2}{z}(x + \tilde{x}_2) - 1 - \frac{d}{z} + \frac{2}{z} \quad (3.152)$$

instead of (2.172). LSI reproduces correctly the result (3.76) if we set $g(u) = 1$, with the parameters (3.148) and (3.150) and the choice

$$\xi = \tilde{\xi} = \tilde{\xi}_2 = 0, \quad x = \tilde{x} = \tilde{x}_2 = \frac{d}{2} \quad (\Leftrightarrow b_{th} = d/4 - 1/2), \quad b'_{th} = 0 \quad (3.153)$$

This can be seen by scaling out the factor $s(y+1-2\theta)$ from the integral over \mathbf{k} in (3.151). Then, with the given identification, (3.151) reduces exactly to (3.76).

In a similar way, equation (2.156) for the preparation part gets modified to

$$\begin{aligned} C_{init}(t, s; \mathbf{r}) &= c_0 s^{-2(2\tilde{\xi} + x + \tilde{x})/z + 2\beta/z + 2d/z} y^{-2(\tilde{x} + 2\tilde{\xi} - \xi)/z + \beta/z + d/z} (y-1)^{-2(x-\tilde{x})/z - 4(\xi-\tilde{\xi})/z} \\ &\times \int_{\mathbb{R}^d} \frac{d\mathbf{k}}{(2\pi)^d} |\mathbf{k}|^{2\beta} \exp \left(-\alpha |\mathbf{k}|^z (t+s) - \kappa_0 |\mathbf{k}|^2 (t^{F^2} + s^{F^2}) \right) e^{i\mathbf{r}\cdot\mathbf{k}} \hat{a}(\mathbf{k}) \end{aligned} \quad (3.154)$$

which reduces to the subleading part (3.75) for the choices (3.148) and (3.153).

model	a	b	λ_R	λ_C	Reference
cons. spherical	$d/4 - 1/2$	$d/4 - 1/2$	$d + 2$	$d + 2$	[45, 19]
cons. Mullins-Herring	$d/4 - 1/2$	$d/4 - 1/2$	$d + 2$	$d + 2$	[45, 19]
non-cons. Mullins-Herring	$d/4 - 1$	$d/4 - 1$	d	d	[207]

Table 3.2: Exponents $a, b, \lambda_R, \lambda_C$ of the conserved spherical model and the Mullins-Herring model at criticality. For all models, the dynamical exponent is $z = 4$.

3.2.7 Conclusions of this section

In this section, we have been exploring the idea presented in chapter 2 that dynamical scaling might be generalisable to a larger algebraic structure of local scale-transformations. Since values of z quite distinct from two can be obtained for a conserved order-parameter, this motivated our choice to study the kinetics of such systems. The spherical model, quenched to $T = T_c$ from a fully disordered initial state and the Mullins-Herring model with conserved noise are useful first tests, since their scaling behaviour is non-trivial, yet the models do remain analytically treatable.

We have shown, that both the old version LSI and the new version presented in chapter 2 are fully compatible with the exactly known results in the spherical model. Together with the Mullins-Herring growth model, these are the first analytically solved examples which confirm LSI for a dynamical exponent $z = 4$.¹⁰ In table 3.2 we collect the values of the exponents of the conserved spherical model and the conserved and the non-conserved Mullins-Herring models.

That confirmation was possible because the deterministic part of the Langevin equation is still a linear equation. Numerical simulations in models where this is no longer so will inform us to what extent LSI with $z \neq 2$ can be confirmed in a more general context.

3.3 Spherical model with long-range interactions

3.3.1 Introduction

The two examples considered in sections 3.1 and 3.2 both provided examples for models with $z = 4$. The results of these models are reproduced by both versions of LSI. In this section, we look at the spherical model with long-range interactions, which provides an example for a model where z takes a value between 0 and 2. In this model, only the 'new' version of LSI, proposed in chapter 2 reproduces the right result.

Generalising expressions (1.11) and (1.12), we define response- and correlation functions

$$R(t, s) = \left. \frac{\delta \langle \mathcal{O}(t, \mathbf{r}) \rangle}{\delta h(s, \mathbf{r})} \right|_{h=0} = s^{-a-1} f_R \left(\frac{t}{s} \right), \quad f_R(y) \stackrel{y \rightarrow \infty}{\sim} y^{-\lambda_R/z}, \quad (3.155)$$

$$C(t, s) = \langle \mathcal{O}(t, \mathbf{r}) \mathcal{O}(s, \mathbf{r}) \rangle = s^{-b} f_C \left(\frac{t}{s} \right), \quad f_C(y) \stackrel{y \rightarrow \infty}{\sim} y^{-\lambda_C/z}, \quad (3.156)$$

¹⁰Another example of a system with a dynamical exponent far from 2 which appears to be compatible with LSI is the bond-diluted 2D Ising-model quenched to $T < T_c$ [121].

where the observable $\mathcal{O}(t, \mathbf{r})$ (at time t and location \mathbf{r}) can be the order-parameter $\phi(t, \mathbf{r})$ as before, but in this section, we shall also study composite fields such as the energy density. We denote by h the field conjugate to \mathcal{O} (and when \mathcal{O} is the order-parameter the conjugate field h is the associated magnetic field). The dynamical scaling forms (3.155,3.156) are expected to hold in the scaling limit where both $t, s \gg t_{\text{micro}}$ and also $t - s \gg t_{\text{micro}}$, where t_{micro} is some microscopic time scale. In writing eqs. (3.155,3.156), it is implicitly assumed that the underlying dynamics is such that there is a single relevant length-scale $L = L(t) \sim t^{1/z}$, where z is the dynamical exponent. Non-equilibrium universality classes are distinguished by different values of exponents such as $a, b, \lambda_C, \lambda_R$ (which will depend on the observable \mathcal{O} and the field h used and also on whether $T < T_c$ or $T = T_c$). For reviews, see [37, 94, 45, 60, 122].

All existing tests for $z \neq 2$, except the two cases with $z =$ discussed in sections 3.1 and 3.2, merely tested the LSI prediction for the autoresponse function, and this for the order-parameter *only*, see [124, 125] for a detailed discussion.

A fuller picture on the validity of the several technical assumptions which are needed for the precise formulation of the theory of local scale-invariance (LSI) can only come from more systematic tests of its predictions. To this end, we shall study in this section the ageing behaviour of the spherical model with long-range interactions. It was shown by Cannas, Stariolo and Tamarit [48] that for quenches to $T < T_c$, if the exchange couplings decay sufficiently slowly with the distance then the dynamical exponent z becomes a continuous function of the control parameters of the model and that the scaling forms (3.155,3.156) hold for the order-parameter. Here we shall also extend these considerations to the critical case $T = T_c$ and shall further look at further look at the scaling behaviour of composite operators (i.e. energy density). Specifically, we shall inquire

1. whether dynamical scaling holds, and if so, what are the values of the corresponding non-equilibrium exponents ?
2. what is the form of the scaling functions of responses and correlators ?
3. which of the composite operators, if any, transform as quasi-primary fields under local scale-invariance ?

In subsection 3.3.2, we review the exact solution of the kinetic long-range spherical model and list our results for the non-equilibrium exponents and the scaling functions for the order-parameter and for composite fields. Some of the details can be found in the appendix of [20]. In subsection 3.3.3, we first show that the presently available formulation [109] of local scale-invariance cannot explain our results on the space-time form of the response functions when $z \neq 2$. We then recall some results from chapter 2 and [21] on the general reformulation of local scale-invariance for $z \neq 2$ before comparing our explicit results with the corresponding predictions of that general theory. In subsection 3.3.4 we conclude.

3.3.2 Exact solution of the long-range spherical model

The two-time correlation- and response-functions of the order-parameter in the spherical model when quenched either to $T = T_c$ or else to $T < T_c$ are well-known in the case of nearest-neighbour interactions [136, 176, 93, 5]. These are also known for the long-range model when quenched to $T < T_c$ [48]. Here, we shall derive the response and correlation

functions of the order-parameter and of certain composite operators in the long-range mean spherical model quenched to $T \leq T_c$.

Long-range spherical model

The long-range spherical model is defined in terms of a real spin variable $S(t, \mathbf{x})$ at time t and on the sites \mathbf{x} of a d -dimensional hypercubic lattice $\Lambda \subset \mathbb{Z}^d$, subject to the (mean) spherical constraint

$$\left\langle \sum_{\mathbf{x} \in \Lambda} S(t, \mathbf{x})^2 \right\rangle = \mathcal{N}, \quad (3.157)$$

where \mathcal{N} is the number of sites of the lattice¹¹. The Hamiltonian is given by [140]

$$\mathcal{H} = -\frac{1}{2} \sum_{\mathbf{x}, \mathbf{y}} J(\mathbf{x} - \mathbf{y}) S_{\mathbf{x}} (S_{\mathbf{y}} - S_{\mathbf{x}}), \quad (3.158)$$

where the sum extends over all pairs (\mathbf{x}, \mathbf{y}) such that $\mathbf{x} - \mathbf{y} \neq \mathbf{0}$. The coupling constant $J(\mathbf{x})$ of the model is defined by

$$J(\mathbf{x}) = \left(\sum'_{\mathbf{y} \in \Lambda} |\mathbf{y}|^{-(d+\sigma)} \right)^{-1} |\mathbf{x}|^{-(d+\sigma)}, \quad (3.159)$$

when $\mathbf{x} \neq 0$ and vanishes when $\mathbf{x} = 0$; the summation is over all lattice sites except $\mathbf{y} = 0$. The last term in (3.158), $\sum_{\mathbf{x}, \mathbf{y}} J(\mathbf{x} - \mathbf{y}) S_{\mathbf{x}}^2$, can also be absorbed into the Lagrange multiplier that imposes the spherical constraint, see below.

The ‘usual’ spherical model with short-range interactions is given by $J_{sr}(\mathbf{x} - \mathbf{y}) = J \sum_{\boldsymbol{\mu}(\mathbf{x})} \delta_{\mathbf{y}, \mathbf{x} + \boldsymbol{\mu}(\mathbf{x})}$, where $\mathbf{x} + \boldsymbol{\mu}(\mathbf{x})$ runs over all the neighbouring sites of \mathbf{x} . When $\sigma \geq 2$, the relevant large-scale behaviour of the above model, (3.158) and (3.159), is governed by this short-range model. Here we shall focus on truly long-range interactions such that $0 < \sigma < 2$. In this case, the dynamical exponent $z = \sigma$ can be continuously varied by tuning this parameter, see [140, 48] and below.

The dynamics is governed by the Langevin equation¹²

$$\partial_t S(t, \mathbf{x}) = - \left. \frac{\delta \mathcal{H}}{\delta S_{\mathbf{x}}} \right|_{S_{\mathbf{x}} \rightarrow S(t, \mathbf{x})} - \mathfrak{z}(t) S(t, \mathbf{x}) + \eta(t, \mathbf{x}), \quad (3.160)$$

where the coupling to the heat bath at temperature T is described by a Gaussian noise η of vanishing average and a variance

$$\langle \eta(t, \mathbf{x}) \eta(t', \mathbf{x}') \rangle = 2T \delta(t - t') \delta(\mathbf{x} - \mathbf{x}'). \quad (3.161)$$

The Lagrange multiplier $\mathfrak{z}(t)$ is fixed by the mean spherical constraint.

¹¹For short-ranged interactions, a careful analysis [86] has shown that the long-time behaviour is not affected whether (3.157) is assumed exactly or on average.

¹²In eq. (3.160), fluctuations in the Lagrange multiplier $\mathfrak{z}(t)$ are neglected. As pointed out in [5], these must be taken into account when treating non-local observables involving spins from the entire lattice or if the initial magnetisation is nonzero. Here we are only interested in local quantities and use a vanishing initial magnetisation. See [8] for a careful discussion on the applicability of Langevin equations in long-ranged systems.

The Langevin equation and the variance of the noise in the Fourier space read

$$\partial_t \widehat{S}(t, \mathbf{k}) = -\left(\omega(\mathbf{k}) + \mathfrak{z}(t)\right) \widehat{S}(t, \mathbf{k}) + \widehat{\eta}(t, \mathbf{k}), \quad (3.162)$$

$$\langle \widehat{\eta}(t, \mathbf{k}) \widehat{\eta}(t', \mathbf{k}') \rangle = 2T(2\pi)^d \delta(t - t') \delta(\mathbf{k} + \mathbf{k}'), \quad (3.163)$$

where $\omega(\mathbf{k}) = \widehat{J}(\mathbf{0}) - \widehat{J}(\mathbf{k})$. The hatted functions denote the Fourier transform of the corresponding functions. In the long-wavelength limit $|\mathbf{k}| \rightarrow 0$, the function $\omega(\mathbf{k}) \rightarrow B|\mathbf{k}|^\sigma$, where the constant B is given by [48] $B = \lim_{|\mathbf{k}| \rightarrow 0} (\widehat{J}(\mathbf{0}) - \widehat{J}(\mathbf{k})) |\mathbf{k}|^{-\sigma}$. The solution of the above equation is

$$\widehat{S}(t, \mathbf{k}) = \frac{e^{-\omega(\mathbf{k})t}}{\sqrt{g(t; T)}} \left[\widehat{S}(0, \mathbf{k}) + \int_0^t d\tau e^{\omega(\mathbf{k})\tau} \sqrt{g(\tau; T)} \widehat{\eta}(\tau, \mathbf{k}) \right], \quad (3.164)$$

with the constraint function $g(t; T) = \exp(2 \int_0^t d\tau \mathfrak{z}(\tau))$. The system is assumed to be quenched from far above the critical temperature, hence $\langle \widehat{S}(0, \mathbf{k}) \rangle = 0$; and the spins are assumed to be uncorrelated initially, hence the spherical constraint implies $\langle \widehat{S}(0, \mathbf{k}) \widehat{S}(0, \mathbf{k}') \rangle = (2\pi)^d \delta(\mathbf{k} + \mathbf{k}')$. Therefore, the spin-spin correlation function when $t > s$ is

$$\langle \widehat{S}(t, \mathbf{k}) \widehat{S}(s, \mathbf{k}') \rangle = (2\pi)^d \delta(\mathbf{k} + \mathbf{k}') \widehat{C}(t, s; \mathbf{k}), \quad (3.165)$$

where

$$\widehat{C}(t, s; \mathbf{k}) = \frac{e^{-\omega(\mathbf{k})(t+s)}}{\sqrt{g(t; T)g(s; T)}} \left[1 + 2T \int_0^s d\tau e^{2\omega(\mathbf{k})\tau} g(\tau; T) \right]. \quad (3.166)$$

The spherical constraint implies $1 = (2\pi)^{-d} \int d\mathbf{k} \widehat{C}(t, t; \mathbf{k})$ and gives $g(t; T)$ as the solution to the Volterra integral equation [93, 48]

$$g(t; T) = f(t) + 2T \int_0^t d\tau f(t - \tau) g(\tau; T), \quad (3.167)$$

with $g(0; T) = 1$, and $f(t) = f(t, \mathbf{0})$ is obtained from the function

$$f(t; \mathbf{r}) := \int_{\Lambda_{\mathbf{k}}} d\mathbf{k} \exp(i\mathbf{k} \cdot \mathbf{r} - 2\omega(\mathbf{k})t), \quad (3.168)$$

where $\Lambda_{\mathbf{k}}$ denotes the first Brillouin zone of the lattice Λ .

Composite operators: Correlations and responses

We shall now consider not only the spin operator $S(t, \mathbf{r})$ but also some composite fields, specifically the spin-squared (spin²) operator and the energy-density operator. We denote the spin and spin² operators by

$$\mathcal{O}_1(t, \mathbf{x}) := S(t, \mathbf{x}), \quad (3.169)$$

$$\mathcal{O}_2(t, \mathbf{x}) := S^2(t, \mathbf{x}) - \langle S^2(t, \mathbf{x}) \rangle, \quad (3.170)$$

respectively. The energy-density operator is defined as

$$\begin{aligned} \mathcal{O}_\epsilon(t, \mathbf{x}) &:= \mathcal{E}(t, \mathbf{x}) - \langle \mathcal{E}(t, \mathbf{x}) \rangle, \\ \mathcal{E}(t, \mathbf{x}) &:= \sum_{\mathbf{x}'} J(\mathbf{x} - \mathbf{x}') S(t, \mathbf{x}) (S(t, \mathbf{x}') - S(t, \mathbf{x})). \end{aligned} \quad (3.171)$$

These composite operators are defined in such a way that their average value is zero, and hence their correlation functions are essentially the *connected* correlation-functions. Also note that since energy is defined only up to a constant there is no unique definition of the energy-density operator.

The distinction between \mathcal{O}_2 and \mathcal{O}_ϵ and \mathcal{E} in (3.171) might be better understood as follows. We look into the continuum limit of the energy-density operator, at least for the short-range model, for we shall later discuss that this operator is not quasi-primary under local-scale transformations. In the short-range model, the expression for energy in lattice models is usually taken as

$$\mathcal{H} = -J \sum_{\mathbf{x}, \boldsymbol{\mu}(\mathbf{x})} S_{\mathbf{x}} S_{\mathbf{x}+\boldsymbol{\mu}(\mathbf{x})}, \quad (3.172)$$

where $\mathbf{x} + \boldsymbol{\mu}(\mathbf{x})$ runs over the neighbouring sites of \mathbf{x} . In such a case, the energy density could be defined as $\tilde{\epsilon}(\mathbf{x}) = -J \sum_{\boldsymbol{\mu}} S_{\mathbf{x}} S_{\mathbf{x}+\boldsymbol{\mu}}$, which in the continuum limit would reduce to $\tilde{\epsilon}(\mathbf{x}) = -J(2S_{\mathbf{x}}^2 + \mu^2 S_{\mathbf{x}} \nabla^2 S_{\mathbf{x}})$, where μ is the lattice constant. But if we had added an overall constant $E_0 = \mathcal{N} = \sum_{\mathbf{x}} S_{\mathbf{x}}^2$ then the energy density could be defined as

$$\epsilon(\mathbf{x}) = -J \sum_{\boldsymbol{\mu}} S_{\mathbf{x}} (S_{\mathbf{x}+\boldsymbol{\mu}} - S_{\mathbf{x}}) \rightarrow -J\mu^2 S_{\mathbf{x}} \nabla^2 S_{\mathbf{x}} (1 + \mathcal{O}(\mu)). \quad (3.173)$$

Hence $\mathcal{H}_{\text{sr}} = \sum_{\mathbf{x}} \epsilon(\mathbf{x}) = J\mu^2 \sum_{\mathbf{x}} (\nabla S_{\mathbf{x}})^2$, up to boundary terms. Therefore, for our model (3.158) the two operators $\mathcal{O}_2(t, \mathbf{x})$ and $\mathcal{O}_\epsilon(t, \mathbf{x})$ must be distinguished.

The connected two-point correlation functions of the composite operators

$$\mathcal{C}_{ab}(t, s; \mathbf{x} - \mathbf{x}') := \langle \mathcal{O}_a(t; \mathbf{x}) \mathcal{O}_b(s; \mathbf{x}') \rangle \quad (3.174)$$

are obtained by making use of Wick's contraction as detailed in the appendix of [20]. Throughout it is implicitly assumed that $t > s$ unless stated otherwise. As we have spatial-translation invariance in our system, we shall find that all two-point quantities depend merely on the difference $\mathbf{r} := \mathbf{x} - \mathbf{x}'$ of the spatial coordinates.

The response functions of the fields $\{\mathcal{O}_a(t, \mathbf{x})\}$ to the conjugate fields $\{h_a(t, \mathbf{x})\}$

$$\mathcal{R}_{ab}(t, s, \mathbf{x} - \mathbf{x}') := \left. \frac{\delta \langle \mathcal{O}_a(t, \mathbf{x}) \rangle_{\{h\}}}{\delta h_b(s, \mathbf{x}')} \right|_{\{h\}=\{0\}}, \quad (3.175)$$

are obtained by linearly perturbing the Hamiltonian, $\mathcal{H} \rightarrow \mathcal{H} - \sum_{a,t,\mathbf{x}} h_a(t, \mathbf{x}) \mathcal{O}_a(t, \mathbf{x})$, as detailed in the appendix of [20]. The above defined response function can be interpreted as the susceptibility of the expectation value of a field to near-equilibrium fluctuations.

Finally, we also obtain out-of-equilibrium responses of the fields $\{\mathcal{O}_a(t, \mathbf{x})\}$ to local temperature fluctuations. This we do by perturbing the noise strength $T \rightarrow T + \delta T(t, \mathbf{x})$ and then evaluating the response functions

$$\mathcal{R}_a^{(T)}(t, s, ; \mathbf{x} - \mathbf{x}') := \left. \frac{\delta \langle \mathcal{O}_a(t, \mathbf{x}) \rangle_{\delta T}}{\delta T(s, \mathbf{x}')} \right|_{\delta T=0}. \quad (3.176)$$

Let us specify at this point the asymptotic scaling forms that we expect for the auto-correlation function $\mathcal{C}_{ab}(t, s) := \mathcal{C}_{ab}(t, s; \mathbf{0})$ and the autoresponse functions $\mathcal{R}_{ab}(t, s) := \mathcal{R}_{ab}(t, s; \mathbf{0})$ and $\mathcal{R}_a^{(T)}(t, s) := \mathcal{R}_a^{(T)}(t, s; \mathbf{0})$. They are expected to behave as

$$\mathcal{C}_{ij}(t, s) = s^{-b_{ij}} f_C^{ij}(t/s), \quad f_C^{ij}(y) \stackrel{y \rightarrow \infty}{\sim} y^{-\lambda_C^{ij}/z}, \quad (3.177)$$

$$\mathcal{R}_{ij}(t, s) = s^{-a_{ij}-1} f_R^{ij}(t/s), \quad f_R^{ij}(y) \stackrel{y \rightarrow \infty}{\sim} y^{-\lambda_R^{ij}/z}, \quad (3.178)$$

$$\mathcal{R}_i^{(T)}(t, s) = s^{-a_i^{(T)}-1} f_R^{(T)i}(t/s), \quad f_R^{(T)i}(y) \stackrel{y \rightarrow \infty}{\sim} y^{-\lambda_R^{(T)i}/z}, \quad (3.179)$$

in the scaling regime where t, s and $t - s$ are simultaneously large. This also defines the nonequilibrium critical exponents $a_{ij}, b_{ij}, a_i^T, \lambda_R^{ij}, \lambda_C^{ij}, \lambda_R^{(T)i}$.

We now write the correlation and response functions of some of the fields $\{\mathcal{O}_a(t, \mathbf{x})\}$ in terms of the spin-spin correlator $C(t, s; \mathbf{r})$, the constraint function $g(t; T)$ and $f(t; \mathbf{r})$. The details of these computations are given in the appendix of [20], while the explicit forms of these functions and their asymptotics are spelt out in the next subsection.

The correlation functions:

We obtain the following expressions for the non-vanishing correlation functions of the composite fields.

- The spin²-spin² correlation function is found to be

$$\mathcal{C}_{22}(t, s; \mathbf{r}) = \langle \mathcal{O}_2(t, \mathbf{r}) \mathcal{O}_2(s, \mathbf{0}) \rangle = 2 \left[C(t, s; \mathbf{r}) \right]^2. \quad (3.180)$$

For the short-range case, this formula has already been found in [44].

- The spin²-energy-density correlation functions are

$$\mathcal{C}_{2\epsilon}(t, s; \mathbf{r}) = \langle \mathcal{O}_2(t, \mathbf{r}) \mathcal{O}_\epsilon(s, \mathbf{0}) \rangle = \frac{-1}{2g(t; T)} \partial_t \left(g(t; T) \mathcal{C}_{22}(t, s; \mathbf{r}) \right), \quad (3.181)$$

and

$$\mathcal{C}_{\epsilon 2}(t, s; \mathbf{r}) = \mathcal{C}_{2\epsilon}(t, s; \mathbf{r}). \quad (3.182)$$

This is a stronger result than the obvious relation $\mathcal{C}_{\epsilon 2}(t, s; \mathbf{r}) = \mathcal{C}_{2\epsilon}(s, t; -\mathbf{r})$ and follows from $\omega(\mathbf{k}) = \omega(-\mathbf{k})$.

- The energy-density-energy-density correlation function is given by

$$\mathcal{C}_{\epsilon\epsilon}(t, s; \mathbf{r}) = \frac{-1}{2g(t; T)} \partial_t \left(g(t; T) \mathcal{C}_{2\epsilon}(t, s; \mathbf{r}) \right). \quad (3.183)$$

The response functions:

For the response functions, we obtain the following expressions. Because of causality, in all expressions given below the factor $\Theta(t - s)$ is implied, where the step function $\Theta(t - s) = 1$ for $t > s$, and zero otherwise.

- Responses to the magnetic field $h_1(t, \mathbf{x})$, which are obtained when $\mathcal{H} \rightarrow \mathcal{H} - \sum_{t, \mathbf{x}} h_1(t, \mathbf{x}) S(t, \mathbf{x})$, are given by

$$\mathcal{R}_{11}(t, s; \mathbf{r}) = \sqrt{\frac{g(s; T)}{g(t; T)}} f \left(\frac{t - s}{2}, \mathbf{r} \right), \quad (3.184)$$

$$\mathcal{R}_{21}(t, s; \mathbf{r}) = \mathcal{R}_{\epsilon 1}(t, s; \mathbf{r}) = 0. \quad (3.185)$$

- Responses to the conjugate field $h_2(t, \mathbf{x})$ of spin² operator are obtained when $\mathcal{H} \rightarrow \mathcal{H} - \sum_{t, \mathbf{x}} h_2(t, \mathbf{x}) \mathcal{O}_2(t, \mathbf{x})$ and are given by

$$\mathcal{R}_{12}(t, s; \mathbf{r}) = 0, \quad (3.186)$$

$$\mathcal{R}_{22}(t, s; \mathbf{r}) = 4\mathcal{R}_{11}(t, s; \mathbf{r})C(t, s; \mathbf{r}), \quad (3.187)$$

$$\mathcal{R}_{\epsilon 2}(t, s; \mathbf{r}) = -\mathcal{R}_{22}(t, s; \mathbf{r}) \partial_t \ln f\left(\frac{t-s}{2}, \mathbf{r}\right), \quad (3.188)$$

The expression for $\mathcal{R}_{22}(t, s; \mathbf{r})$ has already been given in [44] for the short-range model.

- Responses to the conjugate field $h_\epsilon(t, \mathbf{x})$ of energy-density operator are obtained when $\mathcal{H} \rightarrow \mathcal{H} - \sum_{t, \mathbf{x}} h_\epsilon(t, \mathbf{x}) \mathcal{O}_\epsilon(t, \mathbf{x})$ and are given by

$$\mathcal{R}_{1\epsilon}(t, s; \mathbf{r}) = 0, \quad (3.189)$$

$$\mathcal{R}_{2\epsilon}(t, s; \mathbf{r}) = \frac{-1}{2g(t; T)} \partial_t \left(g(t; T) \mathcal{R}_{22}(t, s; \mathbf{r}) \right), \quad (3.190)$$

$$\mathcal{R}_{\epsilon\epsilon}(t, s; \mathbf{r}) = \frac{-1}{2g(t; T)} \partial_t \left(g(t; T) \mathcal{R}_{2\epsilon}(t, s; \mathbf{r}) \right). \quad (3.191)$$

- The spin, the spin² and the energy-density responses to temperature fluctuation are

$$\mathcal{R}_1^{(T)}(t, s; \mathbf{r}) = 0, \quad (3.192)$$

$$\mathcal{R}_2^{(T)}(t, s; \mathbf{r}) = 2 \left(\mathcal{R}_{11}(t, s; \mathbf{r}) \right)^2, \quad (3.193)$$

$$\mathcal{R}_\epsilon^{(T)}(t, s; \mathbf{r}) = \frac{-1}{2g(t; T)} \partial_t \left(g(t; T) \mathcal{R}_2(t, s; \mathbf{r}) \right), \quad (3.194)$$

respectively.

Late-time behaviour of correlation- and response- functions

In this subsection, we first explicitly evaluate in the scaling limit the quantities specified in the previous subsection, and then identify the critical exponents and scaling functions. The treatment is based on previous results and techniques from [48, 93].

In the late-time limit we can approximate the function $\omega(\mathbf{k}) \approx B|\mathbf{k}|^\sigma$, where $0 < \sigma \leq 2$ [48]. Hence the dynamical exponent in this range of σ is given by

$$z = \sigma. \quad (3.195)$$

Furthermore, the large-time behaviour of $f(t)$ and $g(t; T)$ are as follows. The function $f(t, \mathbf{x})$ in this limit becomes

$$f(t; \mathbf{x}) \approx B_0 t^{-d/\sigma} G(|\mathbf{x}| t^{-1/\sigma}) ; \quad B_0 := \int_{\mathbf{k}} e^{-2B|\mathbf{k}|^\sigma}. \quad (3.196)$$

Here the scaling function $G(|\mathbf{u}| t^{-1/\sigma})$ for any variable \mathbf{u} is defined as

$$G(|\mathbf{u}| t^{-1/\sigma}) := B_0^{-1} t^{d/\sigma} \int_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{u}} e^{-2B|\mathbf{k}|^\sigma t}, \quad (3.197)$$

where $\int_{\mathbf{k}} \cdots = (2\pi)^{-d} \int d^d k \cdots$ denotes an integral over \mathbb{R}^d . The Laplace transform of $f(t)$ is given by the expression

$$f_L(p) = -A_0 p^{-1+d/\sigma} + \sum_{n=1}^{\infty} A_n (-p)^{n-1}, \quad (3.198)$$

where the universal constant $A_0 = |\Gamma(1 - d/\sigma)| B_0$ and the nonuniversal constants $A_n = \int_{\Lambda_{\mathbf{k}}} (2\omega_{\mathbf{k}})^{-n} - \int_{\mathbf{k}} (2B|\mathbf{k}|^\sigma)^{-n}$, for $n = 1, 2, \dots$. We note that $A_1 = 1/2T_c$.

Now the constraint equation (3.167), upon Laplace transforming, becomes

$$g_L(p; T) = \frac{f_L(p)}{1 - 2T f_L(p)}, \quad (3.199)$$

and is solved in the small- p region using equation (3.198). Following a similar analysis as done for $\sigma = 2$ case in [93], we find the large- t limit of the function $g(t; T)$, which is given in equations (3.200), (3.216), and (3.232). This asymptotic constraint function has three different forms depending on the quenched temperature and the lattice dimension, for a given value of the parameter σ . The known case for the short-range model one can obtain by taking the limit $\sigma \rightarrow 2$. The three cases are

- $T < T_c$: This case was treated in [48] for the spin-spin correlator and the spin response. We recover their results and further add other correlation and response functions of the composite fields.
- $T = T_c, \sigma < d < 2\sigma$: To the best of our knowledge the quench to criticality has not been treated before. We must further distinguish two critical cases. In the first case, d can at most be 4 since $\sigma \leq 2$.
- $T = T_c, d > 2\sigma$: In this second case of a critical quench, the space dimension d is not bounded from above. This case includes the mean-field case.

We now discuss the large-time behaviour of the correlation and response functions in these three cases.

Case I: $T < T_c$

Since the system exhibits space-translation invariance we take $\mathbf{x}' = \mathbf{0}$. We denote $y = t/s > 1$. The constraint function for $T < T_c$ in the large-time limit [48] is

$$g(t; T) \approx B_0 \left(1 - \frac{T}{T_c}\right)^{-1} t^{-d/\sigma}, \quad (3.200)$$

and hence the spin-spin correlation function for $T < T_c$ in the scaling regime reduces to

$$\widehat{C}(t, s; \mathbf{k}) = \left(1 - \frac{T}{T_c}\right) B_0^{-1} s^{d/\sigma} y^{d/2\sigma} e^{-B|\mathbf{k}|^\sigma(t+s)}, \quad (3.201)$$

in the Fourier space, or

$$C(t, s; \mathbf{r}) = C_0 y^{d/2\sigma} (y+1)^{-d/\sigma} G(u), \quad (3.202)$$

Function	b		λ_C		
	$T < T_c$	$T = T_c$	$T < T_c$	$T = T_c$	
				$\sigma < d < 2\sigma$	$d > 2\sigma$
\mathcal{C}_{11}	0	$d/\sigma - 1$	$d/2$	$3d/2 - \sigma$	d
\mathcal{C}_{22}	0	$2d/\sigma - 2$	d	$3d - 2\sigma$	$2d$
$\mathcal{C}_{2\epsilon}$	1	$2d/\sigma - 1$	$d + \sigma$	$3d - \sigma$	$2d + \sigma$
$\mathcal{C}_{\epsilon\epsilon}$	2	$2d/\sigma$	$d + 2\sigma$	$3d$	$2d + 2\sigma$

Table 3.3: Non-equilibrium exponents b , λ_C , as defined in (3.177), for several non-equilibrium autocorrelation functions in the long-range spherical model. The exponents for the short-range model can be recovered by taking the limit $\sigma \rightarrow 2$.

in the direct space, where $C_0 = 2^{d/\sigma}(1 - T/T_c)$. Here and below, expressions become shorter with the use of the three related scaling variables u , v , and w , where

$$\begin{aligned} u &= |\mathbf{r}|((t+s)/2)^{-1/\sigma} = w(1+s/t)^{-1/\sigma}, \\ v &= |\mathbf{r}|((t-s)/2)^{-1/\sigma} = w(1-s/t)^{-1/\sigma} \\ w &= |\mathbf{r}|(t/2)^{-1/\sigma} \end{aligned} \quad (3.203)$$

The autocorrelation function can now be directly deduced since the scaling function $G(0) = 1$ for $\mathbf{r} = 0$. Hence one reads off, see (3.177) and table 3.2,

$$b_{11} = 0, \quad \lambda_C^{11} = \frac{d}{2}, \quad f_C^{11}(y) = C_0 y^{d/2\sigma} (y+1)^{-d/\sigma}. \quad (3.204)$$

Below we list the remaining expressions in the scaling limit. The autocorrelation and autoresponse functions are obtained for the composite operators in a similar way as is demonstrated for $C(t, s; \mathbf{r}) = \mathcal{C}_{11}(t, s; \mathbf{r})$. The non-equilibrium ageing exponents are listed in tables (3.3) and (3.4), for future reference.

We first list the non-vanishing correlation functions.

- The spin² – spin² correlator, obtained by substituting equation (3.202) into (3.180), is

$$\mathcal{C}_{22}(t, s; \mathbf{r}) = 2C_0^2 y^{d/\sigma} (y+1)^{-2d/\sigma} G^2(u). \quad (3.205)$$

- The spin² – energy-density correlator, obtained by using equations (3.200, 3.205) in (3.181), is

$$\mathcal{C}_{2\epsilon}(t, s; \mathbf{r}) = \frac{2C_0^2}{\sigma} s^{-1} y^{d/\sigma} (y+1)^{-1-2d/\sigma} G(u) D_u G(u), \quad (3.206)$$

where, the operator D_z is defined as

$$D_z := z\partial_z + d. \quad (3.207)$$

- The energy-density – energy-density correlator, obtained by inserting equations (3.200, 3.206) into (3.183), is given by

$$\mathcal{C}_{\epsilon\epsilon}(t, s; \mathbf{r}) = \frac{C_0^2}{\sigma^2} s^{-2} y^{d/\sigma} (y+1)^{-2-2d/\sigma} (D_u + d + \sigma) [G(u) D_u G(u)]. \quad (3.208)$$

Function	a		λ_R		
	$T < T_c$	$T = T_c$	$T < T_c$	$T = T_c$	
				$\sigma < d < 2\sigma$	$d > 2\sigma$
\mathcal{R}_{11}	$d/\sigma - 1$	$d/\sigma - 1$	$d/2$	$3d/2 - \sigma$	d
\mathcal{R}_{22}	$d/\sigma - 1$	$2d/\sigma - 2$	d	$3d - 2\sigma$	$2d$
\mathcal{R}_{e2}	d/σ	$2d/\sigma - 1$	$d + \sigma$	$3d - \sigma$	$2d + \sigma$
$\mathcal{R}_{2\epsilon}$	d/σ	$2d/\sigma - 1$	$d + \sigma$	$3d - \sigma$	$2d + \sigma$
$\mathcal{R}_{\epsilon\epsilon}$	$d/\sigma + 1$	$2d/\sigma$	$d + 2\sigma$	$3d$	$2d + 2\sigma$
\mathcal{R}_2^T	$2d/\sigma - 1$	$2d/\sigma - 1$	d	$3d - 2\sigma$	$2d$
\mathcal{R}_ϵ^T	$2d/\sigma$	$2d/\sigma$	$d + \sigma$	$3d - \sigma$	$2d + \sigma$

Table 3.4: Nonequilibrium exponents $a = a'$ and λ_R , as defined in (3.178) and (3.179), for several scaling operators in the long-range spherical model. The exponents for the short-range model one obtains by taking the limit $\sigma \rightarrow 2$.

Next we write down the non-vanishing response functions.

- The spin response function, obtained using equations (3.196, 3.200) in (3.184), is given by

$$\mathcal{R}_{11}(t, s; \mathbf{r}) = C_1 s^{-d/\sigma} y^{d/2\sigma} (y - 1)^{-d/\sigma} G(v), \quad (3.209)$$

where $C_1 = \int_{\mathbf{k}} \exp(-B|\mathbf{k}|^\sigma)$, and v was defined in eq. (3.203).

- The non-vanishing response functions to spin² conjugate field, inferred from equations (3.187, 3.188) using (3.196, 3.202, 3.209), are given by

$$\mathcal{R}_{22}(t, s; \mathbf{r}) = 4C_0 C_1 s^{-d/\sigma} y^{d/\sigma} (y^2 - 1)^{-d/\sigma} G(u)G(v), \quad (3.210)$$

$$\mathcal{R}_{e2}(t, s; \mathbf{r}) = \frac{4C_0 C_1}{\sigma} s^{-1-d/\sigma} y^{d/\sigma} (y^2 - 1)^{-d/\sigma} \frac{D_v}{y - 1} G(u)G(v), \quad (3.211)$$

where D_v is as given in (3.207) and u, v were defined in (3.203).

- Responses to the energy-density conjugate field, obtained from equations (3.190, 3.191) using (3.200, 3.210), are given as follows.

$$\begin{aligned} \mathcal{R}_{2\epsilon}(t, s; \mathbf{r}) &= \frac{2C_0 C_1}{\sigma} s^{-1-d/\sigma} y^{d/\sigma} (y^2 - 1)^{-d/\sigma} \\ &\times \left(\frac{D_u}{y + 1} + \frac{D_v}{y - 1} \right) G(u)G(v), \end{aligned} \quad (3.212)$$

$$\begin{aligned} \mathcal{R}_{\epsilon\epsilon}(t, s; \mathbf{r}) &= \frac{C_0 C_1}{\sigma^2} s^{-2-d/\sigma} y^{d/\sigma} (y^2 - 1)^{-d/\sigma} \\ &\times \left(\frac{D_u^2 + \sigma D_u}{(y + 1)^2} + \frac{2D_u D_v}{y^2 - 1} + \frac{D_v^2 + \sigma D_v}{(y - 1)^2} \right) G(u)G(v). \end{aligned} \quad (3.213)$$

- The spin² and energy-density responses to local temperature fluctuations, obtained using equations (3.200, 3.209) in (3.193, 3.194), are

$$\mathcal{R}_2^{(T)}(t, s; \mathbf{r}) = 2C_1^2 s^{-2d/\sigma} y^{d/\sigma} (y-1)^{-2d/\sigma} G^2(v), \quad (3.214)$$

$$\mathcal{R}_\epsilon^{(T)}(t, s; \mathbf{r}) = \frac{2C_1^2}{\sigma} s^{-1-2d/\sigma} y^{d/\sigma} (y-1)^{-1-2d/\sigma} G(v) D_v G(v), \quad (3.215)$$

respectively.

Case IIa: $T = T_c$ and $\sigma < d < 2\sigma$

For $T = T_c$ and $\sigma < d < 2\sigma$, the constraint function has the form

$$g(t; T_c) \approx (4T_c^2 A_0 \Gamma(-1 + d/\sigma))^{-1} t^{-2+d/\sigma}, \quad (3.216)$$

and hence the correlation function in the scaling regime reduces to

$$\widehat{C}(t, s; \mathbf{k}) = 2T_c s y^{1-d/2\sigma} \int_0^1 dz e^{-B|\mathbf{k}|^\sigma(t+s-2sz)} z^{-2+d/\sigma}, \quad (3.217)$$

or in the direct space is given by

$$C(t, s; \mathbf{r}) = 2T_c C_1 s^{1-d/\sigma} y^{1-d/2\sigma} (y+1)^{-d/\sigma} \sum_{n=0}^{\infty} \frac{(y+1)^{-n} G_n(u)}{n!(n-1+d/\sigma)}, \quad (3.218)$$

where u is given in (3.203) and the function $G_n(|\mathbf{v}|t^{-1/\sigma})$ is defined as

$$G_n(|\mathbf{v}|t^{-1/\sigma}) := 4^n t^{n+d/\sigma} B_0^{-1} \int_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{v}} e^{-2B|\mathbf{k}|^\sigma t} (B|\mathbf{k}|^\sigma)^n, \quad (3.219)$$

for any variable \mathbf{v} . The spin-response function in this case has the form

$$\mathcal{R}_{11}(t, s; \mathbf{x}) = C_1 s^{-d/\sigma} y^{1-d/2\sigma} (y-1)^{-d/\sigma} G(v). \quad (3.220)$$

To avoid presenting lengthy expressions we write down only the leading behaviour in y for the correlators and responses in this case. The spin-spin correlation function in this approximation becomes

$$C(t, s; \mathbf{r}) \approx 2\widetilde{T}_c C_1 s^{1-d/\sigma} y^{1-3d/2\sigma} G(w), \quad (3.221)$$

where $\widetilde{T}_c = T_c \sigma / (d - \sigma)$, and w is as given in (3.203). Setting w and v to zero, we can read off the ageing exponents, see tables 3.3 and 3.4.

$$a_{11} = b_{11} = \frac{d}{\sigma} - 1, \quad \lambda_R^{11} = \lambda_C^{11} = \frac{3d}{2} - \sigma, \quad z = \sigma \quad (3.222)$$

The other non-vanishing correlators and responses are given as follows, wherein we first list the correlation functions.

- The spin² – spin² correlator is given by

$$C_{22}(t, s; \mathbf{r}) \approx 8\widetilde{T}_c^2 C_1^2 s^{2-2d/\sigma} y^{2-3d/\sigma} G^2(w). \quad (3.223)$$

- For the spin² – energy correlator we obtain

$$\mathcal{C}_{2\epsilon}(t, s; \mathbf{r}) \approx \frac{8\tilde{T}_c^2 C_1^2}{\sigma} s^{1-2d/\sigma} y^{1-3d/\sigma} G(w) D_w G(w). \quad (3.224)$$

- Finally the energy– energy correlator reads

$$\mathcal{C}_{\epsilon\epsilon}(t, s; \mathbf{r}) \approx \frac{4\tilde{T}_c^2 C_1^2}{\sigma^2} s^{-2d/\sigma} y^{-3d/\sigma} (D_w + d + \sigma) [G(w) D_w G(w)]. \quad (3.225)$$

The non-vanishing response functions are listed below.

- The responses to the spin² conjugate field are given by

$$\mathcal{R}_{22}(t, s; \mathbf{r}) \approx 8\tilde{T}_c C_1^2 s^{1-2d/\sigma} y^{2-3d/\sigma} G^2(w), \quad (3.226)$$

$$\mathcal{R}_{\epsilon 2}(t, s; \mathbf{r}) \approx \frac{8\tilde{T}_c C_1^2}{\sigma} s^{-2d/\sigma} y^{1-3d/\sigma} G(w) D_w G(w). \quad (3.227)$$

- The responses to energy-density conjugate field are

$$\mathcal{R}_{2\epsilon}(t, s; \mathbf{r}) \approx \mathcal{R}_{\epsilon 2}(t, s; \mathbf{r}), \quad (3.228)$$

$$\mathcal{R}_{\epsilon\epsilon}(t, s; \mathbf{r}) \approx \frac{4\tilde{T}_c C_1^2}{\sigma^2} s^{-1-2d/\sigma} y^{-3d/\sigma} (D_w + d + \sigma) [G(w) D_w G(w)]. \quad (3.229)$$

- Lastly, the responses to temperature fluctuations are

$$\mathcal{R}_2^{(T)}(t, s; \mathbf{r}) \approx 2C_1^2 s^{-2d/\sigma} y^{2-3d/\sigma} G^2(w), \quad (3.230)$$

$$\mathcal{R}_\epsilon^{(T)}(t, s; \mathbf{r}) \approx \frac{2C_1^2}{\sigma} s^{-1-2d/\sigma} y^{1-3d/\sigma} G(w) D_w G(w). \quad (3.231)$$

Case IIb: $T = T_c$ and $d > 2\sigma$

For $T = T_c$ and $d > 2\sigma$, the constraint function at large times is

$$g(t; T_c) \approx (4T_c^2 A_2)^{-1}. \quad (3.232)$$

This is just a constant and does not appear in the correlation and response functions to leading order in this large-time limit. In this case, the correlation function in the scaling regime reduces to

$$\hat{C}(t, s; \mathbf{k}) = \frac{T_c}{B|\mathbf{k}|^\sigma} (e^{-B|\mathbf{k}|^\sigma(t-s)} - e^{-B|\mathbf{k}|^\sigma(t+s)}), \quad (3.233)$$

and in the direct space is

$$C(t, s; \mathbf{r}) = 2T_c C_1 s^{1-d/\sigma} \left(\frac{G_{-1}(v)}{(y-1)^{d/\sigma-1}} - \frac{G_{-1}(u)}{(y+1)^{d/\sigma-1}} \right), \quad (3.234)$$

where G_{-1} is as given in (3.219).

The spin-response function in this case is given by

$$\mathcal{R}_{11}(t, s; \mathbf{r}) = C_1 s^{-d/\sigma} (y-1)^{-d/\sigma} G(v). \quad (3.235)$$

Here again we present only the leading behaviour in y of the correlators and responses. The correlation function in this approximation becomes

$$C(t, s; \mathbf{r}) \approx 2T_c s f(t/2, \mathbf{r}) = 2T_c C_1 s^{1-d/\sigma} y^{-d/\sigma} G(w). \quad (3.236)$$

Again we read off the critical exponents after setting $v = w = 0$

$$a_{11} = b_{11} = \frac{d}{\sigma} - 1, \quad \lambda_R^{11} = \lambda_C^{11} = d. \quad (3.237)$$

The other non-vanishing correlation functions are given as follows.

- The spin²–spin² correlation function is

$$\mathcal{C}_{22}(t, s; \mathbf{r}) \approx 8T_c^2 C_1^2 s^{2-2d/\sigma} y^{-2d/\sigma} G^2(w). \quad (3.238)$$

- The spin² -energy correlation function is given by

$$\mathcal{C}_{2\epsilon}(t, s; \mathbf{r}) \approx \frac{8T_c^2 C_1^2}{\sigma} s^{1-2d/\sigma} y^{-1-2d/\sigma} G(w) D_w G(w). \quad (3.239)$$

- The energy-density – energy-density correlation function is

$$\mathcal{C}_{\epsilon\epsilon}(t, s; \mathbf{r}) \approx \frac{4T_c^2 C_1^2}{\sigma^2} s^{-2d/\sigma} y^{-2-2d/\sigma} (D_w + d + \sigma) [G(w) D_w G(w)]. \quad (3.240)$$

The remaining non-vanishing response functions follow.

- The responses to spin² conjugate field are

$$\mathcal{R}_{22}(t, s; \mathbf{r}) \approx 8T_c C_1^2 s^{1-2d/\sigma} y^{-2d/\sigma} G^2(w), \quad (3.241)$$

$$\mathcal{R}_{\epsilon 2}(t, s; \mathbf{r}) \approx \frac{8T_c C_1^2}{\sigma} s^{-2d/\sigma} y^{-1-2d/\sigma} G(w) D_w G(w). \quad (3.242)$$

- The responses to energy-density conjugate field are given by

$$\mathcal{R}_{2\epsilon}(t, s; \mathbf{r}) \approx \mathcal{R}_{\epsilon 2}(t, s; \mathbf{r}), \quad (3.243)$$

$$\mathcal{R}_{\epsilon\epsilon}(t, s; \mathbf{r}) \approx \frac{4T_c C_1^2}{\sigma^2} s^{-1-2d/\sigma} y^{-2-2d/\sigma} (D_w + d + \sigma) [G(w) D_w G(w)]. \quad (3.244)$$

- Finally, the responses to temperature fluctuations are given as

$$\mathcal{R}_2(T)(t, s; \mathbf{r}) \approx 2C_1^2 s^{-2d/\sigma} y^{-2d/\sigma} G^2(w), \quad (3.245)$$

$$\mathcal{R}_\epsilon^{(T)}(t, s; \mathbf{r}) \approx \frac{2C_1^2}{\sigma} s^{-1-2d/\sigma} y^{-1-2d/\sigma} G(w) D_w G(w). \quad (3.246)$$

The exponents of these functions, derived in this subsection, are collected in tables 5.1 and 3.4.

Fluctuation-dissipation ratios

An important quantity, in particular for the case of critical dynamics, is the fluctuation-dissipation ratio of an observable, which is defined as [58, 56]

$$X_{ab}(t, s) := T_c \mathcal{R}_{ab}(t, s; \mathbf{0}) \left(\frac{\partial C_{ab}(t, s; \mathbf{0})}{\partial s} \right)^{-1} \quad (3.247)$$

and its limit value

$$X_{ab}^\infty := \lim_{s \rightarrow \infty} \left(\lim_{t \rightarrow \infty} X_{ab}(t, s) \right) = \lim_{y \rightarrow \infty} \left(\lim_{s \rightarrow \infty} X_{ab}(t, s) |_{y=t/s} \right). \quad (3.248)$$

For case *I*, that is for phase-ordering kinetics, it was already known that in the quasi-static limit $s \rightarrow \infty$ but $t - s$ fixed and $\ll s$, the fluctuation-dissipation theorem still holds [48]. On the other hand, we obtain in the scaling limit $s \rightarrow \infty$ and $y = t/s > 1$ fixed that, for all observables considered here

$$X_{11}(t, s) = X_{22}(t, s) = X_{2\epsilon}(t, s) = X_{\epsilon 2}(t, s) = X_{\epsilon\epsilon}(t, s) = \frac{2\sigma T C_1}{d C_0} s^{1-d/\sigma}. \quad (3.249)$$

For $d > \sigma$ we have therefore in this case that

$$X_{11}^\infty = X_{22}^\infty = X_{2\epsilon}^\infty = X_{\epsilon 2}^\infty = X_{\epsilon\epsilon}^\infty = 0 \quad (3.250)$$

as expected for a low-temperature phase (recall that for $d \leq \sigma$ the critical temperature is zero [140]).

In the case of critical dynamics (case *IIa* and *IIb*) the limit fluctuation-dissipation ratios are universal numbers characterising the critical system [93]. For their calculation, we can use directly the scaling limit $s \rightarrow \infty$ with $y = t/s$ being kept fixed. In case *IIa*, it is convenient to obtain the auto-correlation function $C(t, s)$ by directly integrating eq. (3.217), which leads to

$$C(t, s) = \frac{2T_c C_1 \sigma}{d - \sigma} s^{1-d/\sigma} y^{1-d/2\sigma} (y - 1)^{1-d/\sigma} (y + 1)^{-1}. \quad (3.251)$$

Combining this with eq. (3.220), we get

$$X_{11}(t, s) = X_{11}(y) = \frac{1}{2} (y + 1) \left[1 + \frac{y - 1}{d - \sigma} \left(\frac{d}{2} - \frac{\sigma}{y + 1} \right) \right]^{-1} \quad (3.252)$$

Similarly, in case *IIb*, using equations (3.234) and (3.235), and upon substituting the value of $G_{-1}(0) = \sigma G(0)/(d - \sigma)$, we find

$$X_{11}(t, s) = X_{11}(y) = \left(1 + \left(\frac{y - 1}{y + 1} \right)^{d/\sigma} \right)^{-1} \quad (3.253)$$

In particular, we see that in the quasi-static limit $s \rightarrow \infty$ with $t - s$ being kept fixed (or alternatively $y \rightarrow 1$), $\lim_{y \rightarrow 1} X_{11}(y) \rightarrow 1$ in both critical cases, such that the fluctuation-dissipation theorem holds. Similarly, from the relations (3.180,3.181,3.183) and (3.187,3.190,3.191) we also have $\lim_{y \rightarrow 1} X_{22}(y) = \lim_{y \rightarrow 1} X_{\epsilon\epsilon}(y) = \lim_{y \rightarrow 1} X_{2\epsilon}(y) = 1$. On the other hand, and remarkably, the limit fluctuation-dissipation ratio turns out to be independent of the choice of the considered observable. We find for $y \rightarrow \infty$

$$X_{11}^\infty = X_{22}^\infty = X_{2\epsilon}^\infty = X_{\epsilon^2}^\infty = X_{\epsilon\epsilon}^\infty = \begin{cases} 1 - \sigma/d & \text{for the case } IIa \\ 1/2 & \text{for the case } IIb \end{cases} \quad (3.254)$$

This reduces to the well-known expressions in the short-range model [93] when $z = \sigma \rightarrow 2$. We recall that in [44], a slightly different definition for the energy density was used, in which case the value for the corresponding fluctuation-dissipation ratio may be different.

3.3.3 Local scale-invariance

We will now proceed and compare the results obtained for the spherical model with long-range interactions to the LSI-predictions. In order keep this section selfcontained and to remain in line with the notations of this section, we will repeat some facts from chapter 2. We recall that a quasi-primary scaling operator ϕ is characterised by a set of ‘quantum numbers’ (x, ξ, μ, β) , where x is the ‘scaling dimension’ of ϕ and μ is sometimes referred to as the ‘mass’ of ϕ (not to be confused with the lattice constant μ in subsection 3.3.2).

Response functions

For a given dynamical exponent z , LSI yields the following prediction for the response function of a quasi-primary operator ϕ characterised by the parameters (x, ξ, μ, β) : [109, 207, 21, 126]

$$\begin{aligned} R^{LSI}(t, s; \mathbf{r}) &= \delta_{\mu, -\tilde{\mu}} \delta_{\beta, \tilde{\beta}} R(t, s) \mathcal{F}^{(\mu, \beta)} \left(\frac{|\mathbf{r}|}{(t-s)^{1/z}} \right), \\ R(t, s) &= s^{-1-a} \left(\frac{t}{s} \right)^{1+a'-\lambda_R/z} \left(\frac{t}{s} - 1 \right)^{-1-a'}, \end{aligned} \quad (3.255)$$

where the exponents a, a' and λ_R are related to the parameters (x, ξ, μ) via

$$a + 1 = \frac{1}{z}(x + \tilde{x}), \quad a' + 1 = \frac{1}{z}(x + 2\xi + \tilde{x} + 2\tilde{\xi}), \quad \frac{\lambda_R}{z} = \frac{2x}{z} + \frac{2\xi}{z}, \quad (3.256)$$

and the parameters $(\tilde{x}, \tilde{\xi}, \tilde{\mu}, \tilde{\beta})$ characterise the response field $\tilde{\phi}$. For the ‘old’ version of LSI the space-time part $\mathcal{F}^{(\mu, \beta)}(\rho)$ (where $\rho := |\boldsymbol{\rho}|$ and $\boldsymbol{\rho} = \mathbf{r}(t-s)^{-1/\sigma}$) satisfies the following fractional differential equation

$$(\partial_\rho + z\mu \rho \partial_\rho^{2-z} + [\beta\mu + \mu(2-z)] \partial_\rho^{1-z}) \mathcal{F}^{(\mu, \beta)}(\rho) = 0. \quad (3.257)$$

which also illustrates that the ‘mass’ μ may be interpreted as a generalised diffusion constant. The fractional derivatives ∂_ρ^α are defined and discussed in [109]. Recall, however, that the definition used here is not unique and that different non-equivalent definitions for fractional derivatives exist [174, 200]. If $z = N + p/q$, where $N = [z]$ is the largest

integer less or equal to z , $0 \leq p/q < 1$ and p and q coprime, the solution of (3.257) by series methods is particularly simple, with the result [207]

$$\mathcal{F}^{(\mu, \beta)}(\rho) = \sum_{m \in \mathcal{E}} c_m \phi^{(m)}(\rho), \quad \text{with} \quad \phi^{(m)}(\rho) = \sum_{n=0}^{\infty} b_n^{(m)} \rho^{(n-1)z+p/q+m+1}. \quad (3.258)$$

The constants c_m are not determined by LSI and the set \mathcal{E} is

$$\mathcal{E} = \begin{cases} -1, 0, \dots, N-1 & p \neq 0 \\ 0, \dots, N-1, & p = 0 \end{cases}. \quad (3.259)$$

Finally, the coefficients $b_n^{(m)}$ read

$$b_n^{(m)} = \frac{(-z^2 \mu)^n \Gamma(p/q + 1 + m) \Gamma(n + z^{-1}(p/q + m) + \beta + 2 - z)}{\Gamma((n-1)z + p/q + m + 2) \Gamma(z^{-1}(p/q + m) + \beta + 2 - z)}. \quad (3.260)$$

such that $\phi^{(m)}(\rho)$ has an infinite radius of convergence for $z > 1$.

Let us now consider the magnetic response of the order-parameter, \mathcal{R}_{11} , the result for which we recall from (3.184) is

$$\begin{aligned} \mathcal{R}_{11}(\mathbf{r}; t, s) &= (2\pi)^d s^{-d/\sigma} \left(\frac{t}{s}\right)^{-\hat{\alpha}/2} (t/s - 1)^{-d/\sigma} \int_{\mathbf{k}} e^{i\mathbf{k} \cdot \mathbf{r}(t-s)^{-1/\sigma}} e^{-B|\mathbf{k}|^\sigma} \\ &= R(t, s) \sum_{n=0}^{\infty} a_n \rho^{2n}, \quad \rho = \mathbf{r}(t-s)^{-1/\sigma}, \end{aligned} \quad (3.261)$$

where the exponent $\hat{\alpha}$ is given by

$$\hat{\alpha} = \begin{cases} -d/\sigma & \text{case (I)} \\ -2 + d/\sigma & \text{case (IIa)} \\ 0 & \text{case (IIb)} \end{cases}. \quad (3.262)$$

Clearly, the space-time part of the 'old' LSI-prediction does *not* agree with this result since the exponents of ρ in eqs. (3.82) and (3.258) are linearly independent if z is not an integer. In eq. (3.261), we have expanded the exponential in order to rewrite this as a series in $\rho = |\boldsymbol{\rho}|$. This form of the series is incompatible with the expected form (3.258) for $z < 2$. In fact, it was this disagreement that motivated us to look for the new formulation of LSI, which uses a more appropriate form of fractional derivatives ∇_r^α and which was presented in chapter 2. We recall two more results for the 'new' version of LSI:

1. Generalised Bargmann superselection rule: *Let a system be given with dynamical exponent $z \neq 2$, ($k \in \mathbb{N}$). Let $\{\phi_i\}$ be a set of quasi-primary scaling operators, each characterised by the set $(x_i, \xi_i, \mu_i, \beta_i)$. Then the $(2n)$ -point function*

$$F^{(2n)} := \langle \phi_1(t_1, \mathbf{r}_1) \dots \phi_{2n}(t_{2n}, \mathbf{r}_{2n}) \rangle. \quad (3.263)$$

is zero unless the μ_i form n distinct pairs $(\mu_i, \mu_{\tau(i)})$ ($i = 1, \dots, n$), such that

$$\mu_i = -\mu_{\tau(i)}. \quad (3.264)$$

2. The decomposition (3.255) of the response function remains valid, but its space-time part now satisfies the fractional differential equation, which is quite similar to eq. (3.257)

$$(\partial_\rho + z\mu\rho\nabla_\rho^{2-z} + [\beta\mu + \mu(2-z)]\partial_\rho\nabla_\rho^{-z})\mathcal{F}^{(\mu,\beta)}(\rho) = 0. \quad (3.265)$$

A solution of equation (3.265) reads [21]

$$\mathcal{F}^{(\mu,\beta)}(\rho) = f_0 \int_{\mathbf{k}} e^{i\rho\cdot\mathbf{k}} |\mathbf{k}|^\beta \exp\left(-\frac{1}{z^2 i^{2-z}\mu} |\mathbf{k}|^z\right) \quad (3.266)$$

We see that this prediction of the ‘new’ formulation of LSI is fully compatible with our exact result (3.261) for $\mathcal{R}_{11}(t, s; \mathbf{r})$ if we identify

$$\mu_1 = -\tilde{\mu}_1 = (z^2 B i^{2-z})^{-1}, \quad \beta_1 = \tilde{\beta}_1 = 0, \quad g_0 = (2\pi)^d. \quad (3.267)$$

and set for the critical exponents

$$a_{11} = a'_{11} = \frac{d}{\sigma} - 1, \quad \lambda_R^{11} = d + \frac{\alpha\sigma}{2}. \quad (3.268)$$

This agreement supports the assumption that the fields ϕ and $\tilde{\phi}$ are both quasi-primary with $\mu = -\tilde{\mu}$ and $\beta = \tilde{\beta}$. This is further supported by the fact that $\mathcal{R}_{12}(t, t'; \mathbf{r}) = 0 = \mathcal{R}_{1\epsilon}(t, t'; \mathbf{r})$, which is predicted by LSI because of the generalised Bargmann superselection rule.

Having verified that the response function for the order-parameter field ϕ agrees with LSI, and thus having confirmed that ϕ is indeed quasi-primary, we now inquire whether this holds for composite operators. First, we consider the short-range model $\sigma \geq 2$. The relevant results can be read from those of section 2 if we let $\sigma \rightarrow 2$. Then the response $\mathcal{R}_{11}(t, s; \mathbf{r})$ in eq. (3.261) simplifies to

$$\mathcal{R}_{11}(t, s; \mathbf{r}) = s^{-d/2} \left(\frac{t}{s}\right)^{-\hat{\alpha}/2} \left(\frac{t}{s} - 1\right)^{-d/2} \exp\left(-\frac{1}{4B} \frac{\mathbf{r}^2}{t-s}\right), \quad (3.269)$$

up to a normalisation constant. Similarly, the temperature response of the spin² field, from the above expression and eq. (3.193), becomes

$$\mathcal{R}_2^{(T)}(t, s; \mathbf{r}) = s^{-d} \left(\frac{t}{s}\right)^{-\hat{\alpha}} \left(\frac{t}{s} - 1\right)^{-d} \exp\left(-\frac{1}{2B} \frac{\mathbf{r}^2}{t-s}\right), \quad (3.270)$$

which is of the form predicted by eq. (3.266), if we identify

$$\mu_2 = -\tilde{\mu}_2 = 2\mu_1, \quad \beta_2 = \tilde{\beta}_2 = 0, \quad (3.271)$$

and

$$a_{22} = a'_{22} = 2a_{11} + 1, \quad \lambda_R^{22} = 2\lambda_R^{11}. \quad (3.272)$$

Physically, we can therefore identify temperature changes as the conjugate variable to the spin-squared operator, at least for the short-ranged case. On the other hand, the spin² response \mathcal{R}_{22} to the perturbation $h_2(t, \mathbf{x})$ cannot be cast into that form. This can easily be seen in equation (3.210), which has a dependence on $t+s$, while the LSI-predicted form

does not contain this dependence. Note that this response function in a field-theoretical setting (see for example [226, 228]) corresponds to $\langle \phi^2(t, \mathbf{x})(\tilde{\phi}\tilde{\phi})(s, \mathbf{x} + \mathbf{r}) \rangle$.

Our findings suggest that for the short-range model the operator ϕ^2 , corresponding to spin^2 , is quasi-primary and so is the corresponding response field $\tilde{\phi}^2$ (obtained by locally perturbing the temperature). The parameters of these two fields are related to the fields ϕ and $\tilde{\phi}$ in the following way: If ϕ has the parameters (x, ξ, μ, β) then the parameters of ϕ^2 can be obtained from these by multiplying each parameter by the factor 2. Similarly the parameters of $\tilde{\phi}^2$ are related to those of $\tilde{\phi}$. On the other hand, we see that the composite operator $\phi\tilde{\phi}$ (defined by a perturbation of the external field $h_2(t, \mathbf{x})$) is *not* quasi-primary, and neither is the energy-density operator $\epsilon(\mathbf{x})$, even in the short-range model (that last finding is not surprising, since we have already seen in section 2 that $\epsilon(\mathbf{x})$ is related to the gradient of ϕ).¹³

We now proceed to the long-range model, where $0 < \sigma < 2$. \mathcal{R}_{22} cannot be brought into the LSI-predicted form, for the same reason as mentioned above for the short-range model, namely by comparing the $t+s$ dependence. The response function $\mathcal{R}_2^{(T)}$ cannot be brought into the LSI-predicted form either, since it contains a product of the type $\mathcal{F}^{(\mu, \beta)}(t, s; \mathbf{r})^2$. This again cannot be cast into the general form (3.266), except for $z = 2$. In this exceptional case, the special properties of a Gaussian integral ensure that $\mathcal{F}^{(\mu, \beta)}(t, s; \mathbf{r})^2$ can be rewritten in the form (3.266) upon redefinition of parameters. By a similar analysis we find that \mathcal{R}_{ϵ^2} does not have the LSI-predicted form. We conclude that the operator ϕ^2 is not quasi-primary under LSI for the long-range model, unlike for the short-range case $\sigma \geq 2$.

In a similar way, we also find that the response functions of the operator \mathcal{O}_ϵ , namely \mathcal{R}_{ϵ^2} and $\mathcal{R}_{\epsilon\epsilon}$, also do not have the form (3.255) and (3.266).

Summarising, we have seen that in the long-range model the above composite fields, though made of quasi-primary fields, are not quasi-primary. For the time being, the order-parameter ϕ and the associate response field $\tilde{\phi}$ related to a magnetic perturbation remain the only scaling operators with a simple transformation under local scale-transformations. This is distinct from the short-range case of $z = 2$. It remains an open question in which sense the transformation of, say, ϕ^2 is distinct from the one of ϕ . On the other hand, the generalised Bargman superselection rule (which follows from the weaker Galilei-invariance alone) has been confirmed in all cases, by assigning the following (relative) 'masses' to the fields

$$\mu_\phi = \mu, \quad \mu_{\mathcal{O}_2} = 2\mu, \quad \mu_{\mathcal{O}_\epsilon} = 2\mu, \quad (3.273)$$

and with negative masses to the corresponding response fields. This is natural because of the linear structure of the theory.

Correlation functions

Now we compare the LSI-prediction for the correlation function of the quasi-primary operator $\phi(t, \mathbf{x})$ with our exact result, see (3.202, 3.217, 3.233).

The LSI-prediction for the correlation function, for fully disordered initial conditions with

¹³In the Landau-Ginzburg classification of primary scaling operators in the minimal models of 2D conformal field-theory (Ising, Potts etc.), one usually has that ϕ and eventually a finite number of normal-ordered powers : $\phi :^\ell$ are primary.

white noise, is [21]:

$$C^{LSI}(t, s; \mathbf{r}) = C_{\text{init}}^{LSI}(t, s; \mathbf{r}) + C_{\text{th}}^{LSI}(t, s; \mathbf{r}), \quad (3.274)$$

with the ‘initial’ part

$$C_{\text{init}}^{LSI}(t, s; \mathbf{r}) = c_0 s^{-b_{\text{init}}+2\beta/z+d/z} y^{-b_{\text{init}}+\lambda_R/z+\beta/z} (y-1)^{b_{\text{init}}+d/z-2\lambda_R/z} \\ \times \int_{\mathbf{k}} |\mathbf{k}|^{2\beta} \exp\left(-\frac{|\mathbf{k}|^z}{z^2 \mu i^{2-z}}(t+s)\right) e^{i\mathbf{r}\cdot\mathbf{k}}, \quad (3.275)$$

and the ‘thermal’ part

$$C_{\text{th}}^{LSI}(t, s; \mathbf{r}) = 2T s^{-b_{\text{th}}+2\beta/z+d/z} y^{2\xi/z} (y-1)^{2(1+a')-2\lambda_R/z-4\xi/z} \\ \times \int_0^1 d\theta (y-\theta)^{-2(a'+1)+\lambda_R/z+2\xi/z+\beta/z+d/z} (1-\theta)^{-2(a'+1)+\lambda_R/z+2\xi/z+\beta/z+d/z} \\ \times \theta^{4\tilde{\xi}/z} g\left(\frac{1}{y} \frac{y-\theta}{1-\theta}\right) \int_{\mathbf{k}} |\mathbf{k}|^{2\beta} \exp\left(-\frac{|\mathbf{k}|^z s(y+1-2\theta)}{z^2 \mu i^{2-z}}\right) e^{i\mathbf{r}\cdot\mathbf{k}}. \quad (3.276)$$

Here the function $g(u)$ is not determined by the dynamical symmetries and ξ and $\tilde{\xi}$ can be considered as free parameters (Note that we have set $F = 0$ right from the beginning, as this form suffices to reproduce correctly the results).

In case I, the spin-spin correlation function (3.202) can be rewritten as

$$C(t, s; \mathbf{r}) = s^{-\hat{\alpha}} y^{-\hat{\alpha}/2} \int_{\mathbf{k}} e^{i\mathbf{r}\cdot\mathbf{k}} e^{-B|\mathbf{k}|^\sigma(t+s)}, \quad (3.277)$$

up to a normalisation constant, with $\hat{\alpha}$ given by (3.262). In this case ($T < T_c$), the contribution coming from the initial noise is the relevant one [37], and therefore we should compare with the spin-spin correlator $C_{\text{init}}^{LSI}(t, s; \mathbf{r})$. Indeed we find for the choice of parameters as given in (3.267), (3.268) and $b_{\text{init}} = 0$ that $C_{\text{init}}^{LSI}(t, s; \mathbf{r}) = C(t, s; \mathbf{r})$, as it should be.

In case IIa and IIb, the correlation function, as given in (3.217) and (3.233), can be rewritten in direct space as follows, using again (3.262) and up to normalisation constant,

$$C_{\text{th}}(t, s; \mathbf{r}) = 2T s y^{-\hat{\alpha}/2} \int_0^1 d\theta \theta^{\hat{\alpha}} \int_{\mathbf{k}} e^{-B|\mathbf{k}|^\sigma s(y+1-2\theta)} e^{i\mathbf{r}\cdot\mathbf{k}}. \quad (3.278)$$

For the cases *IIa* ($T = T_c, \sigma < d < 2\sigma$) and *IIb* ($T = T_c, d > 2\sigma$), in the LSI-prediction the term coming from the thermal noise is the relevant one [37, 45]. If we set $g(u) = 1$ and, in addition to the given choice of parameters (3.267) and (3.268), let

$$b_{\text{th}} = \frac{d}{z} - 1, \quad \text{and} \quad \xi = -\frac{1}{4} z \hat{\alpha}, \quad \tilde{\xi} = \frac{1}{4} z \hat{\alpha}, \quad (3.279)$$

we find agreement of the LSI-predicted correlation function $C_{\text{th}}^{LSI}(t, s; \mathbf{r}) = C(t, s; \mathbf{r})$.

3.3.4 Conclusions of this section

We have analysed the kinetics of the spherical model with long-range interactions when quenched onto or below the critical point T_c . For $T < T_c$ we have reproduced the results

of Cannas *et al.* [48] for the order-parameter and for $T = T_c$ we have derived exact results for the response and correlation function of the order parameter. We also considered, for $T \leq T_c$, various composite fields and derived their ageing exponents and scaling functions as listed in section 2. We then have carried out a detailed test of local scale-invariance using our analytical results. For this purpose, the long-range spherical model offers the useful feature that its dynamical exponent $z = \sigma$ depends continuously on one of the control parameters.

We have obtained the following results:

1. Dynamical scaling holds for various composite fields for quenches onto or below the critical temperature. The non-equilibrium exponents are given in table 3.3 and 3.4. The scaling functions also have been determined.
2. In the kinetic spherical model with short-ranged interactions ($\sigma > 2$ and hence $z = 2$), apart from the order-parameter field ϕ , its square too appears to be a quasi-primary scaling operator, as tested through several two-time response and correlation functions.
3. In the long-range spherical model, the first tests of the space-time response in a system with a tunable dynamical exponent have been performed. This shows that the formulation of LSI with $z \neq 2$, which we proposed earlier [109], even with the recent improvements given in [207], does not describe the exact result for \mathcal{R}_{11} when $0 < z < 2$, although that formulation did pass previous tests when $z = 2$ [110] or $z = 4$ [207, 19].
4. As can be seen from the fractional differential equation satisfied by the space-time response function, the precise definition of the fractional derivative used is crucial. We have presented in chapter 2 a systematic construction of new generators of local scale-invariance [21] where we have also shown that *all* previous tests where $z = 2$ or $z = 4$ are passed by the new formulation. Here we have seen that the exact results from the long-range spherical model are completely consistent with the new formulation of local scale-invariance.
5. In contrast to the short-range case where $z = 2$, the spin-squared field in the long-range model is no longer described by a quasi-primary scaling operator. This calls for a more systematic analysis, since it indicates that there might be new ways, not readily realized in conformal invariance, of non-quasi-primary scaling operators.
6. Both the two-time response and the correlation function of the order-parameter field ϕ are fully compatible with local scale-invariance in the entire range $0 < z = \sigma < 2$.

While the analytical results presented here certainly provide useful information, the eventual confirmation of local scale-invariance might appear fairly natural since the underlying Langevin equation is *linear*. Indeed, for linear Langevin equations we have actually *proven* local scale-invariance by using a decomposition of the Langevin equation into a ‘deterministic part’ for which non-trivial local scale-symmetries can be mathematically proven and a ‘noise part’ [192, 126, 21] (see also chapter 2). For non-linear Langevin equations the formal proof of non-trivial symmetries of the ‘deterministic part’ is still difficult, although progress has been made [222]. In the absence of exact solutions for models described

in terms of non-linear Langevin equations numerical tests going beyond merely checking the autoresponse function $R(t, s; \mathbf{0})$ will be required and it will be useful to be able to vary the value of the dynamical exponent z . In this context, a natural candidate for such studies is the disordered Ising model quenched to $T < T_c$, where it is already known that z depends continuously on the disorder and on temperature, see [188, 121, 125] and references therein. Furthermore, its Langevin equation is non-linear. The tests carried out so far in this system will be reported in the final part of this chapter

3.4 The diluted Ising model

All models studied so far have in common that they are based on linear equations of motion (which means, on the level of LSI, that $\beta = 0$). To get further confirmation on the theory, one has to look at nonlinear models, for instance the bond diluted Ising model quenched below the critical temperature. Here we will briefly show results on this model, which have been presented in more detail in [23] (see also [21]). The model is described by the Hamiltonian

$$\mathcal{H} = - \sum_{(i,j)} J_{ij} \sigma_i \sigma_j. \quad (3.280)$$

where the $\sigma_i = \pm 1$ are the usual Ising spin variables and J_{ij} are random variables which

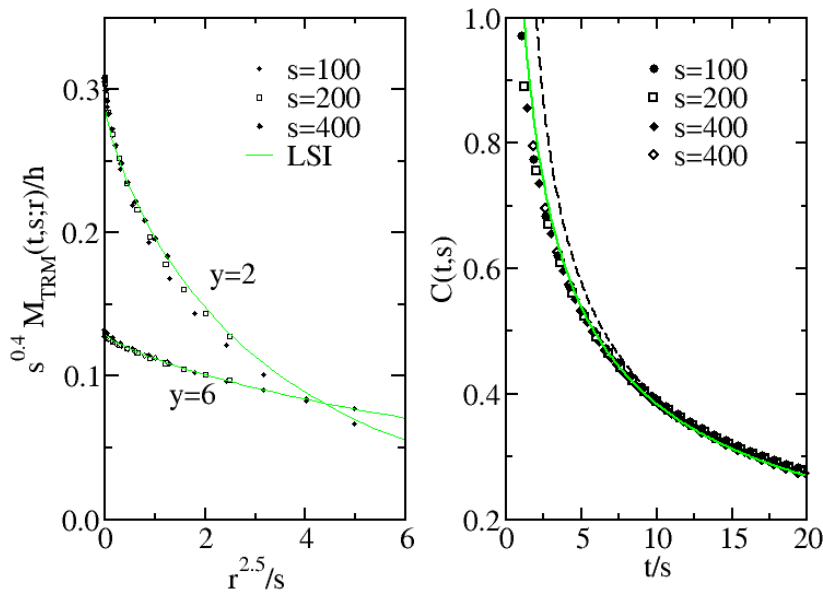


Figure 3.6: In the left panel the space-time behaviour of $M_{TRM}(t, s; \mathbf{r})$ for $z = 2.5$ is shown. The subleading correction term (3.286) has been subtracted to obtain scaling behaviour. In the right panel the predictions (2.158) (dashed line) and (2.167) (full line) for the autocorrelator for $z = 2.5$ are tested. The LSI-parameters used can be found in table 3.6.

are equally distributed over $[1 - \epsilon/2, 1 + \epsilon/2]$ with $0 \leq \epsilon \leq 2$. The kinetics (we suppose

a non-conserved order parameter) is described through a standard heat-bath algorithm. It has been shown [189, 204], that the dynamical exponent is given by the expression $z = 2 + \epsilon/T$, so that one can 'tune' z to values far away from 2 [121, 125] by choosing appropriate values for ϵ and T . In [121, 125], it was also found that there are very strong finite time scaling corrections which have to be subtracted. Also the required computing time to get acceptable data is quite high. In [121, 125] autoresponse and -correlation function were already considered. Here we look mainly at the space-time behaviour of the response function in order to test the LSI-prediction of the 'new' version of LSI as presented in chapter 2.

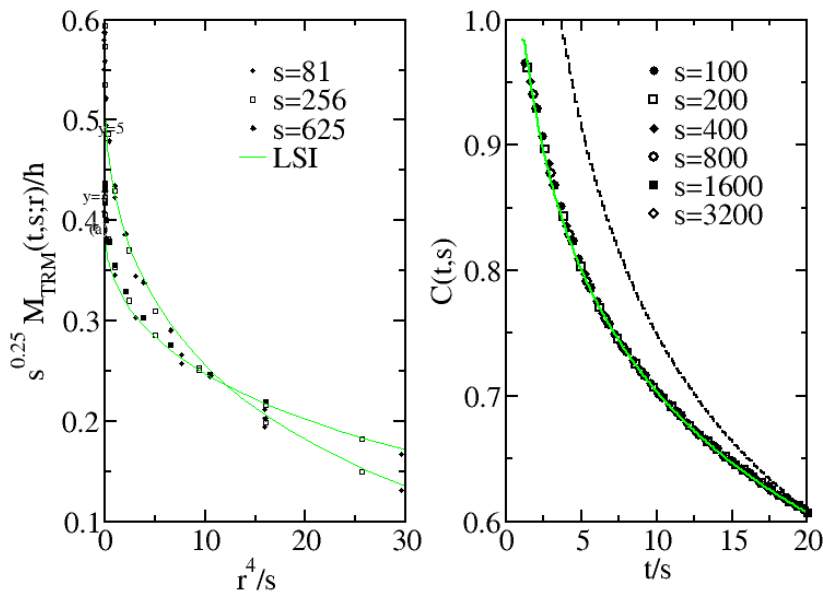


Figure 3.7: In the left panel the space-time behaviour of $M_{TRM}(t, s; \mathbf{r})$ for $z = 4$ is shown. The subleading correction term (3.286) has been subtracted to obtain scaling behaviour. In the right panel the predictions (2.158) (dashed line) and (2.167) (full line) for the autocorrelator for $z = 4$ are tested. The LSI-parameters used can be found in table 3.6.

Instead of measuring the response function directly it is much easier in simulations to measure the time-integrated response function

$$M_{TRM}(t, s; \mathbf{r}) := \int_0^s d\tau R(t, \tau; \mathbf{r}). \quad (3.281)$$

In order to identify the scaling behaviour of this quantity as predicted by LSI one can use the method developed in [112, 113, 110], which also yields the subleading correction terms. We take the form $R(t, s; \mathbf{r}) = R(t, s) \mathcal{F}^{(\mu, \gamma)}(|\mathbf{r}|(t-s)^{-1/z})$ as given in (2.152). Then it is well-known [131] that the response with respect to a fluctuation in the initial state should behave as $t^{-\lambda_R/z}$ for large times, i.e.

$$R(t, 0) \sim t^{-\lambda_R/z}. \quad (3.282)$$

On the other hand, it can be shown [240] that there is a time-scale $t_p \sim s^\zeta$ with $0 < \zeta < 1$ such that for $t - s \leq t_p$ the response function is still the one of the equilibrium system $R(t, s) = R_{gg}(t - s)$. Therefore, we can write

$$\begin{aligned} M_{TRM}(t, s; \mathbf{r}) &= \int_0^s d\tau R(t, s - \tau; \mathbf{r}) = \int_0^{t_p} d\tau R_{gg}(t - s + \tau) \mathcal{F}^{(\mu, \gamma)} \left(\frac{|\mathbf{r}|}{(t - s + \tau)^{1/z}} \right) \\ &+ \int_{t_p}^{t_\epsilon} d\tau R_{age}(t, s - \tau) \mathcal{F}^{(\mu, \gamma)} \left(\frac{|\mathbf{r}|}{(t - s + \tau)^{1/z}} \right) \\ &+ \int_{t_\epsilon}^s d\tau R_{ini}(t, 0) \mathcal{F}^{(\mu, \gamma)} \left(\frac{|\mathbf{r}|}{(t - s + \tau)^{1/z}} \right). \end{aligned} \quad (3.283)$$

where t_ϵ is another time-scale so that $s - t_\epsilon = O(1)$ [60, 240, 112]. $R_{age}(t, s - \tau)$ is the actual ageing part for which we insert the LSI-prediction (2.152). Then we get the

model	z	μ	γ/μ	$a = a'$	b_{th}	λ_R	λ_C	ξ	$\tilde{\xi}_2 = \tilde{\xi}$	ref.
SMc	4	$-\frac{1}{16}$	$\frac{1}{2}$	$\frac{d}{4} - \frac{1}{2}$	$\frac{d}{4} - \frac{1}{2}$	$d + 2$	$d + 2$	0	0	[19]
SMlr	$\sigma \in (0, 2)$	$(\sigma^2 B i^{2-\sigma})^{-1}$	$\frac{1}{2}$	$\frac{d}{4} - 1$	$\frac{d}{4} - 1$	$d + \frac{\hat{\alpha}\sigma}{2}$	$d + \frac{\hat{\alpha}\sigma}{2}$	$-\frac{1}{4}\sigma\hat{\alpha}$	$\frac{1}{4}\sigma\hat{\alpha}$	[20]
MH1	4	$-(16\nu_4)^{-1}$	$\frac{1}{2}$	$\frac{d}{4} - 1$	$\frac{d}{4} - 1$	d	d	0	0	[207]
MH2	4	$-(16\nu_4)^{-1}$	$\frac{1}{2}$	$\frac{d}{4} - 1$	$\frac{d}{4} - 1 - \frac{\rho}{2}$	d	$d - 2\rho$	0	0	[207]
MHc	4	$-(16\nu_4)^{-1}$	$\frac{1}{2}$	$\frac{d}{4} - 1$	$\frac{d}{4} - \frac{1}{2}$	d	$d + 2$	0	0	[207]

Table 3.5: Overview over all critical models with $z \neq 2$ considered in this chapter (SMc = spherical model with conserved order parameter as presented in section 3.2, SMlr = spherical model with long-range interaction as presented in section 3.3, MH1 = Mullins-Herring model with nonconserved noise, MH2 = Mullins-Herring model with coloured noise, MHc = Mullins-Herring model with conserved noise as presented in section 3.1). B is a constant, which can be found in [19], The constants ν_4, ρ and $\hat{\alpha}$ are defined in (3.2), (3.6) and (3.262) respectively. The remaining scaling function $g(u)$ has always been set to unity and $b'_{th} = 0$ everywhere. For the spherical model with conserved order parameter we have $F_2 = 1/2$, for all other models $F = 0$ (recall the definition (2.146) and (3.126) for F and F_2 respectively).

following result:

$$M_{TRM}(t, s; \mathbf{r}) = M_{eq}(t - s; \mathbf{r}) + r_1 t^{-\lambda_R/z} \mathcal{F}^{(\mu, \gamma)} \left(\frac{|\mathbf{r}|}{t^{1/z}} \right) + r_0 s^{-a} f_M \left(\frac{t}{s}, \frac{|\mathbf{r}|}{s^{1/z}} \right) \quad (3.284)$$

where r_1, r_0 are constants, $M_{eq}(t - s; \mathbf{r})$ is the equilibrium contribution and

$$\begin{aligned} f_M(y, w) &= \int_0^1 dv (1 - v)^{-1-a} \left(\frac{y}{1 - v} \right)^{1+a'-\lambda_R/z} \left(\frac{y}{1 - v} - 1 \right)^{-1-a'} \\ &\times \mathcal{F}^{(\mu, \gamma)} (w (y - 1 + v)^{-1/z}). \end{aligned} \quad (3.285)$$

In the scaling regime we do not expect the term $M_{eq}(t - s; \mathbf{r})$ to contribute, whereas the term

$$r_1 t^{-\lambda_R/z} \mathcal{F}^{(\mu, \gamma)} \left(\frac{|\mathbf{r}|}{t^{1/z}} \right) \quad (3.286)$$

gives a subleading contribution, which has to be taken into account. In the left panels of the pictures 3.6 and 3.7 we show plots of the simulated $M_{TRM}(t, s; \mathbf{r})$ for the value $z = 2.5$ and $z = 4$ respectively. From the simulational data the term (3.286) has been subtracted in order to obtain scaling behaviour. The LSI-prediction $s^{-a} f_M(t/s)$ (see (3.285)) was plotted also. The values for the LSI-parameters μ and γ used are given in table 3.6. We see that for both values of z we obtain scaling behaviour and that the LSI-predictions fits reasonably well with the data. In view of the fact that the simulational effort to obtain good data is very high, this is quite satisfying. In particular the relation (2.157) between λ_R and λ_C was confirmed.

model	z	μ	γ/μ	$a = a'$	b_{init}	λ_R	λ_C	ref.
SMlr	4	$-\frac{1}{16}$	$\frac{1}{2}$	$\frac{d}{4} - \frac{1}{2}$	$\frac{d}{4} - \frac{1}{2}$	$d + 2$	$d + 2$	[19]
RBIM	4	-0.42	0.51	0.25	0	1.32	1.28	[20]
RBIM	3	0.56i	0.53	0.25	0	1.53	1.47	[20]
RBIM	2.5	$0.66 \cdot i^{0.5}$	0.6	0.25	0	1.525	1.425	[20]

Table 3.6: Results for the case of phase-ordering dynamics (SMlr = spherical model with long-range interactions, RBIM = random bond diluted Ising model). Recall that the mass μ is related to the LSI-parameter α via $\alpha = (z^2 \mu^{2-z})^{-1}$ and γ/μ is connected to β via $2\gamma/\mu = (1 - \beta/(z - 2))$. The values for RBIM are taken from ([20]), where a more detailed table can be found.

We also compare for the same values of z the LSI-predictions (2.158) (dashed line) and (2.167) (full line) for the autoresponse function to the numerical data. This is shown in the right panels of figure 3.6 and 3.7. Clearly, for (2.158) one has at best a qualitative agreement and particularly for smaller values of $y = t/s$, the data deviate strongly from the the curve (2.158). In [23] we argue that the form (2.167) should be more appropriate and indeed we find for this case a much more convincing agreement with LSI. For more details on this, see [23]

Finally we list in table 3.5 the values of the LSI-parameters (for the 'new' version of LSI) of all critical models with $z \neq 2$ we considered in this chapter. We see that we have always $\gamma/\mu = 1/2$ for this models, as they were all based on linear equations of motion. The values of the LSI-parameters for the models undergoing phase-ordering are given in table 3.6. Here we do encounter cases with $\gamma/\mu \neq 1/2$. For certain values of z the diluted Ising model can have imaginary parameter μ , but the corresponding parameter $\alpha = (z^3 \mu^{2-z})^{-1}$ is always real.

Chapter 4

Ageing in reaction-diffusion systems

In this chapter, a new type of physical system will be considered - so-called reaction-diffusion systems which have already been briefly introduced in the first chapter. Technically, these systems can be microscopically described by a master equation, which can then be turned into a Schrödinger type equation, see [227] and references therein. Starting with this Schrödinger equation, one can then take a continuum limit and describe the system by a field-theoretical action $\mathcal{J}[\phi, \tilde{\phi}]$. We will not enter into the details of how this is done exactly, but refer the reader to the literature [139, 227, 228]. The important point is, that also here, we have the field-theoretical approach at our disposal, which is needed to apply LSI to these systems. Physically the important difference to magnetic systems is the absence of detailed balance, which means that there is no local time-reversal symmetry. This is connected to the existence of an absorbing state - a state which the dynamics of the system can reach, but not leave anymore. Another point which differs from the magnetic systems considered in chapter 3 is the fact, that the expectation value of the order parameter (which corresponds to the particle density in this case) is nonvanishing, in contrast to the situation we typically looked at in chapter 3. This can lead to problems for the application of LSI to these systems, as LSI was only formulated for the case of a vanishing average of the order parameter.

The investigation of ageing phenomena in such systems has started only quite recently in [80, 203], where the fermionic contact process was treated numerically. It was found, that at the critical point, dynamical scaling holds, but that the exponents a and b do not agree, unlike the situation one usually encounters in critical magnetic systems. This work also entailed an discussion about the applicability of LSI for the description of the autoresponse function [103, 123]. We hope to shed some more light on these questions in the present chapter.

We will start in section 4.1 by considering fermionic contact process from a field-theoretical perspective. We will confirm the findings of [80, 203] and discuss some of its consequences, but we will also point out, that LSI in its current state can not appropriately describe this model. In section 4.2 we will then pass to two bosonic reaction-diffusion systems, which can be solved exactly, the bosonic contact and pair-contact processes. Finally, in section 4.3, we will show how LSI can be extended to describe these bosonic systems. To this end we have to extend LSI for the case $z = 2$ to include non-linear Schrödinger equations.

Most of the content of this chapter has been published in the following articles, where also some additional information may be found.

- F. Baumann, M. Henkel, M. Pleimling and J. Richert, *J. Phys. A: Math. Gen.* **38**, 6623 (2005)
- F. Baumann, S. Stoimenov and M. Henkel, *J. Phys. A: Math. Gen.* **39**, 4095 (2006)
- F. Baumann, *J. Phys.: Conf. Ser.* **40**, 86 (2006)
- F. Baumann and A. Gambassi, *J. Stat. Mech.* P01002 (2007)

4.1 The fermionic contact process

4.1.1 Introduction

The contact process (CP) has been introduced long ago as a simple model for the spreading of diseases [101] (see also [139, 227, 228, 102, 178]). It is defined on a d -dimensional hypercubic lattice in which each site x is characterised by an occupation variable n_x and is either active (ill, $n_x = 1$) or inactive (healthy, $n_x = 0$). At each time step of the dynamics a site x is chosen at random. If x is inactive then it becomes active with a rate given by Λ times the fraction of its neighbouring sites which are already active (infection). Otherwise, if originally active, x becomes inactive with rate 1 (healing). In the long-time (non-equilibrium) stationary state all lattice sites will be eventually inactive (*absorbing phase*) if Λ is small enough, whereas for large enough Λ a finite fraction of sites will be active (*active phase*). These two phases are separated by a continuous phase transition for $\Lambda = \Lambda_c$ (with $\Lambda_c \simeq 3.3$ in $d = 1$, see, e.g., [102]) and a suitable order parameter is indeed the average density of active sites $\langle n_x \rangle$ in the stationary state.

Extensive Monte Carlo simulations of the CP have provided a very detailed quantitative description of its dynamical behaviour and of the associated non-equilibrium phase transition, which turns out to be in the same universality class as directed percolation and therefore its universal features are properly captured by the so-called *Reggeon field theory* (see, e.g., [139, 227, 228, 135, 49]).

The directed percolation (DP) universality class has been recently the subject of renewed interest in the context of ageing phenomena [80, 203, 103, 123], characterised by two-time quantities (such as response and correlation functions, see below) which are homogeneous functions of their time arguments and do not display the time-translational invariance which is expected in a stationary state. The two-time quantities of interest are the connected density-density correlation function $^1 C_{x-x'}(t, s) := \langle n_x(t)n_{x'}(s) \rangle - \langle n_x(t) \rangle \langle n_{x'}(s) \rangle$ and the response function $R_{x-x'}(t, s) := \delta \langle n_x(t) \rangle / \delta \kappa_{x'}(s) |_{\kappa=0}$ where $\kappa_{x'}(s)$ is the field conjugate to $n_{x'}(s)$ — corresponding to a local spontaneous activation rate of the lattice site x' at time s — and $\langle \dots \rangle$ stands for the average over the stochastic realization of the process.

In [80, 203] the ageing behaviour of the critical CP was investigated numerically. A system with a homogeneous initial particle density (corresponding to the active phase with $\Lambda \gg \Lambda_c$) was quenched at $t = 0$ to the critical point $\Lambda = \Lambda_c$ and $R_{x=0}(t, s)$ and $C_{x=0}(t, s)$ were determined, finding the following scaling behaviour ($t > s$)

$$R_{x=0}(t, s) = s^{-1-a} f_R(t/s), \quad C_{x=0}(t, s) = s^{-b} f_C(t/s), \quad (4.1)$$

where

$$f_R(y \gg 1) \sim y^{-\lambda_R/z}, \quad f_C(y \gg 1) \sim y^{-\lambda_C/z} \quad (4.2)$$

and $b = 2\beta/(\nu z) = 2\delta$ [β , ν , z and $\delta := \beta/(\nu z)$ are the standard critical exponents of DP, see, e.g., [102] — the values of z and δ for $d = 1, 2$ and 3 are reported in table 4.1]. In particular it was found that $\lambda_C/z = 1.85(10)$ and $\lambda_R/z = 1.85(10)$ for $d = 1$ [80, 203], whereas $\lambda_C/z = 2.75(10)$ and $\lambda_R/z = 2.8(3)$ for $d = 2$ [203]. These results suggest that $\lambda_R = \lambda_C$ independently of the dimensionality $d = 1$ and 2 . On the same numerical footing

¹In this section we will use a slightly different notation than in all other sections for correlation and response functions

it was noticed — with some surprise — that $1 + a = b$, in stark contrast to the case of slow dynamics of systems with detailed balance such as Ising ferromagnets, for which $a = b$ (see, e.g., [93, 45]). The fluctuation-dissipation ratio [57, 58, 93]

$$X(t, s) := T_b R_{x=0}(t, s) / \partial_s C_{x=0}(t, s) \quad (4.3)$$

and its long-time limit $X_\infty := \lim_{s \rightarrow \infty} \lim_{t \rightarrow \infty} X(t, s)$ have been used, for these magnetic systems evolving in contact with a thermal bath of temperature T_b , to detect whether the (equilibrium) stationary state has been reached, in which case the fluctuation-dissipation theorem yields $X_\infty = 1$. Given that $b = a + 1$ for the CP, the fluctuation-dissipation ratio — as defined in equation (4.3) — would always yield a trivial value of X_∞ and therefore it would not serve its purpose. In [80], it was suggested to consider, instead of X ,

$$\Xi(t, s) := \frac{R_{x=0}(t, s)}{C_{x=0}(t, s)} = \frac{f_R(t/s)}{f_C(t/s)} \quad (4.4)$$

and define $\Xi_\infty := \lim_{s \rightarrow \infty} \lim_{t \rightarrow \infty} \Xi(t, s)$, which has now a finite non-trivial value $\Xi_\infty = 1.15(5)$ for the CP in $d = 1$ [80]. (We comment on the meaning of Ξ in subsection 4.1.2.) In addition, the numerical results of [80, 203] support the applicability of the theory of local scale-invariance (LSI) [47, 109, 114, 192] (see chapter 2) to the ageing behaviour of the CP. This theory tries to use *local* space-time symmetries to constrain the form of $f_R(t/s)$ [see equation (2.2)] and has been applied to ageing phenomena in magnetic systems quenched from an initial high-temperature state to and below the critical temperature [47, 114, 192] and bosonic reaction-diffusion systems [17]. In the case of critical ageing of the Ising model with purely relaxational dynamics, early numerical simulations provided support to the predictions of LSI [47]. Subsequently, discrepancies were found both analytically [45, 43] (via a field-theoretical calculation at two loops) and numerically [198, 157] (via dedicated simulations). A more general version of LSI [123] — the version we shall refer to in this section — improved considerably the agreement with simulations while the disagreement with field-theoretical predictions remained. We point out that LSI in the present form [123] deals only with cases (such as those just mentioned) in which the relaxation of the system starts from a state with a vanishing mean value m_0 of the order parameter. In spite of this fact, the predictions of LSI are seemingly confirmed also in the CP [80, 203] and in the parity conserving non-equilibrium kinetic Ising model [179], for which $m_0 \neq 0$. Recent numerical simulations of the CP indicate, however, that the scaling function f_R predicted by LSI is incorrect for $t \simeq s$ [103, 123]. It was suggested in [123, 124] that one could possibly account for this discrepancy by extending LSI to include also the case $m_0 \neq 0$. As this extension is at present still lacking, in what follows we shall refer to the available version of LSI.

The previously mentioned (numerical) works leave some questions open:

- (i) Could the relations $1 + a = b$ and $\lambda_R = \lambda_C$ have been expected?
- (ii) Is $\lambda_R (= \lambda_C)$ an independent critical exponent?
- (iii) Is Ξ_∞ a *universal* quantity like X_∞ in ageing systems with detailed balance?
- (iv) To what extent does LSI (with $m_0 = 0$) actually describe some of the features of the ageing behaviour in the CP (with $m_0 \neq 0$)?

The aim of this part of the thesis is to answer these questions by adopting a field-theoretical approach.

The rest of the section is organised as follows. In subsection 4.1.2 we introduce the field-theoretical model (Reggeon field theory), the formalism and we set up the general framework for the perturbative expansion. In addition we discuss the expected scaling forms for the two-time response and correlation functions, the relation among the different ageing exponents and between X and Ξ , providing complete answers to the questions (i), (ii) and (iii). In subsection 4.1.3, we calculate the response function and its long-time ratio Ξ_∞ to the correlation function up to first order in the ϵ -expansion ($\epsilon = 4 - d$) and then we compare our results to the predictions of LSI ², providing an answer to question (iv). In subsection 4.1.4 we summarise our findings and present our conclusions. Some details of the calculation are reported in the appendix of [18].

4.1.2 The field-theoretical approach

As explained in detail in [139, 227, 228], the universal scaling properties of the CP (more generally, of the DP universality class) in the stationary state are captured by a Reggeon field-theoretical action S . In the critical case it reads

$$S[\varphi, \tilde{\varphi}] = \int d^d x dt \{ \tilde{\varphi} [\partial_t - D\nabla^2] \varphi - u(\tilde{\varphi} - \varphi)\tilde{\varphi}\varphi - h\tilde{\varphi} \}, \quad (4.5)$$

where $\varphi(x, t)$ and $h(x, t)$ are the coarse-grained versions of the particle density $n_x(t)$ and of the spontaneous activation rate of lattice sites $\kappa_x(t)$ (external perturbation), respectively, whereas $\tilde{\varphi}(x, t)$ is the response field, $u > 0$ the bare coupling constant of the theory and D the diffusion coefficient ($D = 1$ in what follows, unless differently stated).

In terms of the action (4.5), the average of an observable \mathcal{O} over the possible stochastic realizations of the process is given by $\langle \mathcal{O} \rangle = \int [d\varphi d\tilde{\varphi}] \mathcal{O} e^{-S[\varphi, \tilde{\varphi}]}$. As a result, the response of $\langle \mathcal{O} \rangle$ to the external perturbation h can be computed as $\delta \langle \mathcal{O} \rangle / \delta h(x, t) = \langle \tilde{\varphi}(x, t) \mathcal{O} \rangle$, leading to the following expression for the (linear) response function $R_{x-x'}(t, s) := \delta \langle \varphi(x, t) \rangle / \delta h(x', s)|_{h=0} = \langle \varphi(x, t) \tilde{\varphi}(x', s) \rangle_{h=0}$.

The action (4.5) with $h = 0$ and $t \in (-\infty, \infty)$ is invariant under the duality transformation

$$\tilde{\varphi}(x, t) \xleftrightarrow{\text{RR}} -\varphi(x, -t) \quad (4.6)$$

(the so-called *rapidity reversal* — RR) which implies that the scaling dimensions $[\dots]_{\text{scal}}$ of the fields φ and $\tilde{\varphi}$ are equal (see, e.g., [139, 227, 228]):

$$[\varphi(x, t)]_{\text{scal}} = [\tilde{\varphi}(x, t)]_{\text{scal}} = \beta/\nu. \quad (4.7)$$

Note that, as in the case of systems with detailed balance (DB), the scaling dimensions of the fields (with $t > 0$) do not change if RR (alternatively, DB) is broken by the presence of *initial conditions* (at time $t = 0$). If RR is a symmetry of S , then

$$\begin{aligned} C_{x-x'}(t, s) &:= \langle \varphi(x, t) \varphi(x', s) \rangle_{h=0} - \langle \varphi(x, t) \rangle_{h=0} \langle \varphi(x', s) \rangle_{h=0} \\ &\stackrel{\text{RR}}{=} \langle \tilde{\varphi}(x, -t) \tilde{\varphi}(x', -s) \rangle_{h=0} - \langle \tilde{\varphi}(x, -t) \rangle_{h=0} \langle \tilde{\varphi}(x', -s) \rangle_{h=0} = 0, \end{aligned} \quad (4.8)$$

²Notice that we compare here only to the LSI-prediction of the *autoresponse* function, which is the same for both versions of LSI

where the last equality is a consequence of causality [239] and therefore correlations vanish in the stationary state of the CP. On the other hand, a suitable initial condition (say, at time $t = 0$) can effectively generate correlations which decay for $t > 0$. Generally speaking one expects this decay to be exponential in t for $\Lambda \neq \Lambda_c$, due to a finite relaxation time both in the absorbing and active phase, whereas an algebraic decay is expected in the critical case $\Lambda = \Lambda_c$ we are interested in. (This picture is indeed confirmed by the numerical results of [80].) Accordingly, $C_{x=0}(t, s) := \langle \varphi(x, t)\varphi(x, s) \rangle - \langle \varphi(x, t) \rangle \langle \varphi(x, s) \rangle$ does no longer vanish during the relaxation from the initial condition and for $t, s \neq 0$ it has the same scaling dimension as $R_{x=0}(t, s)$. Two straightforward consequences of this fact are:

- (A) $1 + a = b$ [see equation (2.2)], which could have been expected on this basis and therefore is valid beyond the mere numerical coincidence³ and
- (B) $\Xi(t, s)$ [see equation (4.4)] — and therefore Ξ_∞ — is a ratio of two quantities with the same engineering and scaling dimensions and therefore it is a *universal* function (see, e.g., [202]) which takes the same value in all the models belonging to the same universality class (in particular, the lattice CP, the DP and the model (4.5) on the continuum). This is analogous to the case of X_∞ in systems with DB.

Scaling forms

The non-equilibrium dynamics of the CP after a sudden quench (at time $t = 0$) from the active phase $\Lambda \gg \Lambda_c$ (characterised by $\langle n_x(t < 0) \rangle = 1$ on the lattice and $\langle \varphi(x, t < 0) \rangle \neq 0$ on the continuum) to the critical point $\Lambda = \Lambda_c$ is partly analogous to the non-equilibrium relaxation of Ising systems with dissipative dynamics after a quench from a magnetised state (e.g., a low-temperature one with $T \ll T_c$, where T_c is the critical temperature) to the critical point $T = T_c$ [46]. In both cases the order parameter $m(t) := \langle \varphi(x, t) \rangle$ ^{4 5} provides a background for the fluctuations, with a *universal* scaling behaviour [229, 136, 137]

$$m(t) = A_m m_0 t^{\theta + \hat{a}} \mathcal{F}_M(B_m m_0 t^\varsigma) \quad (4.9)$$

where $m_0 := \langle \varphi(x, t = 0) \rangle$ is the initial value of the order parameter, \hat{a} is related to the scaling dimensions of the fields φ and $\tilde{\varphi}$ in real space via $\hat{a} = (d - [\varphi]_{\text{scal}} - [\tilde{\varphi}]_{\text{scal}})/z$ (we recall that $[\varphi]_{\text{scal}} = \beta/\nu$), θ is the so-called initial-slip exponent [136, 137] and $\varsigma = \theta + \hat{a} + \beta/(\nu z)$. In equation (4.9), $\mathcal{F}_M(v)$ is a universal scaling function once the non-universal amplitudes A_m and B_m have been fixed by suitable normalisation conditions, e.g., $\mathcal{F}_M(0) = 1$ and $\mathcal{F}_M(v \rightarrow \infty) = v^{-1} + O(v^{-2})$. [Note that $\mathcal{F}_M(v \rightarrow \infty) \sim v^{-1}$ is required in order to recover the well-know long-time decay of the order parameter $m(t) \sim t^{-\beta/(\nu z)}$.] Within the Ising universality class $\hat{a} = (2 - \eta - z)/z$ and $\theta \neq 0$ [136, 137, 45] whereas within the DP class $\hat{a} = -\eta/z$ (indeed $[\varphi]_{\text{scal}} = [\tilde{\varphi}]_{\text{scal}} = (d + \eta)/2$ [139]) and $\theta = 0$ [229]. In both cases it turns out that the width $\Delta_0 = \langle [\varphi(x, 0) - m_0]^2 \rangle$ of the initial distribution of the order parameter φ — assumed with short-ranged spatial correlations — is irrelevant [136, 137, 229] and controls only corrections to the leading

³The same conclusion can be drawn from the analysis presented in [180] (see also [139, 227, 228])

⁴For magnetic systems φ represents the local magnetisation whereas in the present case $\langle \varphi \rangle$ is the coarse-grained density of active sites.

⁵Hereafter we assume invariance of the system under space translations.

scaling behaviour, so that an initial state with $\Delta_0 \neq 0$ is asymptotically equivalent to one with no fluctuations $\Delta_0 = 0$. Equation (4.9) clearly shows that a non-vanishing value of the initial order parameter introduces an additional time scale in the problem $\tau_m = (B_m m_0)^{-1/\zeta}$ [139, 229, 46]. The long-time limit we are interested in is characterised by times $\gg \tau_m$ and therefore the relevant scaling properties can be formally explored in the limit $m_0 \rightarrow \infty$, i.e., $\tau_m \rightarrow 0$.

According to the analogy discussed above one expects the following scaling form for the two-time response function in momentum space (see, e.g., [139, 229] and subsection 3 in [46])

$$R_{q=0}(t > s, s) = A_R (t - s)^{\hat{a}} (t/s)^{\theta} F_R(s/t, B_m m_0^{1/\zeta} t), \quad (4.10)$$

where F_R is a universal scaling function once the non-universal amplitude A_R has been fixed by requiring, e.g., $F_R(0, 0) = 1$. In the case of the DP universality class, the two-time Gaussian correlation function $C_x^{(0)}(t, s)$ vanishes for $m_0 = 0$ — apart from irrelevant corrections due to a finite Δ_0 — whereas the two-time Gaussian response function $R_x^{(0)}(t, s)$ is invariant under time translations. Taking into account causality, it is easy to realize that all the diagrammatic contributions to the full response function (with $u \neq 0$) have the same invariance and therefore $\theta = 0$ and $F_R(s/t, 0) = 1$. (As opposed to the case of the Ising universality class, where $\theta \neq 0$ and $F_R(s/t, 0) \neq 1$ [41, 42, 43, 45, 198].) In fact, the case $m_0 = 0$ would correspond on the lattice to an initially empty system with $\Lambda = \Lambda_c$ where nothing happens as long as one does not switch on the external field $\kappa_{x'}(s)$. Accordingly, the response to $\kappa_{x'}(s)$ at time $s + \Delta t$ has to depend only on Δt and no ageing is observed.

In the long-time limit $t > s \gg \tau_m$ one expects F_R to become independent of the actual value of m_0 and therefore

$$F_R(x, v \rightarrow \infty) = \frac{\mathcal{A}_R}{A_R} x^{\theta - \bar{\theta}} \mathcal{F}_R(x), \quad (4.11)$$

where $\bar{\theta}$ is an additional exponent [related to λ_R , cf equation (4.18)], so that the resulting scaling is

$$R_{q=0}(t > s, s) = \mathcal{A}_R (t - s)^{\hat{a}} (t/s)^{\bar{\theta}} \mathcal{F}_R(s/t). \quad (4.12)$$

\mathcal{A}_R is a *non-universal* constant which can be fixed by requiring $\mathcal{F}_R(0) = 1$ and which has a *universal* ratio to A_R [see equation (4.11)]. For the Ising universality class, is was found [46]

$$\bar{\theta} = - \left(1 + \hat{a} + \frac{\beta}{\nu z} \right). \quad (4.13)$$

On the other hand, it is easy to see that the scaling arguments which were used to drawn this conclusion for the response function (see subsection 3 in [46]) are valid also for the CP.

In [180] the scaling behaviour of the two-time correlation function $C_{q=0}(t, s)$, after a quench from the active phase to the critical point, has been discussed with the result that (see equations (3.3) and (4.14) in [180])

$$C_{q=0}(t > s, s) = \mathcal{A}_C (t - s)^{\hat{a}} (t/s)^{\bar{\theta}} \mathcal{F}_C(s/t) \quad (4.14)$$

where the non-universal amplitude \mathcal{A}_C can be fixed by requiring $\mathcal{F}_C(0) = 1$, and $\bar{\theta}$ is indeed given by equation (4.13). Note that in analogy with Ξ [see equation (4.4)] one can

also define (we assume $t > s \gg \tau_m$)

$$\widehat{\Xi}(t, s) := \frac{R_{q=0}(t, s)}{C_{q=0}(t, s)} = \frac{\mathcal{A}_R \mathcal{F}_R(s/t)}{\mathcal{A}_C \mathcal{F}_C(s/t)} \quad (4.15)$$

[where we have used the scaling forms (4.12) and (4.14)] and

$$\widehat{\Xi}_\infty := \lim_{s \rightarrow \infty} \lim_{t \rightarrow \infty} \widehat{\Xi}(t, s) = \frac{\mathcal{A}_R}{\mathcal{A}_C} \quad (4.16)$$

which are, as $\Xi(t, s)$ and Ξ_∞ , a *universal* function and amplitude ratio, respectively. Although in general $\Xi(t, s) \neq \widehat{\Xi}(t, s)$, the argument discussed in [42, 41, 45] can be used to conclude that $\Xi_\infty = \widehat{\Xi}_\infty$ also in this case.

In what follows we focus on $R_{q=0}$ and $C_{q=0}$, i.e., the response and correlation function of the spatial average of the density of active sites ($N^{-1} \langle \sum_x n_x \rangle$ on a lattice with N sites). On the other hand, the corresponding scaling forms equation (4.12) and (4.14) can be easily generalised to $q \neq 0$ taking into account that this amounts to the introduction of an additional scaling variable $y = A_D D q^z (t - s)$ where A_D is a dimensional non-universal constant which can be fixed via a suitable normalisation condition. Accordingly, the scaling behaviour of the autoresponse $R_{x=0}$ and autocorrelation $C_{x=0}$ functions can be easily worked out from equations (4.12) and (4.14), leading to the identification of the exponents a , b and $\lambda_{R,C}$ in equations (2.2) and (4.2) as

$$1 + a = b = \frac{d}{z} - \hat{a} = \frac{2\beta}{\nu z} = 2\delta \quad (4.17)$$

and

$$\frac{\lambda_C}{z} = \frac{\lambda_R}{z} = \frac{d}{z} - \hat{a} - \bar{\theta} = 1 + \delta + \frac{d}{z}. \quad (4.18)$$

Therefore we conclude that:

- (C) λ_R is *equal* to λ_C beyond the mere numerical coincidence observed in [80, 203] and
- (D) $\lambda_R = \lambda_C$ is *not* an independent critical exponent but it is given by

$$\lambda_R = z + z\delta + d. \quad (4.19)$$

In table 4.1 we compare the values of $\lambda_{R,C}$ obtained from this scaling relation and the available estimates of δ and z to the results of fitting the asymptotic behaviour of the scaling functions $f_{C,R}$ [see equations (2.2) and (4.2)] from numerical data [80, 203]. The results reported in the last three columns are in quite good agreement both for $d = 1$ and 2.

The conclusions (A–D) we have drawn so far provide complete answers to the questions (*i–iii*) which we have posed at the end of the Introduction.

d	δ	z	$1 + \delta + d/z$	λ_R/z	λ_C/z
1	0.159464(6)	1.580745(10)	1.792077(10)	1.85(10) [80]	1.85(10) [80]
				1.9(1) [203]	1.9(1) [203]
				1.76(5) [103]	
2	0.451	1.76(3)	2.58(2)	2.75(10) [203]	2.8(3) [203]
3	0.73	1.90(1)	3.30(1)	not available	

Table 4.1: Comparison between the direct numerical estimates of $\lambda_{R,C}/z$ and the predictions of the scaling relation $\lambda_R/z(= \lambda_C/z) = 1 + \delta + d/z$ [see equation (4.18)] in which the available estimates of δ and z (taken from table 2 in [102]) are used. The values of $\lambda_{R,C}/z$ reported in the last two columns have been obtained by fitting the scaling behaviour of the autoresponse and autocorrelation function determined via density-matrix renormalisation-group computation [80] and by Monte Carlo simulations [203, 103] of the contact process.

Relation between X and Ξ

In [80] Ξ has been introduced on the basis of a formal analogy with the fluctuation-dissipation ratio $X(t, s)$. Here we argue that indeed X and Ξ play the same role in different circumstances.

The stationary state of a system with detailed balance is characterised by the time-reversal (TR) symmetry of the dynamics, which qualifies the state as an *equilibrium* one with a certain temperature T . Time-translational invariance (TT) and TR symmetry of the dynamics in the equilibrium state imply the fluctuation-dissipation theorem $TR_{x,q}(t, s) = \partial_s C_{x,q}(t, s)$, leading to $X = 1$ [see equation (4.3)]. In this sense $X \neq 1$ is a signature of the fact that the system has not reached its stationary (equilibrium) state. (This is usually due to slowly relaxing modes which prevent the system from “forgetting” the initial conditions of the dynamics [60, 45].) When detailed balance does not hold, TR is no longer a symmetry of the stationary state. In the specific case of the DP universality class, however, the *non-equilibrium* stationary state is characterised by a different symmetry, the rapidity-reversal [RR, see equation (4.6)], which leads — as discussed in subsection 4.1.2, equation (4.8) — to vanishing correlations and therefore to $\Xi^{-1}, \widehat{\Xi}^{-1} = 0$. Accordingly, $\Xi^{-1}, \widehat{\Xi}^{-1} \neq 0$ provides a signature of the fact that the system is not in its stationary state. In this sense Ξ ($\widehat{\Xi}$) is analogous to X for both of them indicate if the stationary state is eventually reached. In particular this occurs *generically* after a perturbation (e.g., a sudden change in the temperature T or the spreading rate Λ) and therefore $X_\infty = 1$ or $\Xi_\infty^{-1} = \widehat{\Xi}_\infty^{-1} = 0$. On the other hand, it may happen that for particular choices of the external parameters (e.g., T or Λ), slow modes emerge which prevent the system from achieving its stationary state. As a consequence, during this neverending relaxation of the system, TT is broken together with the possible additional symmetries which characterise the stationary state.⁶ This is what happens when ageing takes place in critical systems with detailed balance. In the next part we explicitly show that this is also the case for the contact process.

⁶The one described here is the typical pattern of the spontaneous breaking of a symmetry. See, e.g., [60].

The Gaussian approximation

The analytic computation of the response function follows the same steps as those discussed in [46] (see also [180]) for the non-equilibrium evolution of the Ising model relaxing from a state with non-vanishing value of the magnetisation. Here we briefly outline the calculation. We assume that the initial state has a non-vanishing order parameter $m_0 = \langle \varphi(x, t = 0) \rangle$ which is spatially homogeneous, so that the ensuing relaxation is characterised by translational invariance in space. It is convenient to subtract from the order parameter field $\varphi(x, t)$ its average value $m(t) = \langle \varphi(x, t) \rangle$, by introducing

$$\psi(x, t) := \varphi(x, t) - m(t) \quad \text{and} \quad \tilde{\psi}(x, t) := \tilde{\varphi}(x, t), \quad (4.20)$$

leading to $\langle \psi(x, t) \rangle = 0$ during the relaxation. The action S [see equation (4.5)] becomes, in terms of these fields,

$$S[\psi, \tilde{\psi}] = \int d^d x dt \left\{ \tilde{\psi} [\partial_t - \nabla^2 + 2\sigma] \psi - \sigma \tilde{\psi}^2 - u(\tilde{\psi} - \psi)\tilde{\psi}\psi \right\}, \quad (4.21)$$

where $\sigma(t) := u m(t)$ satisfies the equation of motion (no-tadpole condition)

$$\partial_t \sigma + \sigma^2 + u^2 \langle \psi^2 \rangle = 0. \quad (4.22)$$

Equations (4.22) and (4.21) are the starting point for our calculations. The Gaussian response and correlation function are obtained by neglecting anharmonic terms in equation (4.21):

$$R_q^{(0)}(t, s) = \theta(t - s) \exp \left\{ -q^2(t - s) - 2 \int_s^t dt' \sigma(t') \right\} \quad \text{and} \quad (4.23)$$

$$C_q^{(0)}(t, s) = 2 \int_0^{t <} dt' R_q^{(0)}(t, t') \sigma(t') R_q^{(0)}(s, t') \quad (4.24)$$

where $t < := \min\{t, s\}$. [In what follows we denote the results of the Gaussian approximation with the superscript (0).] In particular, solving (4.22) with $u = 0$ one finds (see also [180] and the appendix of [203]) $\sigma^{(0)}(t) = (t + \sigma_0^{-1})^{-1}$, which scales according to (4.9) ($\beta^{(0)} = 1$, $\nu^{(0)} = 1/2$, $z^{(0)} = 2$ and $\eta^{(0)} = 0$, see, e.g., [239]) with $A_m^{(0)} = 1$, $B_m^{(0)} = u$ and $\mathcal{F}_M^{(0)}(x) = (1 + x)^{-1}$. As explained in subsection 4.1.2, the leading behaviour for $t > s \gg \tau_m = (B_m m_0)^{-1/\zeta} = \sigma_0^{-1}$ can be explored by taking the limit $m_0 \propto \sigma_0 \rightarrow \infty$ from the very beginning. Accordingly, $\sigma^{(0)}(t) = t^{-1}$ and

$$R_q^{(0)}(t, s) = \theta(t - s) \left(\frac{s}{t} \right)^2 e^{-q^2(t-s)}, \quad (4.25)$$

$$C_q^{(0)}(t, s) = 2e^{-q^2(t+s)} (ts)^{-2} \int_0^{t <} dt' t'^3 e^{2q^2 t'}, \quad (4.26)$$

which (for $q = 0$) display the expected scaling behaviours (4.12) and (4.14) with $\mathcal{A}_R^{(0)} = 1$, $\mathcal{A}_C^{(0)} = 1/2$ and $\mathcal{F}_{C,R}^{(0)}(x) \equiv 1$. Equations (4.15) and (4.16) yield $\widehat{\Xi}^{(0)}(t, s) = \widehat{\Xi}_\infty^{(0)} = 2$, which is exact for $d > 4$ but it is almost twice as large as the result which was found in $d = 1$, $\widehat{\Xi}_\infty = 1.15(5)$ [80]. As explained in subsection 4.1.2, $\Xi^{-1} \neq 0$ is a signal of the breaking of the RR symmetry characterising the non-equilibrium stationary state of the

CP (and of the DP universality class in general). Here we show explicitly (within the Gaussian approximation — though the conclusion is expected to be valid also beyond the approximation) that only the homogeneous fluctuation mode $q = 0$ is, at criticality, responsible for such a breaking, as in the case of systems with detailed balance (see, e.g. [45, 43, 46, 42, 41]). Indeed, let us generalise equation (4.15) to modes with $q \neq 0$:

$$\widehat{\Xi}_q^{-1}(t > s, s) := \frac{C_q(t, s)}{R_q(t, s)}. \quad (4.27)$$

Within the Gaussian approximation one readily finds [see equations (4.25) and (4.26)]

$$\left[\widehat{\Xi}_q^{(0)}(t, s)\right]^{-1} = \frac{1}{2} \frac{4!}{y^4} \left(e^{-y} - 1 + y - \frac{y^2}{2!} + \frac{y^3}{3!} \right) \Big|_{y=2Dq^2s}, \quad (4.28)$$

where the additional scaling variable $y = A_D D q^2 s = D q^2 s$ appears. This expression

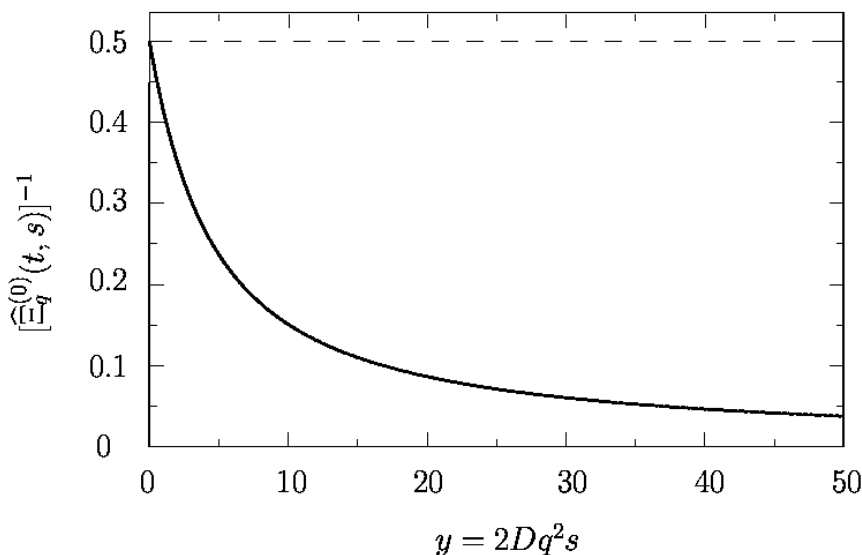


Figure 4.1: Ratio $[\widehat{\Xi}_q^{(0)}(t, s)]^{-1}$ of the correlation function to the response function [see equation (4.27)] within the Gaussian approximation (which becomes exact for $d > 4$). In the long-time limit $s \rightarrow \infty$, $[\widehat{\Xi}_q^{(0)}(t, s)]^{-1}$ vanishes, unless $q = 0$, in which case it takes the value $1/2$. $[\widehat{\Xi}_q^{(0)}]^{-1} \neq 0$ signals the breaking of RR [see equation (4.6) and subsection 4.1.2].

— as the Gaussian fluctuation-dissipation ratio for systems with detailed balance (see, e.g. [42, 41]) — is independent of t and depends on y only. In particular, in the long-time limit $s \gg q^{-2}$ one has $[\widehat{\Xi}_q^{(0)}(y \gg 1)]^{-1} \sim 1/y \rightarrow 0$, for any mode with $q \neq 0$, indicating that the RR symmetry is asymptotically realized. On the other hand, for $q = 0$, $[\widehat{\Xi}_q^{(0)}(y = 0)]^{-1} = 1/2$, independently of s . For a quench into the active phase $\Lambda > \Lambda_c$ the action S and the propagators (4.25) and (4.26) get modified according to $q^2 \rightarrow q^2 + r$, with $r > 0$ (see, e.g., [227, 228, 139]). Therefore in this case, $y = 2D(q^2 + r)s$, yielding $[\widehat{\Xi}_q^{(0)}(y \gg 1)]^{-1} \rightarrow 0$ for $s \gg r^{-1}$ and independently of q , in agreement with what has been stated before and with the available numerical evidences [80].

4.1.3 The response function

In this subsection we determine the response function up to first order in $\epsilon = 4 - d$ (4 being the upper critical dimension d_{ucd} of the model [227, 228], above which the Gaussian results become exact). Some of the details of the calculation are provided in the appendix of [18].

For future reference we recall that the critical exponents of the DP universality class are [139, 102, 227, 228] $\eta = -\epsilon/6 + O(\epsilon^2)$, $z = 2 - \epsilon/12 + O(\epsilon^2)$, $\beta/\nu = (d + \eta)/2$ and therefore [see equation (4.13)]

$$\hat{a} = -\frac{\eta}{z} = \frac{\epsilon}{12} + O(\epsilon^2) \quad \text{and} \quad \bar{\theta} = -2 + \frac{\epsilon}{6} + O(\epsilon^2). \quad (4.29)$$

The expression for the renormalised response function is (where $x := s/t \leq 1$)

$$\begin{aligned} R_{R,q=0}(t, s) &= x^2 \left\{ 1 + \epsilon \left[-\frac{1}{4} \ln x + \frac{1}{12} \ln s \right. \right. \\ &\quad \left. \left. + \frac{\pi^2}{12} + \frac{\ln(1-x)}{x} - \frac{1}{2} \text{Li}_2(x) - \frac{11}{12} \ln(1-x) + \frac{x}{12} \right] \right\} + O(\epsilon^2), \end{aligned} \quad (4.30)$$

(see the appendix of [18] for details) which can be cast in the expected scaling form (4.12) with

$$\mathcal{A}_R = 1 - \epsilon \left(1 - \frac{\pi^2}{12} \right) + O(\epsilon^2), \quad (4.31)$$

$$\mathcal{F}_R(x) = 1 + \epsilon \left[1 + \frac{x}{12} + \left(\frac{1}{x} - 1 \right) \ln(1-x) - \frac{1}{2} \text{Li}_2(x) \right] + O(\epsilon^2), \quad (4.32)$$

[note that $\mathcal{F}_R(0) = 1$ and $\mathcal{F}_R(x \rightarrow 1^-) = 1 + \epsilon(13 - \pi^2)/12 + O(\epsilon^2)$] and the proper exponents (4.29).

Comparison with LSI

For the response function, LSI (with $m_0 \neq 0$) provides the following prediction [123]:

$$R_{q=0}(t > s, s) = r_0 s^A x^B (1-x)^C, \quad (4.33)$$

where $x := s/t$ and A , B , C and r_0 are free parameters. In a first version of LSI it was assumed $A = C$ but more recently it has been suggested that this constraint can be relaxed [192, 123]. On the other hand, requiring $R_{q=0}$ to have the correct scaling dimension (see subsection 4.1.2), leads to $A = \hat{a} = -2\delta + d/z$. In addition, the well-established short-time behaviour $s/t \rightarrow 0$, from equation (4.12), leads to $B = -\bar{\theta} - \hat{a} = 1 + \delta$. The last free parameter, C , can be in principle fixed by requiring the response function to display a *quasi-stationary* regime (analogous to the quasi-equilibrium regime in systems with detailed balance, see, e.g., subsection 2.5 in [45]) for $\Delta t := t - s \ll s$, in which the behaviour of the system depends only on Δt and not on s . This would require $C = A$ [103]. In turn, comparing with equation (4.12), this would imply $\mathcal{F}_R(x) = 1$, $\forall x \in [0, 1]$ which is in contrast with the analytical expression in equation (4.32). The discrepancy between the actual scaling behaviour of the CP and the prediction of LSI with $A = C$, was originally overlooked in [80] but then it became apparent for $t/s \lesssim 2$ in the detailed numerical

analysis carried out in [103], which is also supported by our analytical result. On the other hand, if one questions the existence of such a quasi-stationary regime in the CP, C remains an available fitting parameter. By adjusting it the agreement between numerical data and LSI improves significantly [123], down to $t/s - 1 \simeq 10^{-1}$, being discrepancies observed only for smaller $t/s - 1$ [103]. It has been suggested [123] that such discrepancies might be caused by corrections to scaling due to having $t - s$ of the order of microscopic time scales when exploring the regime $t/s - 1 \simeq 0$ with finite s — However, this does not seem to be the case for the data reported in [103].

In order to compare the analytic expression of $R_{q=0}(t, s)$ to the prediction of LSI with $C \neq A$ we introduce the quantity $\mathcal{R}(x) := \mathcal{A}_R^{-1}(t-s)^{-\hat{a}}(t/s)^{-\hat{\theta}} R_{q=0}(t, s)$ where \mathcal{A}_R is fixed by the requirement $\mathcal{R}(x \rightarrow 0) = 1$. Accordingly, the field-theoretical prediction (4.12), yields (for $d < 4$)

$$\mathcal{R}_{\text{FT}}(x) = \mathcal{F}_R(x) = 1 + \epsilon \mathfrak{f}(x) + O(\epsilon^2) \quad (4.34)$$

where $\mathfrak{f}(x)$ is given by the expression in square brackets in equation (4.32):

$$\mathfrak{f}(x) := 1 + \frac{x}{12} + \left(\frac{1}{x} - 1\right) \ln(1-x) - \frac{1}{2} \text{Li}_2(x), \quad (4.35)$$

with $\mathfrak{f}(1) = (13 - \pi^2)/12$. LSI predicts, instead,

$$\mathcal{R}_{\text{LSI}}(x) = (1-x)^{\Delta C} \quad (4.36)$$

where $\Delta C := C - A$. Above the upper critical dimension $d_{\text{ucd}} = 4$, $\mathcal{R}_{\text{FT}}(x) \equiv 1$ and \mathcal{R}_{LSI} fit it with $\Delta C = 0$. Assuming continuity of critical exponents, one expects for $d < 4$ (i.e., $\epsilon > 0$), $\Delta C = c_1 \epsilon + O(\epsilon^2)$, — where c_1 is a fitting coefficient — and therefore $\mathcal{R}_{\text{LSI}}(x) = 1 + \epsilon c_1 \ln(1-x) + O(\epsilon^2)$. Of course $\mathcal{R}_{\text{FT}} - \mathcal{R}_{\text{LSI}} = \epsilon[\mathfrak{f}(x) - c_1 \ln(1-x)] + O(\epsilon) \neq 0$ for $\epsilon > 0$ (i.e., $d < 4$) whatever the choice of c_1 is, as it is clear by inspecting the expression (4.35). Strictly speaking LSI in its present form *is not* a symmetry of $R_{q=0}(t, s)$, whatever ΔC is, at least sufficiently close to d_{ucd} (small ϵ). Nonetheless, the shape of $\mathfrak{f}(x)$ is such that a proper choice of c_1 can reduce the difference $\mathcal{R}_{\text{FT}} - \mathcal{R}_{\text{LSI}}$. In figure 4.2 we report the comparison between $\ln \mathcal{R}_{\text{FT}}(x) = \epsilon \mathfrak{f}(x) + O(\epsilon^2)$ and $\ln \mathcal{R}_{\text{LSI}}(x) = \epsilon c_1 \ln(1-x) + O(\epsilon^2)$ with $c_1 = 0$ (i.e., $C = A$) and $c_1 = -0.081(2)$ (corresponding to $C \neq A$). This plot clearly indicates that the scaling function $\mathcal{R}_{\text{FT}}(x)$ shows corrections to the behaviour predicted by LSI with $C = A$ already for $t/s - 1 \lesssim 8$, i.e., $0.11 \lesssim x \leq 1$, for which $\mathcal{R}_{\text{FT}}(x)/\mathcal{R}_{\text{LSI}}(x) \gtrsim 1 + 0.01\epsilon + O(\epsilon^2)$. On the other hand the same discrepancy is observed only for $t/s - 1 \lesssim 0.2[0.13]$, i.e., $0.83[0.88] \lesssim x \leq 1$ for $c_1 = -0.083[-0.079]$ and therefore a suitable choice of c_1 (i.e., C) reduces by more than one order of magnitude the value of $t/s - 1$ below which the difference between the predicted scaling behaviour and LSI becomes sizable. This is analogous to what has been observed in numerical data [103, 81] for the scaling of the autoresponse function $R_{x=0}(t, s)$. (See, e.g., figure 2 in [103].) On the other hand, the field-theoretical results presented here are free from numerical artefacts and corrections to scaling, which were invoked in [123] to explain the findings of [103].

As a result of our fitting procedure, we have determined the “ ϵ -expansion” of the exponent ΔC , finding $\Delta C = -0.081(2)\epsilon + O(\epsilon^2)$. According to the notations adopted in [123] $\Delta C = -(a' - a)$ and therefore we conclude that $a' - a = +0.081(2)\epsilon + O(\epsilon^2)$. For the one-dimensional contact process it was found $a' - a = +0.270(10)$ [123, 103]⁷, whose

⁷Note that in [103] the value of a' is reported with the wrong sign.

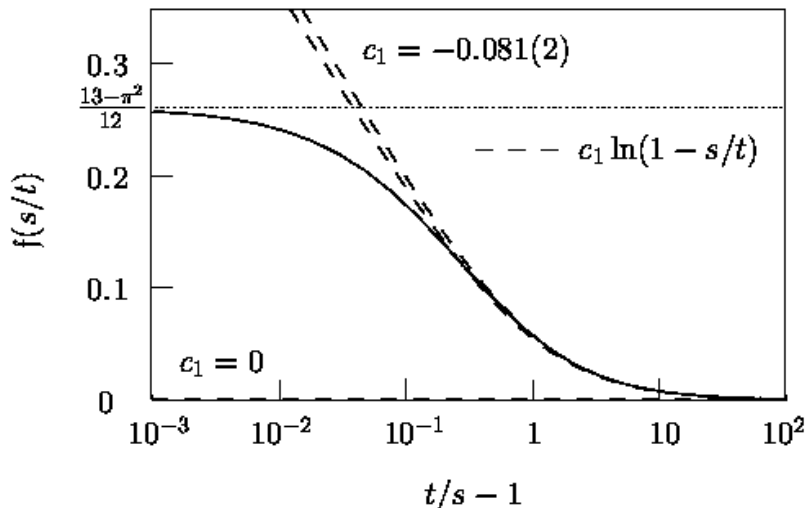


Figure 4.2: Comparison between $\epsilon^{-1} \ln \mathcal{R}_{\text{FT}}(x)$ and $\epsilon^{-1} \ln \mathcal{R}_{\text{LSI}}(x)$ for two different values of the fit-parameter c_1 .

sign is indeed in agreement with our result (generally speaking, the sign of the correction to the Gaussian behaviour is correctly captured by the lowest non-trivial order in the standard ϵ -expansion). Insisting in interpreting our result as an ϵ -expansion we can even attempt an estimate of $a' - a$ in physical dimensions $\epsilon = 1, 2$ and 3 . It comes as a surprise that not only the order of magnitude is the correct one but also the estimate for the one-dimensional CP (i.e., $\epsilon = 3$) $a' - a \simeq +0.24$ is in very good agreement with the actual numerical result.

In passing, we note that a mechanism similar to the one described here could possibly explain the (apparent) agreement between LSI with $C \neq A$ and the scaling form of the integrated response function of the magnetisation in the Ising model quenched from high temperatures to the critical point [198, 123].

One-loop prediction for Ξ

The correlation function was already calculated in [180], up to one loop in the ϵ -expansion, with the result

$$2\mathcal{A}_C = A \times \left[1 - \frac{\epsilon}{6} F(\infty) \right] + O(\epsilon^2) = 1 + \frac{\epsilon}{6} \left(\frac{9\pi^2}{20} - \frac{361}{80} \right) + O(\epsilon^2) \quad (4.37)$$

and

$$\mathcal{F}_C(x) = 1 - \frac{\epsilon}{6} [F(x^{-1}) - F(\infty)] + O(\epsilon^2) \quad (4.38)$$

where A and F are given, respectively, in equation (4.4) and (3.5) therein. Accordingly, we obtain for the ratio $\widehat{\Xi}_\infty$ in (4.16) the value

$$\widehat{\Xi}_\infty = 2 \left[1 - \epsilon \left(\frac{119}{480} - \frac{\pi^2}{120} \right) \right] + O(\epsilon^2). \quad (4.39)$$

Clearly the Gaussian value of $\widehat{\Xi}_\infty$ gets a downward correction ($119/480 - \pi^2/120 \simeq 0.166$) for $\epsilon > 0$. This is qualitatively satisfying, as it brings the theoretical estimate closer to

the value which was determined numerically for $d = 1$ [$\Xi_\infty = 1.15(5)$]. In addition, a direct extrapolation of equation (4.39) to $\epsilon = 3$ (neglecting possible $O(\epsilon^2)$ terms) yields $\widehat{\Xi}_\infty^{d=1} = 1.01$ which is — for a one-loop calculation — in a surprisingly good agreement with the actual value.⁸ More reliable theoretical estimates can only be based on the knowledge of higher-loop contributions.

4.1.4 Conclusions of this section

In this section we have studied the ageing behaviour in the contact process by adopting a field-theoretical approach. The results presented here equally apply to all the models belonging to the same universality class as the contact process, such as the directed percolation.

We confirmed analytically the scaling behaviour

$$R_{x=0}(t, s) = s^{-1-a} f_R(t/s), \quad C_{x=0}(t, s) = s^{-b} f_C(t/s), \quad (4.40)$$

which was observed numerically for the two-time response and correlation functions [80, 203] after a quench from the active phase to the critical point. In addition we have shown that:

- (a) The relation $b = 1 + a$ — due to the rapidity-reversal symmetry — and $\lambda_R = \lambda_C$ [see equation (4.2)] hold beyond the numerical evidences provided in [80, 203].
- (b) $\lambda_{R,C}$ are related to known static and dynamic exponents via $\lambda_{R,C} = z(1 + \delta) + d$ [see equation (4.19)], which is confirmed by the available numerical data (see table 4.1).⁹
- (c) The ratio Ξ of the response to the correlation function [equation (4.4)] defines a *universal function* and its long-time limit Ξ_∞ a *universal amplitude ratio*, which can therefore be studied within a field-theoretical approach.

The result of the ϵ -expansion around $d = 4$ [see equation (4.39)] is in qualitative agreement with the numerical estimate of $\Xi_\infty^{d=1}$ [80].

- (d) After a quench, $\Xi_\infty^{-1} \neq 0$ for the CP, like $X_\infty - 1 \neq 0$ for systems satisfying detailed balance, is a signature of the spontaneous breaking of the symmetry \mathfrak{S} associated with the corresponding non-equilibrium ($\mathfrak{S} =$ rapidity-reversal) and equilibrium ($\mathfrak{S} =$ time-reversal) stationary states.

⁸Extrapolating the result (4.39) as $\widehat{\Xi}_\infty^{(\text{extr})} = 2/[1 + \epsilon(119/480 - \pi^2/120)]$ would give 1.33 for $\epsilon = 3$, still not too far from the numerical result.

⁹In passing we mention that the relation $\lambda_R/z = 1 + \beta/(\nu z) + d/z$ (see equations (4.13) and (4.18)) — as derived in [46] — is generically valid for critical models with relaxational dynamics (irrespective of DB and of the relation between a and b defined in equation (2.2)), short-range correlations of the order parameter in the initial state and in which the average value $m(t)$ of the order parameter decays in time according to equation (4.9) with $m_0 \neq 0$. In addition to the DP universality class discussed in this note, this fact has been confirmed analytically and/or numerically for vector models with $O(N)$ symmetry [123] ($N = 1$ corresponds to the Ising universality class [46]) and for the parity-conserving non-equilibrium kinetic Ising model (PCNEKIM) in one spatial dimension [179]. The same relation for λ_C (which implies $\lambda_C = \lambda_R$), instead, has been derived in less generality for $O(N)$ vector models [46, 123] and for the CP [180] by taking advantage of some of their specific properties. The corresponding proofs do not seem to have a straightforward extension to other cases. On the other hand, the fact that $\lambda_C = \lambda_R$ also in the one-dimensional PCNEKIM (see the numerical evidences in [179]) suggests that such an extension might exist.

In general, whenever the (non-equilibrium) stationary state of a model is characterised by a symmetry \mathfrak{S} , every (universal) quantity whose value is constrained by \mathfrak{S} plays the same role as X_∞ and Ξ_∞^{-1} in detecting the onset of slow dynamics.

- (e) The *universal* scaling function $\mathcal{F}_R(x)$ — describing the ageing behaviour of the response function $R_{q=0}(t, s)$ [see equation (4.12)] — *does not* agree with the prediction of the theory of local scale-invariance when the non-Gaussian fluctuations are taken into account [specifically already at $O(\epsilon)$ for $\epsilon > 0$, see equation (4.32)]. It remains to be seen whether an extension of LSI to systems with nonvanishing order parameter will be able to describe correctly the scaling function of the CP.

4.2 Exactly solvable models

4.2.1 Introduction

We have seen in the previous section, that one of the most prominent reaction diffusion system, the fermionic contact process, shows dynamical scaling behaviour at the critical point. In contrast to systems satisfying detailed balance the equality $a = b$ was broken, whereas $\lambda_G = \lambda_R$ remained true. In this section we will consider two *bosonic* reaction-diffusion systems. This means, that there is *no restriction* on the number of particles on a lattice sites. Particle annihilation and creation processes take place at one lattice point now and the possible offspring particle is placed on the same lattice site as the parent particle(s). These models offer the great advantage that they can be solved analytically, which will help to shed more light on the issues raised in the previous sections.

As we said before, an important ingredient in the ageing studies of magnetic systems is the assumption of detailed balance for the dynamics. This begs the question what might happen if that condition is relaxed. Indeed, numerical and field-theoretical studies of the contact process - as discussed in section 4.1 - gave the following results [80, 203, 207]:

1. Dynamical scaling and ageing only occur *at* the critical point. This is expected since both inside the active and the inactive phases there merely is a single stable stationary state.
2. At criticality, the scaling forms eqs. (1.11) hold true for the (connected) autocorrelator and the response function, but with the scaling relation

$$a + 1 = b = \frac{2\beta}{\nu_\perp z}, \quad (4.41)$$

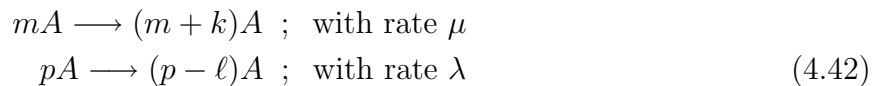
in contrast to eq. (1.15), with β and ν_\perp being now standard steady-state exponents.

In order to get a better understanding of these results, it would be helpful to study the ageing behaviour in exactly solvable but non-trivial models without detailed balance. Remarkably, it has been realized by Houchmandzadeh [129] and by Paessens and Schütz [184] that the bosonic versions of the contact process and of the critical pair-contact process (where an arbitrary number of particles are allowed on each lattice site) are exactly solvable, at least to the extent that the dynamical scaling behaviour of equal-time correlators can be analysed exactly [129, 184, 185]. Here we extend their work by

means of an exact calculation of the two-time correlation and response functions for the bosonic contact process and the critical bosonic pair-contact process. In subsection 4.2.2, we define the models and write down the closed systems of equations of motion for the correlation and response functions. We also recall the existing results on the single-time correlators [129, 184]. In subsection 4.2.3, we discuss the bosonic contact process and in subsection 4.2.4, we describe our results for the critical pair-contact process. In subsection 4.2.5 we give the results for the two-time response functions. As we shall see, the critical bosonic pair-contact process provides a further example of a model where a and b are different. In subsection 4.2.6 we conclude. A detailed discussion of local scale-invariance in these models is presented in section 4.3 of this chapter.

4.2.2 The models

Consider the following stochastic process: on an infinite d -dimensional hypercubic lattice particles move diffusively with rate D in each spatial direction. Each site may contain an arbitrary non-negative number of particles. Furthermore, on any given site the following reactions for the particles A are allowed



It is to be understood that on a given site, out of any set of m particles k additional particles are created with rate μ and ℓ particles are destroyed out of any set of $p \geq \ell$ particles with rate λ . Diffusion applies on single particles. We shall be concerned with two special cases:

1. the *bosonic contact process*, where $p = m = 1$, hence $\ell = 1$. The value of k is unimportant and will be fixed to $k = 1$ as well.
2. the *bosonic pair-contact process*, where $p = m = 2$.

While the bosonic contact process arose from a study on the origin of clustering in biology [129], the bosonic pair-contact process as defined here [184] is an offshoot of a continuing debate about the critical behaviour of the diffusive pair-contact process (PCPD), see [115] for a recent review. Initially, this model was introduced [130] in an attempt to understand the meaning of ‘imaginary’ versus ‘real’ noise but the associated field theory turned out to be unrenormalizable [130, 138]. A lattice version (with the ‘fermionic’ constraint of not more than one particle per site) of the model contains the reactions $2A \rightarrow \emptyset$ and $2A \rightarrow 3A$ together with single-particle diffusion $A\emptyset \leftrightarrow \emptyset A$ and was first studied numerically in [52]. An intense debate on the universality class of this model followed, see [115], and several mutually exclusive conclusions on the critical behaviour continue to be drawn, see [138, 12, 148, 187, 225, 104] for recent work. The bosonic pair-contact process has a dynamic exponent $z = 2$ [184] and is hence distinct from the PCPD where $z < 2$. Its study will not so much shed light on any open question concerning the PCPD but it should rather be viewed as a non-trivial example of an exactly solvable non-equilibrium many-body system to be studied in its own right.

The master equation is written in a quantum hamiltonian formulation as $\partial_t |P(t)\rangle = -H |P(t)\rangle$ [73, 217] where $|P(t)\rangle$ is the time-dependent state vector and the

hamiltonian H can be expressed in terms of annihilation and creation operators $a(\mathbf{x})$ and $a^\dagger(\mathbf{x})$. We define also the particle number operator as $n(\mathbf{x}) = a^\dagger(\mathbf{x})a(\mathbf{x})$. Then the Hamiltonian of the model (4.42) reads [184]

$$\begin{aligned}
H = & -D \sum_{r=1}^d \sum_{\mathbf{x}} [a(\mathbf{x})a^\dagger(\mathbf{x} + \mathbf{e}_r) + a^\dagger(\mathbf{x})a(\mathbf{x} + \mathbf{e}_r) - 2n(\mathbf{x})] \\
& -\lambda \sum_{\mathbf{x}} \left[(a^\dagger(\mathbf{x}))^{p-\ell} (a(\mathbf{x}))^p - \prod_{i=1}^p (n(\mathbf{x}) - i + 1) \right] \\
& -\mu \sum_{\mathbf{x}} \left[(a^\dagger(\mathbf{x}))^{m+k} (a(\mathbf{x}))^m - \prod_{i=1}^m (n(\mathbf{x}) - i + 1) \right] - \sum_{\mathbf{x}} h(\mathbf{x}, t) a^\dagger(\mathbf{x})
\end{aligned} \tag{4.43}$$

where \mathbf{e}_r is the r^{th} unit vector. For later use in the calculation of response functions we have also added an external field which describes the spontaneous creation of a single particle $\emptyset \rightarrow A$ with a site-dependent rate $h = h(\mathbf{x}, t)$ on the site \mathbf{x} .

Single-time observables $g(\mathbf{x}, t)$ can be obtained from the time-independent quantities $g(\mathbf{x})$ by switching to the Heisenberg picture. They satisfy the usual Heisenberg equation of motion, from which the differential equations for the desired quantities can be obtained. The space-time-dependent particle-density $\rho(\mathbf{x}, t) := \langle a^\dagger(\mathbf{x}, t)a(\mathbf{x}, t) \rangle = \langle a(\mathbf{x}, t) \rangle$ satisfies

$$\frac{\partial}{\partial t} \langle a(\mathbf{x}, t) \rangle = D \Delta_{\mathbf{x}} \langle a(\mathbf{x}, t) \rangle - \lambda \ell \langle a(\mathbf{x}, t)^p \rangle + \mu k \langle a(\mathbf{x}, t)^m \rangle + h(\mathbf{x}, t) \tag{4.44}$$

where we have used the short-hand

$$\Delta_{\mathbf{x}} f(\mathbf{x}) := \sum_{r=1}^d (f(\mathbf{x} - \mathbf{e}_r, t) + f(\mathbf{x} + \mathbf{e}_r, t) - 2f(\mathbf{x}, t)) \tag{4.45}$$

and similar equations hold for the equal-time two-point correlation functions, see [184]. It turns out that for the bosonic contact process $p = m = 1$ these equations close for arbitrary values of the rates. On the other hand, for the bosonic pair-contact process where $p = m = 2$ a closed system of equations is only found along the critical line given by [184]

$$\ell \lambda = \mu k. \tag{4.46}$$

This line separates an active phase with a formally infinite particle-density in the steady-state from an absorbing phase where the steady-state particle-density vanishes, see figure 4.3 for the schematic phase-diagrams. In what follows, the essential control parameter is

$$\alpha := \mu k(k + \ell)/(2D) \tag{4.47}$$

The physical nature of this transition becomes apparent when equal-time correlations are studied [129, 184] and can be formulated in terms of a *clustering transition*. By clustering we mean that particles accumulate on very few lattice sites while the other ones remain empty. Now, for the bosonic contact process, the behaviour along the critical line is independent of α . If $d \leq 2$, there is always clustering, while there is no clustering for $d > 2$. On the other hand, in the bosonic pair-contact process, there is on the critical line a multicritical point at $\alpha = \alpha_C$, with

$$\alpha_C = \alpha_C(d) = \frac{1}{2A_1}, \quad A_1 := \int_0^\infty du (e^{-4u} I_0(4u))^d \tag{4.48}$$

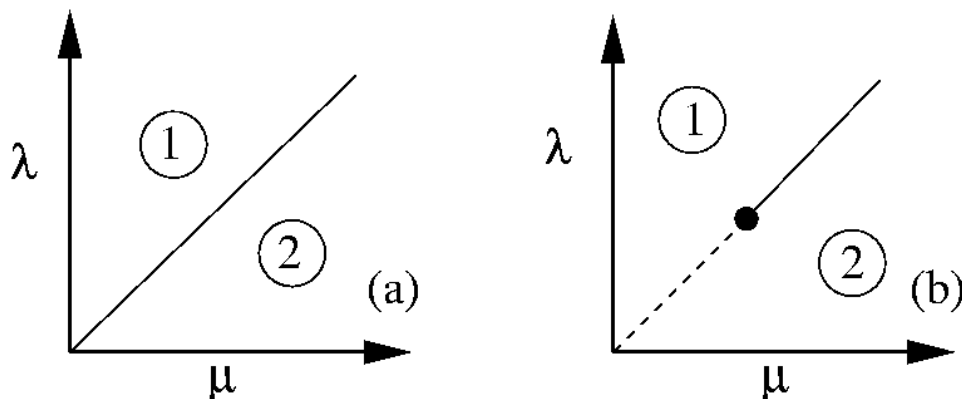


Figure 4.3: Schematic phase-diagrams for $D \neq 0$ of (a) the bosonic contact process and the bosonic pair-contact process in $d \leq 2$ dimensions and (b) the bosonic pair-contact process in $d > 2$ dimensions. The absorbing region 1, where $\lim_{t \rightarrow \infty} \rho(\mathbf{x}, t) = 0$, is separated by the critical line eq. (4.46) from the active region 2, where $\rho(\mathbf{x}, t) \rightarrow \infty$ as $t \rightarrow \infty$. On the critical line $\rho(t) := \int d\mathbf{x} \rho(\mathbf{x}, t)$ remains constant. By varying α one moves along the critical line. Along the critical line, one may have clustering (full lines in (a) and (b)), but in the bosonic pair-contact process with $d > 2$ the steady-state may also be homogeneous (broken line in (b)). These two regimes are separated by a multicritical point.

and where $I_0(u)$ is a modified Bessel function [2], such that clustering occurs for $\alpha > \alpha_C$ only and with a more or less homogeneous state for $\alpha \leq \alpha_C$. Specific values are $\alpha_C(3) \approx 3.99$ and $\alpha_C(4) \approx 6.45$ and $\lim_{d \searrow 2} \alpha_C(d) = 0$. This clustering transition is illustrated in chapter (1) in figure 1.10. We are interested in studying the impact of this clustering transition on the two-time correlations and linear responses.

In order to obtain the equations of motion of the two-time correlator, the time-ordering of the operators $a(\mathbf{x}, t)$ must be taken in account. From the Hamiltonian eq. (4.43) without an external field h , we get the following equations of motion for the two-time correlator, after rescaling the times $t \mapsto t/(2D)$, $s \mapsto s/(2D)$, and for $t > s$, [90] (for a detailed computation, see [14])

$$\begin{aligned} & \frac{\partial}{\partial t} \langle a(\mathbf{x}, t) a(\mathbf{y}, s) \rangle \\ &= \frac{1}{2} \Delta_{\mathbf{x}} \langle a(\mathbf{x}, t) a(\mathbf{y}, s) \rangle - \frac{\lambda \ell}{2D} \langle a(\mathbf{x}, t)^p a(\mathbf{y}, s) \rangle + \frac{\mu k}{2D} \langle a(\mathbf{x}, t)^m a(\mathbf{y}, s) \rangle \end{aligned} \quad (4.49)$$

which we are going to study in the next sections.

4.2.3 The bosonic contact process

For the bosonic contact process, we have $p = m = 1$, hence also $\ell = k = 1$. We first consider the critical case $\lambda \ell = \mu k$. We shall assume throughout that spatial translation-invariance holds and use the notation

$$F(\mathbf{r}; t, s) := \langle a(\mathbf{x}, t) a(\mathbf{x} + \mathbf{r}, s) \rangle. \quad (4.50)$$

Then F satisfies¹⁰ a diffusion equation which is solved in a standard way by Fourier transforms. It is easy to see that the solution of the equations of motion (4.49) involves the single-time correlator $F(\mathbf{r}, t) := F(\mathbf{r}; t, t)$ which satisfies the equation of motion, after the usual rescaling $t \mapsto t/(2D)$ [184, eq. (10)],

$$\frac{\partial}{\partial t} F(\mathbf{r}, t) = \Delta_{\mathbf{r}} F(\mathbf{r}, t) + \alpha \rho_0 \delta_{\mathbf{r}, \mathbf{0}} \quad (4.51)$$

and the parameter α was defined in (4.47). As initial conditions, we shall use throughout the Poisson distribution $F(\mathbf{r}, 0) = \rho_0^2$. Hence one arrives at the following expression of our main quantity of interest, the connected correlator¹¹

$$G(\mathbf{r}; t, s) := F(\mathbf{r}; t, s) - \rho_0^2 = \alpha \rho_0 \int_0^s d\tau b\left(\mathbf{r}, \frac{1}{2}(t+s) - \tau\right) \quad (4.52)$$

where ($I_r(t)$ being a modified Bessel function)

$$b(\mathbf{r}, t) = e^{-2dt} I_{r_1}(2t) \dots I_{r_d}(2t). \quad (4.53)$$

We evaluate this expression in two cases

- $\mathbf{r} = 0$, t and s in the ageing regime:

In this case both s and $t - s$ are large, so that we can use the asymptotic behaviour $I_0(t) \simeq (2\pi t)^{-1/2} e^t$ for t large [97] for the expression $b(\mathbf{0}, \frac{1}{2}(t+s) - \tau)$ under the integral in (4.52). We have to distinguish the cases $d > 2$, $d = 2$ and $d < 2$. For $d > 2$ we obtain

$$\begin{aligned} G(\mathbf{0}, t, s) &\simeq \frac{\alpha \rho_0}{(4\pi)^{\frac{d}{2}}} \int_0^s d\tau \left(\frac{1}{2}(t+s) - \tau\right)^{-\frac{d}{2}} \\ &= \frac{\alpha \rho_0}{(4\pi)^{\frac{d}{2}} (\frac{d}{2} - 1)} \left(\left(\frac{t-s}{2}\right)^{-\frac{d}{2}+1} - \left(\frac{t+s}{2}\right)^{-\frac{d}{2}+1} \right). \end{aligned} \quad (4.54)$$

By analogy with the first equation in (1.11) and with (1.12), we expect the scaling behaviour $G(t, s) := G(\mathbf{0}; t, s) = s^{-b} f_G(t/s)$. We read off the value $b = \frac{d}{2} - 1$ and the scaling function

$$f_G(y) = \frac{\alpha \rho_0}{2(2\pi)^{\frac{d}{2}} (\frac{d}{2} - 1)} \left((y-1)^{-\frac{d}{2}+1} - (y+1)^{-\frac{d}{2}+1} \right). \quad (4.55)$$

From the expected asymptotics $f_G(y) \sim y^{-\lambda_G/z}$ for $y \gg 1$, we obtain

$$\lambda_G = d \quad (4.56)$$

¹⁰With the same technique as outlined in [184] for the derivation of the differential equations, one can prove for the bosonic systems at hand that the density-density correlator $\langle n(t, \mathbf{x}) n(s, \mathbf{y}) \rangle$ is related to the correlation function and the response function (introduced below) via the expression $\langle n(t, \mathbf{x}) n(s, \mathbf{y}) \rangle = F(\mathbf{r}, t, s) + \rho_0 R(\mathbf{r}, t - s)$ for the critical case $\lambda \ell = \mu k$. Note that this relation entails the inequality $b \leq a + 1$.

¹¹In [80, 203] this same quantity was denoted by $\Gamma(t, s)$ which we avoid here in order not to create confusion with the incomplete gamma function [2].

as can be seen from the asymptotic development of (4.55) and where we anticipated that the dynamical exponent $z = 2$, see also [129] and below.

For $d = 2$ the integral in (4.54) gives a different result. We find

$$G(t, s) = f_G(t/s) \quad , \quad f_G(y) = \frac{\alpha\rho_0}{2(2\pi)^{\frac{d}{2}}} \ln\left(\frac{y+1}{y-1}\right) \quad (4.57)$$

and we have the exponents $b = 0$ and $\lambda_G = 2$. The logarithmic divergence of the single-time correlator [129] reflects itself here in the logarithmic form of the scaling function.

Finally, for $d < 2$ the same computation as for $d > 2$ goes through. Now, the exponent $b = \frac{d}{2} - 1$ is *negative* which means that the two-time autocorrelator diverges, in agreement with the earlier results for the equal-time correlators in $1D$ [129].

- \mathbf{r} -dependence for $s, t - s \gg 1$

We use the asymptotic expression, valid for $u \gg 1$ and \mathbf{r}^2/u fixed

$$e^{-dz} I_{r_1}(u) \cdots I_{r_d}(u) \simeq \frac{1}{(2\pi u)^{\frac{d}{2}}} \exp\left(-\frac{\mathbf{r}^2}{2u}\right) \quad (4.58)$$

which yields for arbitrary dimension d , when introduced into (4.52),

$$G(\mathbf{r}; t, s) \simeq \frac{\alpha\rho_0}{(4\pi)^{\frac{d}{2}}} \left(\frac{\mathbf{r}^2}{4}\right)^{-\left(\frac{d}{2}-1\right)} \left[\Gamma\left(\frac{d}{2}-1, \frac{1}{2} \frac{\mathbf{r}^2}{t+s}\right) - \Gamma\left(\frac{d}{2}-1, \frac{1}{2} \frac{\mathbf{r}^2}{t-s}\right) \right] \quad (4.59)$$

The incomplete Gamma function $\Gamma(\kappa, x)$ is defined by [2]

$$\Gamma(\kappa, x) := \int_x^\infty dt e^{-t} t^{\kappa-1} \quad (4.60)$$

and has the following asymptotic behaviour for large or small arguments

$$\Gamma(\kappa, x) \stackrel{|x| \gg 1}{\approx} x^{\kappa-1} e^{-x}, \quad \Gamma(\kappa, x) \stackrel{0 < x \ll 1}{\approx} \Gamma(\kappa) - \frac{x^\kappa}{\kappa}. \quad (4.61)$$

In the limit where both s and $t - s$ become large, we recover eq. (4.54) as it should be. Furthermore, we explicitly see that the dynamical exponent $z = 2$.

For illustration, we have also evaluated the integral (4.52) numerically (with $\alpha\rho_0 = 1$). In Figure 4.4a we compare the numerical results, for several values of s in three dimensions, with the analytical result eq. (4.54). We see that already for quite small values of s one has a nice data collapse which confirms the expected scaling behaviour. Furthermore, the agreement with the analytically calculated scaling function is perfect. In figure 4.4b we display the dependence on \mathbf{r} , evaluated along the line $\mathbf{r} = (r, 0, \dots, 0)$. Again, the expected scaling behaviour is also confirmed and the curves agree with the analytical expression eq. (4.59).

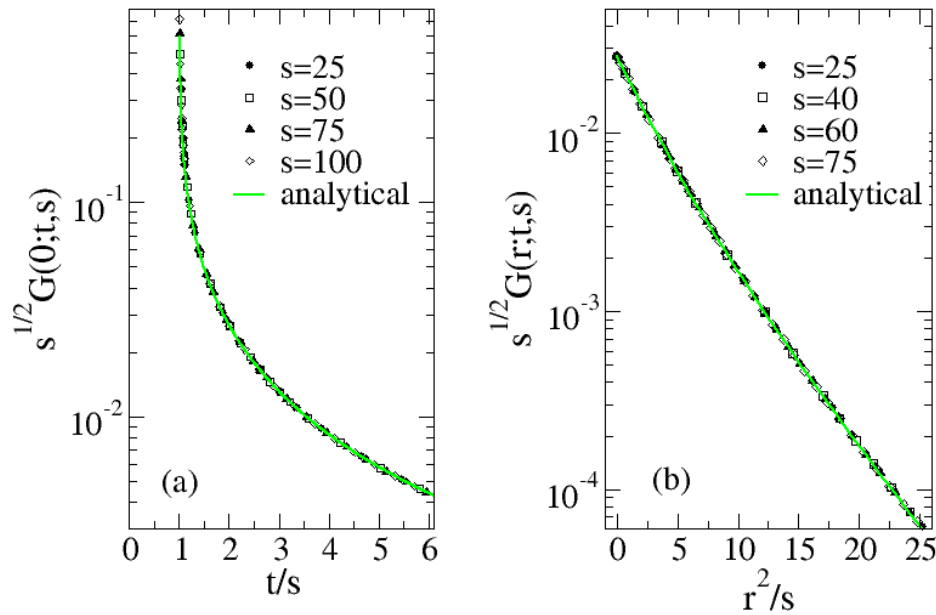


Figure 4.4: Scaling plots of (a) the autocorrelation function $G(0; t, s)$ and (b) the space-dependent correlation function $G(\mathbf{r}; t, s)$ for the critical bosonic contact process in three dimensions with $\alpha\rho_0 = 1$. In (b), the value of $y = t/s = 2$ was used.

In the non-critical case, we have for the density, after rescaling $t \rightarrow t/(2D)$

$$\frac{\partial}{\partial t}\rho(\mathbf{x}, t) = \frac{1}{2}\Delta_{\mathbf{x}}\rho(\mathbf{x}, t) + \frac{1}{2}\eta\rho(\mathbf{x}, t) \quad \text{with} \quad \eta := \frac{\mu k - \lambda \ell}{D} \quad (4.62)$$

This is easily solved and yields

$$\rho(\mathbf{x}, t) = \rho_0 e^{\frac{1}{2}\eta t} \quad (4.63)$$

if we choose again a homogeneous initial distribution with mean density ρ_0 . Depending on whether particle creation or annihilation dominates the density increases or decreases exponentially. Next, for the single-time correlator $F(\mathbf{r}, t)$ we use [184, eqs. (7,8)] which can be written after rescaling as (recall $\ell = 1$)

$$\frac{\partial}{\partial t}F(\mathbf{r}, t) = \Delta F(\mathbf{r}, t) + \eta F(\mathbf{r}, t) + \alpha\delta_{\mathbf{r},0}\rho(t) \quad (4.64)$$

which is easily solved by introducing the particle-density (4.63) and performing a Fourier transform. This in turn allows to solve the equation of motion (4.49) for the two-time correlator and we find

$$F(\mathbf{r}; t, s) = \rho_0^2 e^{\frac{1}{2}\eta(t+s)} + \alpha\rho_0 e^{\frac{1}{2}\eta(t+s)} \int_0^s d\tau e^{-\frac{1}{2}\eta\tau} b\left(\mathbf{r}; \frac{1}{2}(t+s) - \tau\right). \quad (4.65)$$

We consider the case $\mathbf{r} = 0$ and t and s in the ageing regime. As before, we use the asymptotic expression for $b(\mathbf{0}, \frac{1}{2}(t+s) - \tau)$ and find for the connected autocorrelator

$$\begin{aligned}
G(\mathbf{0}; t, s) &:= F(\mathbf{0}; t, s) - \rho_0^2 e^{\frac{1}{2}\eta(t+s)} \\
&= \frac{\alpha \rho_0 e^{\frac{1}{4}\eta(t+s)}}{(4\pi)^{d/2}} \left[\Gamma\left(-\frac{d}{2} + 1, -\frac{\eta}{4}(t+s)\right) - \Gamma\left(-\frac{d}{2} + 1, -\frac{\eta}{4}(t-s)\right) \right]. \quad (4.66)
\end{aligned}$$

Using the asymptotic behaviour eq. (4.61) for the Gamma-function for large arguments we obtain

$$G(\mathbf{0}; t, s) = -\frac{2\alpha\rho_0}{(2\pi)^{d/2}\eta} \left[(t-s)^{-d/2} \exp\left(\frac{\eta}{2}t\right) - (t+s)^{-d/2} \exp\left(\frac{\eta}{2}(t+s)\right) \right]. \quad (4.67)$$

If η is positive, then particle-creation outweighs particle-annihilation. The second term dominates and leads to an exponential divergence. On the other hand, if η is negative, the first term involving $e^{\eta t/2}$ is the dominant one. At first sight, these results appear curious, since the leading exponential behaviour merely depends on $t+s$ and t , respectively, and not on $t-s$, as might have been anticipated.

A similar result had already been found in the inactive phase of the ordinary contact process [80, 203] and we can understand the present result along similar lines. Consider the limits where $|\eta| \rightarrow \infty$, such that diffusion plays virtually no role in comparison with the creation or annihilation processes. Then merely the creation and annihilation processes on a single site need to be considered. Correlators are given in terms of conditional probabilities and we now consider the two cases $\eta > 0$ and $\eta < 0$. First, for $\eta < 0$, annihilation dominates and at late times there are only few particles left in the system. This is the same situation as in the inactive phase of the ordinary contact process. Then $G(\mathbf{0}; t, s)$ can only be non-vanishing if at time s a particle was present and it should only depend on t . On the other hand, for $\eta > 0$, the particle-density diverges exponentially and the number of possible reactions is conditioned by the density at time s , proportional to $e^{\eta s/2}$, hence the dependence on $t+s$. Finally, the power-law prefactors relate to the diffusion between different sites.

4.2.4 The bosonic critical pair-contact process

For the bosonic pair-contact process, we have $p = m = 2$. The system (4.49) of differential equations closes only for the critical case, i.e. for $\lambda\ell = \mu k$, and we shall restrict to this situation throughout. At criticality, the values of ℓ and k do not influence the scaling behaviour. It was shown in [184] that in dimensions $d > 2$ there is a phase transition along the critical line and we must therefore distinguish three cases, according to whether the reduced control parameter

$$\alpha' := \frac{\alpha - \alpha_C}{\alpha_C}. \quad (4.68)$$

is negative, zero, or positive and where α was defined in (4.47) and α_C in (4.48). For $d \leq 2$ one is always in the situation $\alpha' > 0$. We recall the known results for the single-time autocorrelator $F(\mathbf{0}, t)$ which for large times behaves as [184]

- $\alpha < \alpha_C$:

$$F(\mathbf{0}, t) \stackrel{t \rightarrow \infty}{\approx} -\frac{\rho_0^2}{\alpha'}. \quad (4.69)$$

- $\alpha = \alpha_C$:

$$F(\mathbf{0}, t) \stackrel{t \rightarrow \infty}{\approx} \begin{cases} \frac{(4\pi)^{\frac{d}{2}} \rho_0^2}{|\Gamma(1-d/2)| \alpha_C} t^{\frac{d}{2}-1} & \text{for } 2 < d < 4 \\ \frac{\rho_0^2}{4A_2 \alpha_C} t & \text{for } d > 4 \end{cases} \quad (4.70)$$

where A_2 is a known constant which is defined in [184].

- $\alpha > \alpha_C$ or $d < 2$:

$$F(\mathbf{0}, t) \stackrel{t \rightarrow \infty}{\approx} A \rho_0^2 \exp(t/\tau_{ts}). \quad (4.71)$$

The known prefactor A and the time-scale τ_{ts} are dimension-dependent and positive. The exact expressions for them are not essential for our considerations and can be found in [184].

The solution of the equations of motion is quite analogous to the one of the bosonic contact process and the results from subsection 4.2.3 can be largely taken over. We find, again for initially uncorrelated particles of mean density ρ_0 ,

$$F(\mathbf{r}; t, s) = \rho_0^2 + \alpha \int_0^s d\tau F(\mathbf{0}, \tau) b\left(\mathbf{r}, \frac{1}{2}(t+s) - \tau\right) \quad (4.72)$$

For $t = s$ this formula agrees with [184, eq. (21)] as it should. We are interested in the behaviour of the connected correlation function, see (4.52), in the ageing regime. The analysis of eq. (4.72) is greatly simplified by recognising that, quite in analogy with ageing in simple ferromagnets, there is some intermediate time-scale t_p such that for times $\tau \lesssim t_p$, one still is in some quasi-stationary regime while for $\tau \gtrsim t_p$ one goes over into the ageing regime and that furthermore, the cross-over between these regimes occurs very rapidly [240]. We denote by $F_{age}(\mathbf{0}, \tau)$ the asymptotic ageing form of $F(\mathbf{0}, \tau)$ and write

$$\begin{aligned} & \int_0^s d\tau F(\mathbf{0}, \tau) b\left(\mathbf{0}, \frac{1}{2}(t+s) - \tau\right) \\ &= \int_0^{t_p} d\tau F(\mathbf{0}, \tau) b\left(\mathbf{0}, \frac{1}{2}(t+s) - \tau\right) + s \int_{t_p/s}^1 dv F_{age}(\mathbf{0}, sv) b\left(\mathbf{0}, \frac{1}{2}(t+s) - \tau v\right). \end{aligned} \quad (4.73)$$

We denote the first term of the last line by $C_1(t, s, t_p)$. Since we expect that $t_p \sim s^\zeta$ with $0 < \zeta < 1$ [240], we can replace the lower integration limit by 0 in the second integral. This leaves us with the result

$$G(\mathbf{0}; t, s) = C_1(t, s, t_p) + \int_0^s d\tau F_{age}(\mathbf{0}, \tau) b\left(\mathbf{0}, \frac{1}{2}(t+s) - \tau\right). \quad (4.74)$$

On the other hand, we have the following rough estimate

$$\begin{aligned} |C_1(t, s, t_p)| &\leq t_p \max_{\tau \in [0, t_p]} \left| F(\mathbf{0}, \tau) b\left(\mathbf{0}, \frac{1}{2}(t+s) - \tau\right) \right| \\ &\stackrel{s \gg 1}{\approx} t_p \max_{\tau \in [0, t_p]} |F(\mathbf{0}, \tau)| s^{-\frac{d}{2}} \left(4\pi \left(\frac{1}{2}(t/s + 1) - \frac{t_p}{s} \right) \right)^{-\frac{d}{2}} \end{aligned} \quad (4.75)$$

In the three cases (i) $\alpha < \alpha_C$ and $d > 2$, (ii) $\alpha = \alpha_C$ and $2 < d < 4$ and (iii) $\alpha = \alpha_C$ and $d > 4$ this leads by eqs. (4.69, 4.70), respectively, to the upper bounds $|C_1| \lesssim s^{\zeta-d/2}$,

$s^{(\zeta-1)d/2}$ and $s^{2\zeta-d/2}$ which vanish for s large more rapidly than $G(\mathbf{0}; t, s) \sim s^{1-d/2}$, s^0 and $s^{2-d/2}$, respectively and which are derived below. Hence $C_1(t, s, t_p)$ is irrelevant for the determination of b and the scaling functions and will be dropped in what follows. Similarly, because of (4.71), $C_1(t, s, t_p)$ is non-leading if $\alpha > \alpha_C$.

We have also checked that for $d > 4$ this same result can be derived more explicitly using a Laplace transformation, along the lines of [184]. For the sake of brevity, these relatively straightforward calculations will not be reproduced here [14].

Ageing regime: $r = 0$ and $s, t - s \gg 1$

The most interesting cases are $d > 2$ and $\alpha \leq \alpha_C$, which we will treat first. The asymptotic expression for $F(\mathbf{0}, t)$ is of the form $F_{age}(\mathbf{0}, t) = \mathcal{A}\rho_0^2 t^\xi$, where ξ and the prefactor \mathcal{A} can be read off from equations (4.69)-(4.70). We therefore get for the connected autocorrelator

$$\begin{aligned} G(\mathbf{0}; t, s) &= \frac{\alpha\rho_0^2\mathcal{A}}{(4\pi)^{\frac{d}{2}}} \int_0^s d\tau \tau^\xi \left(\frac{1}{2}(t+s) - \tau \right)^{-\frac{d}{2}} \\ &= \frac{\alpha\rho_0^2\mathcal{A}}{(\xi+1)(4\pi)^{\frac{d}{2}}} s^{\xi+1-\frac{d}{2}} \left(\frac{1}{2}(y+1) \right)^{-\frac{d}{2}} {}_2F_1 \left(\frac{d}{2}, \xi+1; \xi+2; \frac{2}{y+1} \right) \end{aligned} \quad (4.76)$$

where $y = t/s$ and ${}_2F_1$ is a hypergeometric function. We deduce the general form of the scaling function

$$f_G(y) = \frac{\alpha\rho_0^2\mathcal{A}}{(\xi+1)(4\pi)^{\frac{d}{2}}} \left(\frac{1}{2}(y+1) \right)^{-\frac{d}{2}} {}_2F_1 \left(\frac{d}{2}, \xi+1; \xi+2; \frac{2}{y+1} \right). \quad (4.77)$$

and the exponents

$$b = -\xi - 1 + \frac{d}{2} \quad \text{and} \quad \lambda_G = d \quad (4.78)$$

and furthermore $z = 2$, see [184] and below. For the different cases we obtain the following explicit expressions:

- $\alpha < \alpha_C$ and $d > 2$: Here we have $\xi = 0$ and the prefactor is $\mathcal{A} = -\frac{1}{\alpha}$. Therefore, we have a value of

$$b = \frac{d}{2} - 1. \quad (4.79)$$

The ${}_2F_1$ -function can be rewritten with the help of the relation (9.121,5) from [97], so that we obtain an elementary expression for the scaling function:

$$f_G(y) = \frac{\rho_0^2\alpha}{\alpha'(2\pi)^{\frac{d}{2}}(d-2)} \left((y+1)^{-\frac{d}{2}+1} - (y-1)^{-\frac{d}{2}+1} \right). \quad (4.80)$$

- $\alpha = \alpha_C$ and $d > 2$: Here we have $\xi = \frac{d}{2} - 1$ and $\xi = 1$ for $2 < d < 4$ and $d > 4$ respectively. This implies for b

$$b = \begin{cases} 0 & \text{for } 2 < d < 4 \\ \frac{d}{2} - 2 & \text{for } d > 4 \end{cases}. \quad (4.81)$$

For $2 < d < 4$ the scaling function is (with the prefactor $\mathcal{A} = \frac{(4\pi)^{\frac{d}{2}}}{|\Gamma(1-\frac{d}{2})|^{\alpha_C}}$ [184])

$$f_G(y) = \frac{2^{\frac{d}{2}+1}\rho_0^2}{d|\Gamma(1-\frac{d}{2})|} (y+1)^{-\frac{d}{2}} {}_2F_1\left(\frac{d}{2}, \frac{d}{2}; \frac{d}{2} + 1; \frac{2}{y+1}\right). \quad (4.82)$$

For $d > 4$, the scaling function (4.77) can again be written as an elementary function with the help of a Gauß recursion relation (eq. (9.137,4) from [97]):

$$f_G(y) = \frac{\rho_0^2}{4A_2(2\pi)^{\frac{d}{2}}(d-2)(d-4)} \times \left((y+1)^{-\frac{d}{2}+2} - (y-1)^{-\frac{d}{2}+2} + (d-4)(y-1)^{-\frac{d}{2}+1} \right). \quad (4.83)$$

- $\alpha > \alpha_C$ or $d < 2$: Due to the exponential behaviour of $F(\mathbf{0}, \tau)$ we do not have a scaling behaviour in these cases. The integrals which enter the calculation are similar to those encountered in (4.66) and where the time-scale τ_{ts} and the factor A are defined in eq. (4.71):

$$G(\mathbf{0}; t, s) = \frac{\alpha\rho_0^2 A e^{t+s/(2\tau)}}{(4\pi)^{d/2}} \tau_{ts}^{\frac{d}{2}} \left[\Gamma\left(-\frac{d}{2} + 1, \frac{t+s}{2\tau_{ts}}\right) - \Gamma\left(-\frac{d}{2} + 1, \frac{t-s}{2\tau_{ts}}\right) \right]. \quad (4.84)$$

Using the asymptotic behaviour of the the Gamma function (4.61), we see that the leading term in the scaling limit is

$$G(\mathbf{0}; t, s) \simeq \frac{\alpha\rho_0^2 A}{(2\pi)^{\frac{d}{2}}} (t-s)^{-d/2} \exp \frac{s}{\tau_{ts}}. \quad (4.85)$$

In contrast with the other cases treated before, the connected autocorrelator *increases* exponentially with the waiting time s .

\mathbf{r} -dependence for $s, t \gg 1$

In order to compute the \mathbf{r} -dependence of the correlator, we follow the same strategy as in the last section. We use the approximation (4.58) which can be justified by an argument relying on an inequality similar to (4.75). We obtain the following results.

- $\alpha < \alpha_C$ and $d > 2$: As we have $F(\mathbf{0}, \tau) \approx -\rho_0^2/\alpha'$ the computation is the same as for the contact process, compare equation (4.59). The result is

$$G(\mathbf{r}; t, s) = \frac{-\alpha\rho_0^2}{(4\pi)^{\frac{d}{2}}\alpha'} \left(\frac{\mathbf{r}^2}{4}\right)^{-\left(\frac{d}{2}-1\right)} \times \left[\Gamma\left(\frac{d}{2}-1, \frac{\mathbf{r}^2}{2(t+s)}\right) - \Gamma\left(\frac{d}{2}-1, \frac{\mathbf{r}^2}{2(t-s)}\right) \right]. \quad (4.86)$$

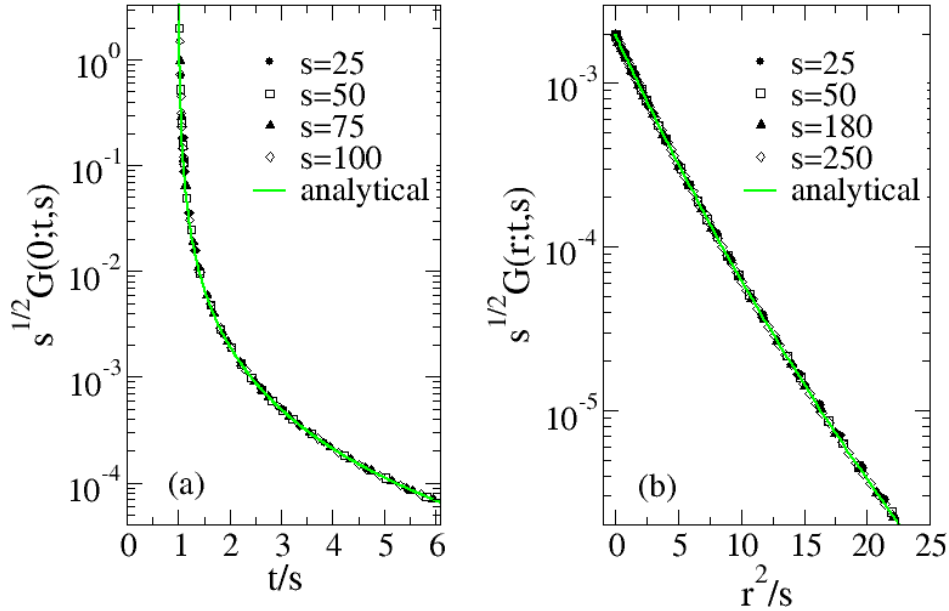


Figure 4.5: Scaling plots for the case $\alpha' < 0$ of (a) the autocorrelation function $G(0; t, s)$ and (b) the space-dependent correlation function $G(\mathbf{r}; t, s)$ for the bosonic pair-contact process in five dimensions and with $\alpha\rho_0 = 1$. In (b), the value of $y = t/s = 2$ was used.

- $\alpha = \alpha_C$ and $d > 4$: We find the following result

$$\begin{aligned}
 G(\mathbf{r}; t, s) &= \frac{\rho_0^2}{4A_2(4\pi)^{\frac{d}{2}}} \left(\frac{\mathbf{r}^2}{4}\right)^{-\left(\frac{d}{2}-1\right)} \\
 &\times \left[\frac{t+s}{2} \left(\Gamma\left(\frac{d}{2}-1, \frac{\mathbf{r}^2}{2(t+s)}\right) - \Gamma\left(\frac{d}{2}-1, \frac{\mathbf{r}^2}{2(t-s)}\right) \right) \right. \\
 &\quad \left. - \left(\frac{\mathbf{r}^2}{4}\right) \left(\Gamma\left(\frac{d}{2}-2, \frac{\mathbf{r}^2}{2(t+s)}\right) - \Gamma\left(\frac{d}{2}-2, \frac{\mathbf{r}^2}{2(t-s)}\right) \right) \right]. \quad (4.87)
 \end{aligned}$$

It is straightforward to check consistency with (4.83) for the case s and $t-s$ much larger than \mathbf{r}^2 by using the asymptotic form (4.61) of the Gamma function.

- $\alpha = \alpha_C$ and $2 < d < 4$:

$$G(\mathbf{r}; t, s) = \frac{\rho_0^2}{(d/2)|\Gamma(\frac{d}{2}-1)|} \int_0^s d\tau \tau^{\frac{d}{2}-1} \left(\frac{1}{2}(t+s) - \tau \right)^{-\frac{d}{2}} \exp\left(-\frac{\mathbf{r}^2}{2(t+s-2\tau)}\right).$$

We develop now the exponential function. The integrals are similar to those already seen so that we merely state the result

$$G(\mathbf{r}; t, s) = \frac{2\rho_0^2}{d|\Gamma(\frac{d}{2}-1)|} \sum_{n=0}^{\infty} \frac{1}{n!} \left(-\frac{\mathbf{r}^2}{4s}\right)^n \left(\frac{t/s+1}{2}\right)^{-\frac{d}{2}-n} \times {}_2F_1\left(\frac{d}{2}+n, \frac{d}{2}; \frac{d}{2}+1; \frac{2}{t/s+1}\right). \quad (4.88)$$

- $\alpha > \alpha_C$ or $d < 2$: Here again we develop the exponential function and obtain as final result

$$G(\mathbf{r}; t, s) = \frac{\alpha\rho_0^2 A}{(4\pi)^{\frac{d}{2}}} \sum_{n=0}^{\infty} \frac{1}{n!} \left(-\frac{\mathbf{r}^2}{4}\right)^n \exp\left(\frac{t+s}{2\tau_{ts}}\right) \tau_{ts}^{\frac{d}{2}+n} \times \left(\Gamma\left(-\frac{d}{2}-n+1, \frac{t+s}{2\tau_{ts}}\right) - \Gamma\left(-\frac{d}{2}-n+1, \frac{t-s}{2\tau_{ts}}\right)\right). \quad (4.89)$$

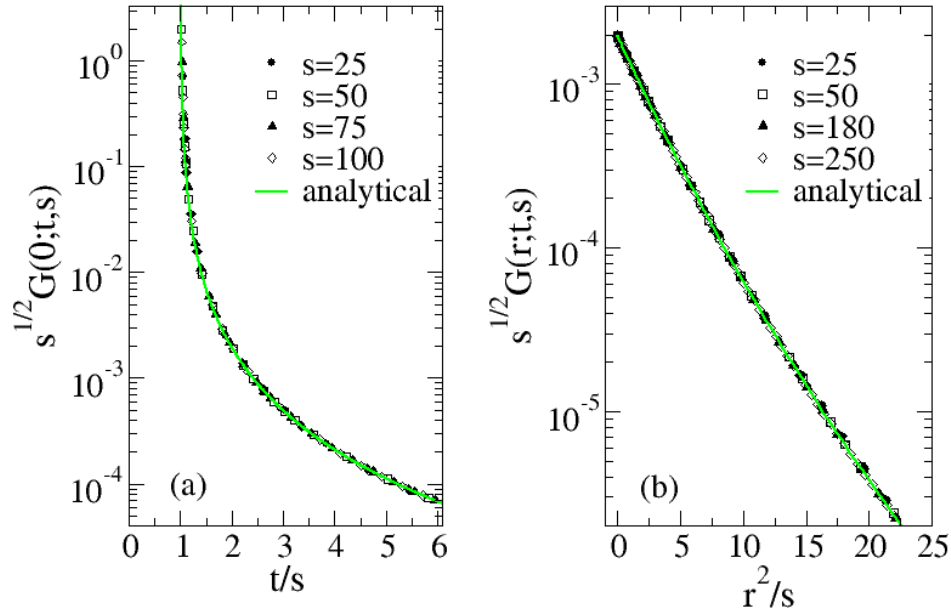


Figure 4.6: Scaling plots for the case $\alpha' = 0$ of (a) the autocorrelation function $G(0; t, s)$ and (b) the space-dependent correlation function $G(\mathbf{r}; t, s)$ for the bosonic pair-contact process in five dimensions and with $\alpha\rho_0 = 1$. In (b), the value of $y = t/s = 2$ was used.

In view of the numerous approximations needed to derive these results, it is of interest to check them numerically. In figure 4.5, we compare the results of the numerical integration of (4.72) with the analytical predictions (4.79,4.80,4.86) which apply for $\alpha < \alpha_C$ and $d = 5$. The nice collapse of the data shows that the scaling regime is already reached for the relatively small values of s used. The perfect agreement of the data with the analytical results confirms that dropping the term C_1 in (4.74) is justified (and suggests that C_1 should be considerably smaller than the rough estimate (4.75)). Similarly, we compare data for $\alpha = \alpha_C$ in $5D$ with the predictions (4.83,4.87) in figure 4.6 and similarly in $3D$ in figure 4.7. Again the agreement is perfect.

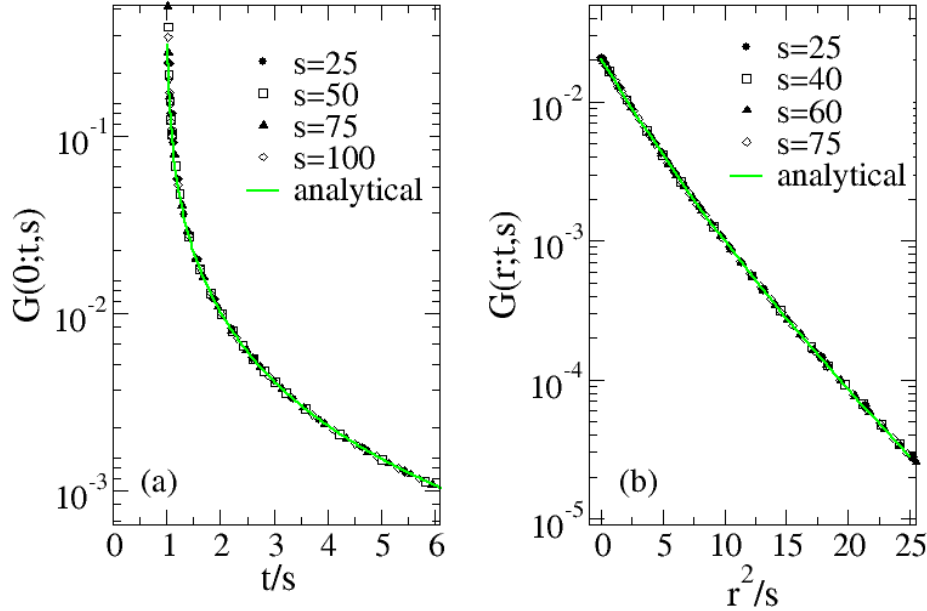


Figure 4.7: Scaling behaviour of the two-time correlator G for the case $\alpha' = 0$ and three dimensions. The value $\alpha\rho_0$ was set to unity. In (b), the value of $y = t/s = 2$ was used. The data collapse occurs for $b = 0$.

4.2.5 Response functions

The response function of the first moment to an external field $h(\mathbf{y}, s)$ is given by

$$R(\mathbf{x}, \mathbf{y}; t, s) := \left. \frac{\delta \langle a(\mathbf{x}, t) \rangle}{\delta h(\mathbf{y}, s)} \right|_{h=0}. \quad (4.90)$$

The contact process

We apply the definition (4.90) on both sides of the equation of motion (4.62) and find, exploiting spatial translation-invariance, with $\mathbf{r} = \mathbf{x} - \mathbf{y}$

$$\frac{\partial}{\partial t} R(\mathbf{r}; t, s) = \frac{1}{2} \Delta R(\mathbf{r}; t, s) + \frac{1}{2} \eta R(\mathbf{r}; t, s) + \delta(t - s). \quad (4.91)$$

This is the defining equation of a diffusion-type Green's function with the solution

$$R(\mathbf{r}; t, s) = r_0 e^{\frac{1}{2}\eta(t-s)} b\left(\mathbf{r}, \frac{1}{2}(t-s)\right) \Theta(t-s). \quad (4.92)$$

where $b(\mathbf{r}, t)$ was given in eq. (4.53) and r_0 is a normalisation constant. This expression is invariant under time-translations and does remain so even at criticality, see below.¹²

¹²Ageing is characterized by the existence of several competing stable stationary states (or a critical point) and time-translation invariance (TTI) can no longer be *requested*. However, that does not mean

	bosonic contact process	bosonic pair-contact process	
		$\alpha < \alpha_C$	$\alpha = \alpha_C$
a	$\frac{d}{2} - 1$	$\frac{d}{2} - 1$	$\frac{d}{2} - 1$
b	$\frac{d}{2} - 1$	$\frac{d}{2} - 1$	0 if $2 < d < 4$ $\frac{d}{2} - 2$ if $d > 4$
λ_R	d	d	d
λ_G	d	d	d
z	2	2	2

Table 4.2: Ageing exponents of the critical bosonic contact and pair-contact processes in the different regimes. The results for the bosonic contact process hold for an arbitrary dimension d , but for the bosonic pair-contact process they only apply if $d > 2$, since $\alpha_C = 0$ for $d \leq 2$.

The critical pair-contact process

The equation of motion for the particle-density on the critical line does not change in comparison with the contact process, so that we can take over the result (4.92) with η set to zero and have

$$R(\mathbf{r}; t, s) = r_0 b \left(\mathbf{r}, \frac{1}{2}(t - s) \right) \Theta(t - s). \quad (4.93)$$

The autoresponse function in the scaling regime is obtained by setting $\mathbf{r} = 0$ and using the known asymptotic behaviour of the Bessel function, with the result ($t > s$)

$$R(t, s) := R(\mathbf{0}; t, s) \simeq r_0 (2\pi(t - s))^{-d/2} \quad (4.94)$$

from which we can read off the scaling function and the exponents a and λ_R

$$a = \frac{d}{2} - 1, \quad f_R(y) = \frac{r_0}{(2\pi)^{d/2}} (y - 1)^{-d/2}, \quad \lambda_R = d \quad (4.95)$$

We collect our results for the ageing exponents $a, b, \lambda_G, \lambda_R, z$ in table 4.2. A few comments are now in order. First, for both the critical bosonic contact process and the critical bosonic pair-contact process with $\alpha < \alpha_C$, we see by comparing the result for a with the corresponding ones for b , see table 4.2, that $a = b$. Together with the identity $\lambda_G = \lambda_R$ the critical ageing behaviour of these systems is quite analogous to the one of simple, reversible ferromagnets quenched to their critical temperature. Second, the critical bosonic pair-contact process with $\alpha = \alpha_C$ furnishes an analytically solved example where a and b are different. This is analogous to the result found for the 1D and 2D critical ordinary contact process, where $a = b - 1$ was observed [80, 203] and where the relation $\lambda_G = \lambda_R$ holds as well. However, there is no apparent simple and general relation between the exponents a and b for ageing systems without detailed balance. Third, our results for the critical bosonic pair-contact process provide further evidence against the generality

that TTI were always impossible and indeed TTI can be recovered as a limit case, for certain specific values of the ageing exponents. A well-known example is the the response function of the spherical model quenched onto criticality ($T = T_c$) in $d > 4$ space dimensions [94].

of a recent proposal by Sastre et al. [212] to define a non-equilibrium temperature which was based on the implicit assumption that $a = b$ would remain true even in the absence of detailed balance. Fourth, we can compare the form of the scaling function $f_R(y)$ of the autoresponse with the prediction of local scale-invariance given in chapter 2. We find perfect agreement and identify $a = a'$. Fifth, we recall that for $z = 2$ there is a variant of local scale-invariance which takes the presence of a discrete lattice into account. It is possible to construct the corresponding representation of the Schrödinger Lie-algebra and then a response function transforming covariantly under it should read for $t > s$ in d spatial dimensions [105]

$$R(\mathbf{r}; t, s) = r_0(t-s)^{(d-2x)/2} \exp\left(\frac{d(t-s)}{\mathcal{M}}\right) \mathcal{I}_{\mathbf{r}}\left(\frac{t-s}{\mathcal{M}}\right) , \quad \mathcal{I}_{\mathbf{r}}(u) := \prod_{j=1}^d I_{r_j}(u) \quad (4.96)$$

where x is a scaling dimension and r_0, \mathcal{M} are constants. Here the spatial distance \mathbf{r} is an integer multiple of the lattice constant. Comparison with eqs. (4.93,4.53) shows complete agreement if we identify $x = d/2$ and $\mathcal{M} = 1/2$.

4.2.6 Conclusions of this section

We have studied the ageing behaviour of the exactly solvable bosonic contact process and of the bosonic critical pair-contact process in order to get a better understanding on how the present scaling description of ageing, which is derived from the study of reversible systems with detailed balance, should be generalised for truly irreversible systems without detailed balance. This more general situation might be closer to what is going on in chemical or biological ageing than the reversible systems undergoing physical ageing, e.g. after a temperature quench. In comparison with the ordinary contact and pair-contact processes, these bosonic models permit an accumulation of many particles on a single site and this possibility does indeed affect the long-time behaviour of these models. Trivially, if either particle production or annihilation dominates, the mean occupation number will either diverge for large times or the population will die out, but if these rates are balanced there is a critical line where the mean particle-density is constant in time and the system's behaviour is more subtle. Indeed, on the critical line the long-time behaviour depends on how effectively single-particle diffusion is capable of homogenising the system, see figure 4.3. For dimensions $d \leq 2$, there is always *clustering* at criticality, that is a few sites are highly populated and the others are empty. On the other hand, for $d > 2$ there is no clustering in the bosonic contact process, but in the bosonic pair-contact process there is a *clustering transition* at some $\alpha = \alpha_C$ such that clustering occurs for $\alpha > \alpha_C$ (where the diffusion is relatively weak) and there is a more or less homogeneous state for $\alpha \leq \alpha_C$.

This behaviour of the models also reflects itself in their ageing behaviour which we studied here. We anticipated in the ageing regime $t, s \gg 1$ and $t - s \gg 1$ the scaling forms for the connected autocorrelator and autoresponse

$$G(t, s) := G(\mathbf{0}; t, s) = s^{-b} f_G(t/s) , \quad R(t, s) := R(\mathbf{0}; t, s) = s^{-1-a} f_R(t/s) \quad (4.97)$$

together with the asymptotics $f_{G,R}(y) \sim y^{-\lambda_{G,R}/z}$ as $y \gg 1$ and our results for the exponents and the scaling functions are listed in tables 4.2 and 4.3. Specifically:

			$f_R(y)$	$f_G(y)$
contact process			$(y-1)^{-\frac{d}{2}}$	$(y-1)^{-\frac{d}{2}+1} - (y+1)^{-\frac{d}{2}+1}$
pair	$\alpha < \alpha_C$	$d > 2$	$(y-1)^{-\frac{d}{2}}$	$(y-1)^{-\frac{d}{2}+1} - (y+1)^{-\frac{d}{2}+1}$
contact process	$\alpha = \alpha_C$	$2 < d < 4$	$(y-1)^{-\frac{d}{2}}$	$(y+1)^{-\frac{d}{2}} {}_2F_1\left(\frac{d}{2}, \frac{d}{2}; \frac{d}{2} + 1; \frac{2}{y+1}\right)$
		$d > 4$	$(y-1)^{-\frac{d}{2}}$	$(y+1)^{-\frac{d}{2}+2} - (y-1)^{-\frac{d}{2}+2} + (d-4)(y-1)^{-\frac{d}{2}+1}$

Table 4.3: Scaling functions of the autoresponse and autocorrelation of the critical bosonic contact and bosonic pair-contact processes. They are only given up to a multiplicative factor, which may depend on the dimension. The logarithmic form (4.57) of $f_G(y)$ for the $2D$ bosonic contact process may be obtained from a $d \rightarrow 2$ limit.

1. For $d > 2$, the ageing of the bosonic pair-contact process for $\alpha < \alpha_C$ lies in the same universality class as the bosonic contact process, since all critical exponents and the scaling functions coincide. Furthermore, the ageing behaviour in the bosonic contact and pair-contact processes does not depend on whether the parity of the total number of particles is conserved or not. All these systems have in common that their behaviour is strongly influenced by single-particle diffusion. One might wonder whether an analogy to the Janssen-Grassberger conjecture [135, 98] could be formulated.¹³
2. While for $d < 2$, we still find a dynamical scaling behaviour in the critical bosonic contact process, there is no such scaling for the bosonic pair-contact process if $\alpha > \alpha_C$, hence in particular for $d \leq 2$. Therefore, although both models have the same topology of their phase-diagrams for $d < 2$, see figure 4.3a, their ageing behaviour is different.
3. At the clustering transition $\alpha = \alpha_C$ in the critical bosonic pair-contact process, dynamical scaling occurs, but the ageing exponents a and b are different. Here the absence of detailed balance leads to a substantial modification of the scaling description with respect to what happens in critical ferromagnets. In particular, there is no non-trivial analogue of the limit fluctuation-dissipation ratio of critical ageing ferromagnets. A relation $a \neq b$, see (4.41), has also been observed in the ordinary critical contact process which also shares the property that $\lambda_G = \lambda_R$ still holds [80, 203]. However, according to the known examples, a simple and general relation between a and b does not seem to exist for systems without detailed balance. Further evidence from other non-equilibrium models would be welcome.
4. On the other hand, the equality $\lambda_G = \lambda_R$ between the autocorrelation and autoresponse exponents, at the critical point of the steady-state and for uncorrelated initial states, seems to be a generic feature even for systems without detailed balance.

¹³An important ingredient of the models studied here seems to be that at criticality the mean particle-density stays constant. On the other hand, even if a ‘soft’ limit on the particle number per site is introduced, e.g. by a further reaction $3A \rightarrow 2A$, the long-time behaviour is likely to be the one of the PCPD, as checked for the particle-density in [186].

5. The form of the response function is in full agreement with local scale-invariance which confirms that the annihilation operator $a(\mathbf{x})$ is a suitable candidate for a quasi-primary field¹⁴ of local scale-invariance. We shall come back to a detailed analysis of the correlators from the point of view of local scale-invariance in the next subsection.

Explicit results were also derived for the space-dependent scaling functions of space-time correlator and responses. For the contact process, the space-dependent response function is given by eq. (4.92) and the space-dependent correlation function by eq. (4.59). For the critical pair-contact process, the space-dependent response function is given by eq. (4.93). The space-dependent correlation function can be found in (i) eq. (4.86) for the case $\alpha < \alpha_C$ and $d > 2$, in (ii) eq. (4.87) for the case $\alpha = \alpha_C$ and $d > 4$, in (iii) eq. (4.88) for the case $\alpha = \alpha_C$ and $2 < d < 4$ and in (iv) eq. (4.89) for the case $\alpha > \alpha_C$ or $d > 2$.

Finally, we comment on a suggested relationship between the bosonic pair-contact process and the spherical model [184]. In the spherical model, a classical result by Berlin and Kac [27] states that the magnetisation is spatially uniform, in particular the possibility that almost the entire macroscopic magnetisation were carried by a single spin can be excluded. This is in remarkable contrast to the clustering transition which occurs in the bosonic pair-contact process. More formally, a closer inspection shows notable differences between the spherical constraint and the analogous equation used to derive the correlator $F(\mathbf{0}, t)$. This suggests that the analogies between the two models do not seem to have a deeper physical basis.

4.3 Extension of local scale-invariance

4.3.1 Introduction

In the final section of this chapter we will demonstrate, how LSI can be extended to describe also the two bosonic reaction-diffusion systems presented in the last section¹⁵. We extend the treatment of local scale-invariance to ageing systems with a dynamical exponent $z = 2$ but without detailed balance. Working with a de Dominicis-Janssen type theory, we find again a decomposition $S[\phi, \tilde{\phi}] = S_0[\phi, \tilde{\phi}] + S_b[\phi, \tilde{\phi}]$ into a ‘deterministic’, Schrödinger-invariant term S_0 and ‘noise’ terms, each of which contains at least one response field more than order-parameter fields (explicit expressions will be given in subsections 4.3.2 and 4.3.3)¹⁶. Then the Bargman superselection rules which follow from the Galilei-invariance of S_0 are enough to establish that again the two-time response function is noise-independent and the two-time correlation function can be reduced to a finite sum of response functions the form of whom is strongly constrained again by the requirement of their Schrödinger-covariance. These developments provide further evidence for a *hidden non-trivial local scale-invariance in ageing systems* which manifests itself directly in the ‘deterministic’ part (see [222] for the construction of Schrödinger-invariant semi-linear

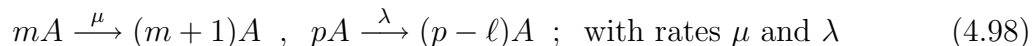
¹⁴In conformal field-theory, a quasi-primary field transforms covariantly under the action of the conformal group [26]. This concept can be generalised to fields transforming covariantly under the action of a group of local scale-transformations, see [109] and references therein for details.

¹⁵As in this case $z = 2$, we do not have to worry about fractional derivatives.

¹⁶We slightly change notation in this section and denote the action with $S[\phi, \tilde{\phi}]$ instead of $\mathcal{J}[\phi, \tilde{\mathcal{J}}]$

kinetic equations) but which strongly constrains the full noisy correlations and responses. Also, this outlines how LSI can be generalised to nonlinear models.

We test the present framework of local scale-invariance in two exactly solvable systems with a non-linear coarse-grained Langevin equation. A convenient set of models with a non-trivial ageing behaviour is furnished by the bosonic contact [129] and pair-contact processes [184] at criticality, presented in section 4.2. We briefly recall their definitions and the results obtained in section 4.2. Consider a set of particles of a single species A which move on the sites of a hypercubic lattice in d dimensions. On any site one may have an arbitrary (non-negative) number of particles.¹⁷ Single particles may hop to a nearest-neighbour site with unit rate and in addition, the following single-site creation and annihilation processes are admitted



where ℓ is a positive integer such that $|\ell| \leq p$. We are interested in the following special cases:

1. *critical bosonic contact process*: $p = m = 1$. Here only $\ell = 1$ is possible. Furthermore the creation and annihilation rates are set equal $\mu = \lambda$.
2. *critical bosonic pair-contact process*: $p = m = 2$. We fix $\ell = 2$, set $2\lambda = \mu$ and define the control parameter¹⁸

$$\alpha := \frac{3\mu}{2D} \quad (4.99)$$

The dynamics is described in terms of a master equation which may be written in a hamiltonian form $\partial_t |P(t)\rangle = -H|P(t)\rangle$ where $|P(t)\rangle$ is the time-dependent state vector and the hamiltonian H can be expressed in terms of creation and annihilation operators $a(\mathbf{x}, t)^\dagger$ and $a(\mathbf{x}, t)$ [73, 217, 227]. It is well-known that these models are critical in the sense that their relaxation towards the steady-state is algebraically slow [129, 184, 15]. In particular, the local particle-density is $\rho(\mathbf{x}, t) := \langle a(\mathbf{x}, t) \rangle$. Its spatial average remains constant in time

$$\int d\mathbf{x} \rho(\mathbf{x}, t) = \int d\mathbf{x} \langle a(\mathbf{x}, t) \rangle = \rho_0 \quad (4.100)$$

where ρ_0 is the initial mean particle-density. We are interested in the two-time connected correlation function

$$G(\mathbf{r}; t, s) := \langle a(\mathbf{x}, t) a(\mathbf{x} + \mathbf{r}, s) \rangle - \rho_0^2 \quad (4.101)$$

and take an uncorrelated initial state, hence $G(\mathbf{r}; 0, 0) = 0$. The linear two-time response function is found by adding a particle-creation term $\sum_{\mathbf{x}} h(\mathbf{x}, t) (a^\dagger(\mathbf{x}, t) - 1)$ to the quantum hamiltonian H and taking the functional derivative

$$R(\mathbf{r}; t, s) := \left. \frac{\delta \langle a(\mathbf{r} + \mathbf{x}, t) \rangle}{\delta h(\mathbf{x}, s)} \right|_{h=0} \quad (4.102)$$

¹⁷This property distinguishes the models at hand from the conventional ('fermionic') contact and pair-contact processes whose critical behaviour is completely different.

¹⁸If instead we would treat a coagulation process $2A \rightarrow A$, where $\ell = 1$, the results presented in the text are recovered by setting $\lambda = \mu$ and $\alpha = \mu/D$.

The previous analysis of these quantities in the scaling limit gave the following results [15]: consider the autocorrelation and autoresponse functions, which satisfy the scaling forms

$$G(t, s) := G(\mathbf{0}; t, s) = s^{-b} f_G(t/s) \quad (4.103)$$

$$R(t, s) := R(\mathbf{0}; t, s) = s^{-1-a} f_R(t/s) \quad (4.104)$$

where the values of the exponents a and b are listed in table 4.2. Here the critical value α_c for the pair-contact process is explicitly given by [184]

$$\frac{1}{\alpha_c} = 2 \int_0^\infty du (e^{-4u} I_0(4u))^d \quad (4.105)$$

where I_0 is a modified Bessel function. The dynamical behaviour of the contact process is independent of α . For the critical bosonic pair-contact process, there is a clustering transition between a spatially homogeneous state for $\alpha < \alpha_c$ and a highly inhomogeneous one for $\alpha > \alpha_c$ where dynamical scaling does not hold. These two transitions are separated by a multicritical point at $\alpha = \alpha_c$. Since our models do not satisfy detailed balance, there is no reason why the exponents a and b should coincide and our result $a \neq b$ for the bosonic pair-contact process is perfectly natural.

While the scaling function $f_R(y) = (y-1)^{-d/2}$ has a very simple form, the autocorrelator scaling function has an integral representation

$$f_G(y) = \mathcal{G}_0 \int_0^1 d\theta \theta^{a-b} (y+1-2\theta)^{-d/2} \quad (4.106)$$

where the values for a and b are given in table 4.2 and \mathcal{G}_0 is a known normalisation constant. The explicit scaling functions are listed up to normalisation in table 4.3 [15]. In this section, we shall study to what extent their form can be understood from local scale-invariance.

This section is organised as follows. In subsection 4.3.2 we treat the bosonic contact process in its field-theoretical formulation. The action is split into a Schrödinger-invariant term S_0 and a noise term S_b and we show how the response and correlation functions can be exactly reduced to certain noiseless three- and four-point response functions. In this reduction the Bargman superselection rules which follow from the Schrödinger-invariance of S_0 play a central rôle. These tools allow us to predict the response- and correlation functions which will be compared to the exact results of table 4.3. In subsection 4.3.3 the same programme is carried out for the bosonic pair-contact process but as we shall see, the Schrödinger-invariant term S_0 of its action is now related to a *non*-linear Schrödinger equation. The treatment of this requires an extension of the usual representation of the Schrödinger Lie-algebra which now includes a dimensionful coupling constant. For the algebraic construction we defer the reader to the appendix B. The required n -point correlation functions coming from this new representation are derived in appendices B and C of [17]. Finally, in subsection 4.3.4 we conclude.

4.3.2 The bosonic contact process

Field-theoretical description

The master equation which describes the critical bosonic contact process as defined in subsection 4.3.1 can be turned into a field-theory in a standard fashion through an operator

formalism which uses a particle annihilation operator $a(\mathbf{r}, t)$ and its conjugate $a^\dagger(\mathbf{r}, t)$, see for instance [73, 227] for detailed discussion of the technique. Since we shall be interested in the connected correlator, we consider the shifted field and furthermore introduce the shifted response field

$$\begin{aligned}\phi(\mathbf{r}, t) &:= a(\mathbf{r}, t) - \rho_0 \\ \tilde{\phi}(\mathbf{r}, t) &:= \bar{a}(\mathbf{r}, t) = a^\dagger(\mathbf{r}, t) - 1\end{aligned}\quad (4.107)$$

such that $\langle \phi(\mathbf{r}, t) \rangle = 0$ (our notation implies a mapping between operators and quantum fields, using the known equivalence between the operator formalism and the path-integral formulation [77, 227]). As we shall see, these fields ϕ and $\tilde{\phi}$ will become the natural quasiprimary fields from the point of view of local scale-invariance. We remark that the response function is not affected by this shift, since

$$R(\mathbf{r}, \mathbf{r}'; t, s) = \frac{\delta \langle a(\mathbf{r}, t) \rangle}{\delta h(\mathbf{r}', s)} = \frac{\delta \langle \phi(\mathbf{r}, t) \rangle}{\delta h(\mathbf{r}', s)} \quad (4.108)$$

Then the field-theory action reads, where μ is the reaction rate [130]

$$\begin{aligned}S[\phi, \tilde{\phi}] &= \int d\mathbf{R} \int du \left[\tilde{\phi}(2\mathcal{M}\partial_u - \nabla^2)\phi - \mu\tilde{\phi}^2(\phi + \rho_0) \right] \\ &= S_0[\phi, \tilde{\phi}] + S_b[\phi, \tilde{\phi}]\end{aligned}\quad (4.109)$$

To keep expressions shorter, we have suppressed the arguments of $\phi(\mathbf{R}, u)$ and $\tilde{\phi}(\mathbf{R}, u)$ under the integrals and we shall also do so often in what follows, if no ambiguity arises. The diffusion constant D is related to the ‘mass’ \mathcal{M} through $D = (2\mathcal{M})^{-1}$. We have decomposed the action as follows:

$$S_0[\phi, \tilde{\phi}] := \int d\mathbf{R} \int du \left[\tilde{\phi}(2\mathcal{M}\partial_u - \nabla^2)\phi \right] \quad (4.110)$$

describes the deterministic,¹⁹ noiseless part whereas the noise is described by

$$S_b[\phi, \tilde{\phi}] := -\mu \int d\mathbf{R} \int du \left[\tilde{\phi}^2(\phi + \rho_0) \right]. \quad (4.111)$$

quite analogously to what happens in the kinetics of simple magnets, see [192] for details. In principle, an initial correlator $G(\mathbf{r}; 0, 0)$ could be assumed and will lead to a further contribution S_{ini} to the action. For critical systems, one usually employs a term of the form $S_{\text{ini, st}} = -\frac{\tau_0}{2} \int d\mathbf{R} (\phi(\mathbf{R}, 0) - \langle \phi(\mathbf{R}, 0) \rangle)^2$, see e.g. [137, 45] but this would have for us the disadvantage that it explicitly breaks Galilei-invariance. We shall rather make use of the Galilei-invariance of the noiseless action $S_0[\phi, \tilde{\phi}]$ and use as an initial term [170, 192]

$$S_{\text{ini}}[\tilde{\phi}] = -\frac{1}{2} \int d\mathbf{R} d\mathbf{R}' \tilde{\phi}(\mathbf{R}, 0) G(\mathbf{R} - \mathbf{R}'; 0, 0) \tilde{\phi}(\mathbf{R}', 0). \quad (4.112)$$

Because of the initial condition $G(\mathbf{R}; 0, 0) = 0$, however, $S_{\text{ini}}[\tilde{\phi}] = 0$ and we shall not need to consider it any further.

¹⁹This terminology is used since the equation of motion of ϕ following from S_0 is a partial differential equation and not a stochastic Langevin equation.

From the action (4.109), n -point functions can then be computed as usual

$$\langle \phi_1(\mathbf{r}_1, t_1) \dots \phi_n(\mathbf{r}_n, t_n) \rangle = \int \mathcal{D}\phi \mathcal{D}\tilde{\phi} \phi_1(\mathbf{r}_1, t_1) \dots \phi_n(\mathbf{r}_n, t_n) \exp\left(-S[\phi, \tilde{\phi}]\right) \quad (4.113)$$

which through the decomposition (4.109) can be written as an average of the noiseless theory

$$\langle \phi_1(\mathbf{r}_1, t_1) \dots \phi_n(\mathbf{r}_n, t_n) \rangle = \left\langle \phi_1(\mathbf{r}_1, t_1) \dots \phi_n(\mathbf{r}_n, t_n) \exp\left(-S_b[\phi, \tilde{\phi}]\right) \right\rangle_0 \quad (4.114)$$

where $\langle \dots \rangle_0$ denotes the expectation value with respect to the noiseless theory.

Symmetries of the noiseless theory

In what follows, we shall need some symmetry properties of the noiseless part described by the action $S_0[\phi, \tilde{\phi}]$ which we now briefly recall from chapter 1. The noiseless equation of motion for the field ϕ is a free diffusion-equation $2\mathcal{M}\partial_t\phi(\mathbf{x}, t) = \nabla^2\phi(\mathbf{x}, t)$. Its dynamical symmetry group is the well-known Schrödinger-group $Sch(d)$ [158, 177] which acts on space-time coordinates (\mathbf{r}, t) as $(\mathbf{r}, t) \mapsto (\mathbf{r}', t') = g(\mathbf{r}, t)$ where

$$t \longrightarrow t' = \frac{\alpha t + \beta}{\gamma t + \delta}, \quad \mathbf{r} \longrightarrow \mathbf{r}' = \frac{\mathcal{R}\mathbf{r} + \mathbf{v}t + \mathbf{a}}{\gamma t + \delta}; \quad \alpha\delta - \beta\gamma = 1 \quad (4.115)$$

and where \mathcal{R} is a rotation matrix. Solutions ϕ of the free diffusion equation are carried to other solutions of the same equation and ϕ transforms as

$$\phi(\mathbf{r}, t) \longrightarrow (T_g\phi)(\mathbf{r}, t) = f_g[g^{-1}(\mathbf{r}, t)]\phi[g^{-1}(\mathbf{r}, t)] \quad (4.116)$$

where the companion function f_g is known explicitly and contains the so-called ‘mass’ $\mathcal{M} = (2D)^{-1}$ [177]. We list the generators of the Lie algebra $\mathfrak{sch}_1 = \text{Lie}(Sch(1))$ in one spatial dimension [106]

$$\begin{aligned} X_{-1} &= -\partial_t \\ X_0 &= -t\partial_t - \frac{1}{2}r\partial_r - \frac{x}{2} \\ X_1 &= -t^2\partial_t - tr\partial_r - xt - \frac{\mathcal{M}}{2}r^2 \\ Y_{-\frac{1}{2}} &= -\partial_r \\ Y_{\frac{1}{2}} &= -t\partial_r - \mathcal{M}r \\ M_0 &= -\mathcal{M} \end{aligned} \quad (4.117)$$

Fields transforming under $Sch(d)$ are characterized by a scaling dimension and a mass. We list in table 4.4 some fields which we shall use below. We remark that for free fields one has

$$\tilde{x}_2 = 2\tilde{x} \quad , \quad x_\Upsilon = 2\tilde{x} + x \quad , \quad x_\Sigma = 3\tilde{x} + x \quad , \quad x_\Gamma = 3\tilde{x} + 2x \quad (4.118)$$

but these relations need no longer hold for interacting fields. On the other hand, from the Bargmann superselection rules (see [11] and below) we expect that the masses of the composite fields as given in table 4.4 should remain valid for interacting fields as well.

field	scaling dimension	mass
ϕ	x	\mathcal{M}
$\tilde{\phi}$	\tilde{x}	$-\mathcal{M}$
$\tilde{\phi}^2$	\tilde{x}_2	$-2\mathcal{M}$
$\Upsilon := \tilde{\phi}^2\phi$	x_Υ	$-\mathcal{M}$
$\Sigma := \tilde{\phi}^3\phi$	x_Σ	$-2\mathcal{M}$
$\Gamma := \tilde{\phi}^3\phi^2$	x_Γ	$-\mathcal{M}$

Table 4.4: Scaling dimensions and masses of some composite fields.

Throughout this section, we shall make the important assumption that the fields ϕ and $\tilde{\phi}$ transform covariantly according to (4.116) under the Schrödinger group. By analogy with conformal invariance, such fields are called *quasiprimary* [109]. For quasiprimary fields the so-called Bargmann superselection rules [11] holds true which state that

$$\langle \underbrace{\phi \dots \phi}_n \underbrace{\tilde{\phi} \dots \tilde{\phi}}_m \rangle_0 = 0 \quad \text{unless } n = m \quad (4.119)$$

We recall the proof of these in appendix B of [17]. Before we consider the consequences of (4.119), we recall the well-known result on the form of noise-less n -point functions in ageing systems.

Since in ageing phenomena, time-translation invariance is broken, we must consider the subalgebra $\mathbf{age}_1 \subset \mathbf{sch}_1$ obtained by leaving out the generator of time-translations X_{-1} [111]. Then the n -point function of quasiprimary fields φ_i , $i = 1, \dots, n$ has to satisfy the covariance conditions [106, 109]

$$\left(\sum_{i=1}^n X_k^{(i)} \right) \langle \varphi_1(\mathbf{r}_1, t_1) \dots \varphi_n(\mathbf{r}_n, t_n) \rangle_0 = 0 \quad ; \quad k \in \{0, 1\} \quad (4.120)$$

$$\left(\sum_{i=1}^n Y_m^{(i)} \right) \langle \varphi_1(\mathbf{r}_1, t_1) \dots \varphi_n(\mathbf{r}_n, t_n) \rangle_0 = 0 \quad ; \quad m \in \left\{ -\frac{1}{2}, \frac{1}{2} \right\} \quad (4.121)$$

where φ_i stands either for a quasiprimary field ϕ_i or a quasiprimary response field $\tilde{\phi}_i$. The φ_i are characterized by their scaling dimension x_i and their mass \mathcal{M}_i . The generators X_k are then the extension of (4.117) to n -body operators and the superscript (i) refers to φ_i . The n -point function is zero unless the sum of all masses vanishes

$$\sum_{i=1}^n \mathcal{M}_i = 0 \quad (4.122)$$

which reproduces the Bargmann superselection rule (4.119). It is well-known [106, 109] that the noiseless two-point function $R_0(\mathbf{r}, \mathbf{r}'; t, s) = \langle \varphi_1(\mathbf{r}, t) \varphi_2(\mathbf{r}', s) \rangle_0$ is completely determined by the equations (4.120) and (4.121) up to a normalisation constant.

$$R_0(\mathbf{r}, \mathbf{r}'; t, s) = R_0(t, s) \exp \left(-\frac{\mathcal{M}_1}{2} \frac{(\mathbf{r} - \mathbf{r}')^2}{(t - s)} \right) \delta(\mathcal{M}_1 + \mathcal{M}_2) \quad (4.123)$$

where the autoresponse function is given by

$$R_0(t, s) = r_0(t - s)^{-\frac{1}{2}(x_1+x_2)} \left(\frac{t}{s}\right)^{-\frac{1}{2}(x_1-x_2)} \quad (4.124)$$

This reproduces the expected scaling form (4.104) together with the scaling function $f_R(y)$ as given in table 4.3 if we identify

$$x = x_1 = x_2, \quad \text{and} \quad x = a + 1 \quad (4.125)$$

For the critical bosonic contact process, we read off from table 4.2 that $a = \frac{d}{2} - 1$. Hence one recovers $x = \frac{d}{2}$, as expected for a free-field theory.

Reduction formulæ

We now show that the Bargmann superselection rule (4.119) implies a reduction of the n -point function of the full theory to certain correlators of the noiseless theory, which is described by S_0 only. This can be done generalising the arguments of [192].

First, to compute the response function, we add the term $\int d\mathbf{R} \int du \tilde{\phi}(\mathbf{R}, u)h(\mathbf{R}, u)$ to the action. As usual the response function is

$$\begin{aligned} R(\mathbf{r}, \mathbf{r}'; t, s) &= \left\langle \phi(\mathbf{r}, t) \tilde{\phi}(\mathbf{r}', s) \right\rangle \\ &= \left\langle \phi(\mathbf{r}, t) \tilde{\phi}(\mathbf{r}', s) \exp \left(-\mu \int d\mathbf{R} \int du \tilde{\phi}^2(\mathbf{R}, u) (\phi(\mathbf{R}, u) + \rho_0) \right) \right\rangle_0 \\ &= \left\langle \phi(\mathbf{r}, t) \tilde{\phi}(\mathbf{r}', s) \right\rangle_0 = R_0(\mathbf{r}, \mathbf{r}'; t, s) \end{aligned} \quad (4.126)$$

where we expanded the exponential and applied the Bargmann superselection rule. Indeed, the two-time response is just given by the response of the (Gaussian) noise-less theory. We have therefore reproduced the exact result of table 4.3 for the response function of the critical bosonic contact process.

Second, we have for the correlator

$$\begin{aligned} G(\mathbf{r}, \mathbf{r}', t, s) &= \left\langle \phi(\mathbf{r}, t) \phi(\mathbf{r}', s) \exp \left(-\mu \int d\mathbf{R} \int du \tilde{\phi}^2(\mathbf{R}, u) \phi(\mathbf{R}, u) \right) \right. \\ &\quad \left. \times \exp \left(-\mu \rho_0 \int d\mathbf{R} \int du \tilde{\phi}^2(\mathbf{R}, u) \right) \right\rangle_0 \end{aligned} \quad (4.127)$$

Expanding both exponentials

$$\begin{aligned} \exp \left(-\mu \int d\mathbf{R} \int du \tilde{\phi}^2(\mathbf{R}, u) \phi(\mathbf{R}, u) \right) &= \sum_{n=0}^{\infty} \frac{(-\mu)^n}{n!} \left(\int d\mathbf{R} \int du \tilde{\phi}^2(\mathbf{R}, u) \phi(\mathbf{R}, u) \right)^n \\ \exp \left(-\mu \rho_0 \int d\mathbf{R} \int du \tilde{\phi}^2(\mathbf{R}, u) \right) &= \sum_{m=0}^{\infty} \frac{(-\rho_0 \mu)^m}{m!} \left(\int d\mathbf{R} \int du \tilde{\phi}^2(\mathbf{R}, u) \right)^m \end{aligned}$$

and using the Bargmann superselection rule (4.119), non-vanishing terms only arise if $2n + 2m = n + 2$ or else

$$n + 2m = 2 \quad (4.128)$$

This can only be satisfied for $n = 0$ and $m = 1$ or for $n = 2$ and $m = 0$. The full noisy correlator hence is the sum of only two terms

$$G(\mathbf{r}, \mathbf{r}'; t, s) = G_1(\mathbf{r}, \mathbf{r}'; t, s) + G_2(\mathbf{r}, \mathbf{r}'; t, s) \quad (4.129)$$

where the first contribution involves a three-point function of the composite field $\tilde{\phi}^2$ of scaling dimension \tilde{x}_2 (see table 4.4)

$$G_1(\mathbf{r}, \mathbf{r}'; t, s) = -\mu\rho_0 \int d\mathbf{R} \int du \left\langle \phi(\mathbf{r}, t) \phi(\mathbf{r}', s) \tilde{\phi}^2(\mathbf{R}, u) \right\rangle_0 \quad (4.130)$$

whereas the second contribution comes from a four-point function and involves the composite field Υ (see table 4.4)

$$G_2(\mathbf{r}, \mathbf{r}'; t, s) = \frac{\mu^2}{2} \int d\mathbf{R} d\mathbf{R}' \int du du' \left\langle \phi(\mathbf{r}, t) \phi(\mathbf{r}', s) \Upsilon(\mathbf{R}, u) \Upsilon(\mathbf{R}', u') \right\rangle_0 \quad (4.131)$$

We see that the connected correlator is determined by three- and four-point functions of the noiseless theory. We now use the symmetries of that noise-less theory to determine the two-, three-, and four-point functions as far as possible.

Correlator with noise

We consider $G_1(\mathbf{r}, \mathbf{r}', t, s)$ first. The appropriate three-point function is given in appendix B of reference [17]:

$$\begin{aligned} \left\langle \phi(\mathbf{r}, t) \phi(\mathbf{r}', s) \tilde{\phi}^2(\mathbf{R}, u) \right\rangle_0 &= (t-s)^{x-\frac{1}{2}\tilde{x}_2} (t-u)^{-\frac{1}{2}\tilde{x}_2} (s-u)^{-\frac{1}{2}\tilde{x}_2} \\ &\times \exp\left(-\frac{\mathcal{M}(\mathbf{r}-\mathbf{R})^2}{2} \frac{1}{t-u} - \frac{\mathcal{M}(\mathbf{r}'-\mathbf{R})^2}{2} \frac{1}{s-u}\right) \Psi_3(u_1, v_1) \Theta(t-u) \Theta(s-u) \end{aligned} \quad (4.132)$$

with

$$\begin{aligned} u_1 &= \frac{u}{t} \cdot \frac{[(s-u)(\mathbf{r}-\mathbf{R}) - (t-u)(\mathbf{r}'-\mathbf{R})]^2}{(t-u)(s-u)^2} \\ v_1 &= \frac{u}{s} \cdot \frac{[(s-u)(\mathbf{r}-\mathbf{R}) - (t-u)(\mathbf{r}'-\mathbf{R})]^2}{(t-u)^2(s-u)} \end{aligned} \quad (4.133)$$

and an undetermined scaling function Ψ_3 . The Θ -functions have been introduced by hand because of causality but this could be justified through a more elaborate argument along the lines of [111]. Introduced into (4.130), this gives the general form for the contribution $G_1(\mathbf{r}, \mathbf{r}'; t, s)$. We concentrate here on the autocorrelator, i.e. $\mathbf{r} = \mathbf{r}'$ and find, with $y = t/s$

$$\begin{aligned} G_1(t, s) &= -\mu\rho_0 s^{-x-\frac{1}{2}\tilde{x}_2+\frac{d}{2}+1} \cdot (y-1)^{-(x-\frac{1}{2}\tilde{x}_2)} \\ &\times \int_0^1 d\theta (y-\theta)^{-\frac{1}{2}\tilde{x}_2} (1-\theta)^{-\frac{1}{2}\tilde{x}_2} \int_{\mathbb{R}^d} d\mathbf{R} \exp\left(-\frac{\mathcal{M}}{2} \mathbf{R}^2 \frac{y+1-2\theta}{(y-\theta)(1-\theta)}\right) \\ &\times H\left(\frac{\theta}{y} \frac{\mathbf{R}^2(y-1)^2}{(y-\theta)(1-\theta)^2}, \theta \frac{\mathbf{R}^2(y-1)^2}{(y-\theta)^2(1-\theta)}\right) \end{aligned} \quad (4.134)$$

where H is an undetermined scaling function. Very much in the same way, we find for $G_2(t, s)$

$$\begin{aligned} G_2(t, s) &= \frac{\mu^2}{2} s^{-x-x_\Gamma+d+2} \cdot (y-1)^{-(x-x_\Gamma)} \int_0^1 d\theta \int_0^1 d\theta' (y-\theta)^{-\frac{1}{2}x_\Gamma} (1-\theta)^{-\frac{1}{2}x_\Gamma} \\ &\quad \times (y-\theta')^{-\frac{1}{2}x_\Gamma} (1-\theta')^{-\frac{1}{2}x_\Gamma} \int_{\mathbb{R}^{2d}} d\mathbf{R}d\mathbf{R}' \exp\left(-\frac{\mathcal{M}}{2} \frac{\mathbf{R}^2}{1-\theta} - \frac{\mathcal{M}}{2} \frac{\mathbf{R}'^2}{1-\theta'}\right) \\ &\quad \times \Psi_4(\tilde{u}_3(\mathbf{R}, \theta, \mathbf{R}', \theta'), \tilde{u}_4(\mathbf{R}, \theta, \mathbf{R}', \theta'), \tilde{v}_3(\mathbf{R}, \theta, \mathbf{R}', \theta'), \tilde{v}_4(\mathbf{R}, \theta, \mathbf{R}', \theta')) \end{aligned} \quad (4.135)$$

where Ψ_4 is another undetermined function and the functions $\tilde{u}_3, \tilde{u}_4, \tilde{v}_3, \tilde{v}_4$ can be worked out from the appropriate expressions for the n -point functions given in the appendix B of [17] by the replacements $\mathbf{r}_3 - \mathbf{r}_2 \rightarrow \mathbf{R}, \mathbf{r}_4 - \mathbf{r}_2 \rightarrow \mathbf{R}', t_2 \rightarrow 1, t_1 \rightarrow y, t_3 \rightarrow \theta, t_4 \rightarrow \theta'$ (remember that $\mathbf{r}_1 = \mathbf{r}_2$)

As we have a free-field theory for the critical bosonic contact process, we expect from table 4.2 and eq. (4.125) that $x = \tilde{x} = d/2$ and hence the following scaling dimensions for the composite fields

$$\tilde{x}_2 = d, \quad x_\Gamma = \frac{3}{2}d \quad (4.136)$$

Consequently, the autocorrelator takes the general form

$$G(t, s) = s^{1-d/2} g_1(t/s) + s^{2-d} g_2(t/s) \quad (4.137)$$

For d larger than the lower critical dimension $d_* = 2$, the second term merely furnishes a finite-time correction. On the other hand, for $d < d_* = 2$, it would be the dominant one and we can only achieve agreement with the known exact result if we assume $\Psi_4 = 0$. In what follows, we shall discard the scaling function g_2 and shall concentrate on showing that our expressions for g_1 are compatible with the exact results given in table 4.3. In order to do so, we choose the following special form for the function Ψ_3

$$\Psi_3(u_1, v_1) = \Xi\left(\frac{1}{u_1} - \frac{1}{v_1}\right) \quad (4.138)$$

where Ξ remains an arbitrary function. Then we are back in the case already treated in [192]. We find

$$\begin{aligned} G_1(t, s) &= -\mu\rho_0 s^{\frac{d}{2}+1-x-\frac{1}{2}\tilde{x}_2} (y-1)^{\frac{1}{2}\tilde{x}_2-x-\frac{d}{2}} \\ &\quad \times \int_0^1 d\theta [(y-\theta)(1-\theta)]^{\frac{d}{2}-\frac{1}{2}\tilde{x}_2} \phi_1\left(\frac{y+1-2\theta}{y-1}\right) \end{aligned} \quad (4.139)$$

where the function ϕ_1 is defined by

$$\phi_1(w) = \int d\mathbf{R} \exp\left(-\frac{\mathcal{M}w}{2} \mathbf{R}^2\right) \Xi(\mathbf{R}^2) \quad (4.140)$$

As in [192] we choose

$$\phi_1(w) = \phi_{0,c} w^{-1-a}. \quad (4.141)$$

This form for $\phi_1(w)$ guarantees that the three-point response function $\langle \phi(\mathbf{r}, t) \phi(\mathbf{r}, s) \phi^2(\mathbf{r}', u) \rangle_0$ is nonsingular for $t = s$. We have thus

$$G(t, s) = G_1(t, s) = s^{-b} f_G\left(\frac{t}{s}\right) \quad (4.142)$$

with

$$\begin{aligned} f_G(y) &= -\mu\rho_0\phi_{0,c} \int_0^1 d\theta (y+1-2\theta)^{-\frac{d}{2}} \\ &= \frac{2\mu\rho_0\phi_{0,c}}{d} \left((y-1)^{-\frac{d}{2}+1} - (y+1)^{-\frac{d}{2}+1} \right) \end{aligned} \quad (4.143)$$

and we have reproduced the corresponding entry in table 4.3 for the critical bosonic contact process.²⁰

4.3.3 The bosonic pair-contact process

Field-theoretical description and reduction formula

For the pair-contact process we have two different cases, namely the case $\alpha < \alpha_c$ and the case at criticality $\alpha = \alpha_c$. The following considerations apply to both cases and we shall for the moment leave the value of α arbitrary and only fix it at a later state.

The action for the pair-contact process on the critical line is [130, eq. (30)]

$$S[a, \bar{a}] = \int d\mathbf{R} \int du [\bar{a}(2\mathcal{M}\partial_t - \nabla^2)a - \alpha\bar{a}^2a^2 - \mu\bar{a}^3a^2] \quad (4.144)$$

As before, see eq. (4.107), we switch to the quasiprimary fields $\phi(\mathbf{r}, t) = a(\mathbf{r}, t) - \rho_0$ and $\tilde{\phi}(\mathbf{r}, t) = \bar{a}(\mathbf{r}, t)$. Then the action becomes

$$\begin{aligned} S[\phi, \tilde{\phi}] &= \int d\mathbf{R} \int du \left[\tilde{\phi}(2\mathcal{M}\partial_t - \nabla^2)\phi - \alpha\tilde{\phi}^2\phi^2 - \alpha\rho_0^2\tilde{\phi}^2 - \right. \\ &\quad \left. - 2\alpha\rho_0\tilde{\phi}^2\phi - \mu\tilde{\phi}^3\phi^2 - 2\mu\rho_0\tilde{\phi}^3\phi - \mu\rho_0^2\tilde{\phi}^3 \right] \\ &= S_0[\phi, \tilde{\phi}] + S_b[\phi, \tilde{\phi}] \end{aligned} \quad (4.145)$$

Also in this model, similarly to the treatment of section 4.3.2, a decomposition of the action into a first term with a non-trivial dynamic symmetry and a remaining noise term is sought such that the correlators and responses can be re-expressed in terms of certain n -point functions which only depend on S_0 . The first term reads

$$S_0[\phi, \tilde{\phi}] := \int d\mathbf{r} \int dt \left[\tilde{\phi}(2\mathcal{M}\partial_t - \nabla^2)\phi - \alpha\tilde{\phi}^2\phi^2 \right]. \quad (4.146)$$

and we derive its Schrödinger-invariance in appendix B. The remaining part is the noise-term which reads

$$S_b[\phi, \tilde{\phi}] = \int d\mathbf{R} \int du \left[-\alpha\rho_0^2\tilde{\phi}^2 - 2\alpha\rho_0\tilde{\phi}^2\phi - \mu\tilde{\phi}^3\phi^2 - 2\mu\rho_0\tilde{\phi}^3\phi - \rho_0^2\tilde{\phi}^3 \right] \quad (4.147)$$

Also in this case the Bargmann superselection rule (4.119) holds true. This means that we can proceed now in a very similar way as before.²¹ First we have to check which n -point

²⁰We remark that for $2 < d < 4$, the same form of the autocorrelation function is also found in the critical voter-model [76].

²¹This argument works provided each term in S_b contains at least one response field $\tilde{\phi}$ more than order-parameter fields ϕ .

contr.	k_1	k_2	k_3	k_4	comp.field	scaling dim.	3-point/4-point
$G_1(t, s)$	1	0	0	0	$\tilde{\phi}^2$	\tilde{x}_2	3-point
$G_2(t, s)$	0	2	0	0	Υ	x_Υ	4-point
$G_3(t, s)$	0	0	2	0	Γ	x_Γ	4-point
$G_4(t, s)$	0	0	0	1	Σ	x_Σ	3-point
$G_5(t, s)$	0	1	1	0	Υ and Γ	x_Υ, x_Γ	4-point

Table 4.5: Contributions to the correlation function: The first column shows how we denote the contribution, the next four columns give the value of the corresponding indices. The sixth column lists the composite field(s) involved, the seventh column how we denote the scaling dimension of that field. The last column lists whether it is a three- or four-point function that contributes.

functions contribute to the response and correlation function. We rewrite $\exp(-S_b[\phi, \tilde{\phi}])$ as a product of five exponentials and expand each factor. The indices of the sums are denoted by k_i for the i -th term in (4.147), for instance for the first term

$$\exp\left(-\int d\mathbf{R} \int du \alpha \rho_0^2 \tilde{\phi}^2(\mathbf{R}, u)\right) = \sum_{k_1=0}^{\infty} \frac{1}{k_1!} \left(-\int d\mathbf{R} \int du \alpha \rho_0^2 \tilde{\phi}^2(\mathbf{R}, u)\right)^{k_1} \quad (4.148)$$

For the response function again only the first term of each sum contributes, that is

$$R(\mathbf{r}, \mathbf{r}'; t, s) = R_0(\mathbf{r}, \mathbf{r}'; t, s) \quad (4.149)$$

is noise-independent. For the correlation function, we have the condition $2k_1 + 2k_2 + 3k_3 + 3k_4 + 3k_5 = 2 + k_2 + 2k_3 + k_4$ or simply

$$2k_1 + k_2 + k_3 + 2k_4 + 3k_5 = 2 \quad (4.150)$$

which implies immediately that

$$k_5 = 0. \quad (4.151)$$

In table 4.5 we list the five different contributions to the correlation function. We denote also the form of the composite field, its scaling dimension and whether it is a three- or four-point function which contributes. A short inspection of the general form of the n -points function given in [17] shows that the contributions have the form (with $y = t/s$)

$$G_1(t, s) = s^{-x - \frac{1}{2}\tilde{x}_2 + \frac{d}{2} + 1} f_1(y) \quad , \quad G_4(t, s) = s^{-x - \frac{1}{2}x_\Sigma + \frac{d}{2} + 1} f_4(y) \quad (4.152)$$

for the 3-point functions and

$$\begin{aligned} G_2(t, s) &= s^{-x - x_\Upsilon + d + 2} f_2(y) \quad , \quad G_3(t, s) = s^{-x - x_\Gamma + d + 2} f_3(y) \\ G_5(t, s) &= s^{-x - \frac{1}{2}x_\Upsilon - \frac{1}{2}x_\Gamma + d + 2} f_5(y) \end{aligned}$$

for the four-point functions. The scaling functions $f_i(y)$ involve an arbitrary functions $\tilde{\Psi}_i$ which are not fixed by the symmetries (see the appendices of [17] for details). As we do not have a free-field theory in this case we can not make any assumptions about the

value of the scaling dimensions of the composite fields. Therefore we do not know which terms will be the leading ones in the scaling regime. However, it turns out that the term $G_1(t, s)$ alone can reproduce our result correctly. Thus we set the scaling functions $f_n=0$ with $n = 2, \dots, 5$ analogously to the last section. We now concentrate on

$$G_1(t, s) = \alpha \rho_0^2 \int d\mathbf{R} \int du \left\langle \phi(\mathbf{r}, t) \phi(\mathbf{r}, s) \tilde{\phi}^2(\mathbf{R}, u) \right\rangle_0 \quad (4.153)$$

Symmetries of the noiseless theory

As in the last chapter, we require for the calculation of the two- and three-point functions the symmetries of the following non-linear ‘Schrödinger equation’ obtained from (4.146)

$$2\mathcal{M}\partial_t\phi(\mathbf{x}, t) = \nabla^2\phi(\mathbf{x}, t) + \mathcal{F}(\phi, \tilde{\phi}) \quad (4.154)$$

with a nonlinear potential

$$\mathcal{F}(\phi, \tilde{\phi}) = -g\phi^2(\mathbf{x}, t)\tilde{\phi}(\mathbf{x}, t) \quad (4.155)$$

While for a constant g the symmetries of this equation are well-known, it was pointed out recently that g rather should be considered as a dimensionful quantity and hence should transform under local scale-transformations as well [222]. This requires an extension of the generators used so far and we shall give this in appendix B. The computation of the n -point functions covariant with respect to these new generators is given in the appendices B and C of [17]. In doing so, we have for technical simplicity assumed that to each field φ_i there is one associated coupling constant g_i and only at the end, we let

$$g_1 = \dots = g_n =: g \quad (4.156)$$

Therefore, from eq. (4.149) we find for the response function (see [17])

$$R_0(\mathbf{r}, \mathbf{r}'; t, s) = (t-s)^{-\frac{1}{2}(x_1+x_2)} \left(\frac{t}{s}\right)^{-\frac{1}{2}(x_1-x_2)} \times \exp\left(-\frac{\mathcal{M}(\mathbf{r}-\mathbf{r}')^2}{2} \frac{t-s}{t-s}\right) \tilde{\Psi}_2\left(\frac{t}{s}, \frac{t-s}{g^{1/y}}, \frac{g}{(t-s)^y}\right) \quad (4.157)$$

with an undetermined scaling function $\tilde{\Psi}_2$. This form is clearly consistent with our results in table 4.3 if we identify

$$x := x_1 = x_2 = a + 1 = \frac{d}{2}, \quad \tilde{\Psi}_2 = \text{const.} \quad (4.158)$$

This holds true for both $\alpha < \alpha_c$ and $\alpha = \alpha_c$. In distinction with the bosonic contact process, the symmetries of the noiseless part S_0 do not fix the response function completely but leave a certain degree of flexibility in form of the scaling function $\tilde{\Psi}_2$.

For the calculation of the correlator we need from eq. (4.153) the following three-point function

$$\left\langle \phi(\mathbf{r}, t) \phi(\mathbf{r}', s) \tilde{\phi}^2(\mathbf{R}, u) \right\rangle_0 = (t-s)^{x-\frac{1}{2}\tilde{x}_2} (t-u)^{-\frac{1}{2}\tilde{x}_2} (s-u)^{-\frac{1}{2}\tilde{x}_2} \times \exp\left(-\frac{\mathcal{M}(\mathbf{r}-\mathbf{R})^2}{2} \frac{t-u}{t-u} - \frac{\mathcal{M}(\mathbf{r}'-\mathbf{R})^2}{2} \frac{t-u}{s-u}\right) \tilde{\Psi}_3(u_1, v_1, \beta_1, \beta_2, \beta_3) \quad (4.159)$$

with

$$u_1 = \frac{u}{t} \cdot \frac{[(s-u)(\mathbf{r}-\mathbf{R}) - (t-u)(\mathbf{r}'-\mathbf{R})]^2}{(t-u)(s-u)^2} \quad (4.160)$$

$$v_1 = \frac{u}{s} \cdot \frac{[(s-u)(\mathbf{r}-\mathbf{R}) - (t-u)(\mathbf{r}'-\mathbf{R})]^2}{(t-u)^2(s-u)} \quad (4.161)$$

$$\beta_1 = \frac{1}{s_2} \cdot \frac{\alpha^{1/y}}{(t-u)^2}, \quad \beta_2 = \frac{1}{s_2} \cdot \frac{\alpha^{1/y}}{(s-u)^2}, \quad \beta_3 = \alpha^{1/y} s_2 \quad (4.162)$$

$$s_2 = \frac{1}{t-u} + \frac{1}{u} \quad (4.163)$$

We choose the following realisation for $\tilde{\Psi}_3$

$$\tilde{\Psi}_3(u_1, v_1, \beta_1, \beta_2, \beta_3) = \Xi \left(\frac{1}{u_1} - \frac{1}{v_1} \right) \left[-\frac{(\sqrt{\beta_1} - \sqrt{\beta_2})\sqrt{\beta_3}}{\beta_3 - \sqrt{\beta_2}\beta_3} \right]^{(a-b)} \quad (4.164)$$

where the scaling function Ξ was already encountered in eq. (4.138) for the bosonic contact process. We now have to distinguish the two different cases $\alpha < \alpha_c$ and $\alpha = \alpha_c$. For the first case $\alpha < \alpha_c$, we have $a - b = 0$ so that the last factor in (4.164) disappears and we simply return to the expressions already found for the bosonic contact process, in agreement with the known exact results. However, at the multicritical point $\alpha = \alpha_c$ we have $a - b \neq 0$ and the last factor becomes important. We point out that only the presence or absence of this factor distinguishes the cases $\alpha < \alpha_c$ and $\alpha = \alpha_c$.

If we substitute the values for β_1, β_2 and β_3 , $\tilde{\Psi}_3$ becomes

$$\tilde{\Psi}_3(u_1, v_1, \beta_1, \beta_2, \beta_3) = \Xi \left(\frac{1}{u_1} - \frac{1}{v_1} \right) \left[\frac{\theta(y-1)}{(y-\theta)(1-\theta)} \right]^{(a-b)} \quad (4.165)$$

This factor does not involve \mathbf{R} so that we obtain in a similar way as before

$$\begin{aligned} G_1(t, s) &= s^{-b}(y-1)^{(b-a)-a-1} \int_0^1 d\theta [(y-\theta)(1-\theta)]^{a-b} \\ &\quad \times \phi_1 \left(\frac{y+1-2\theta}{y-1} \right) \left[\frac{\theta(y-1)}{(y-\theta)(1-\theta)} \right]^{a-b} \end{aligned} \quad (4.166)$$

where we have identified

$$\tilde{x}_2 = 2(b-a) + d \quad (4.167)$$

$G_1(t, s)$ reduces to the expression (4.106) if we choose the same expression for $\phi_1(w)$ as before. We have thus reproduced all scaling functions correctly.

4.3.4 Conclusions of this section

The objective of our investigation has been to test further the proposal of using the non-trivial dynamical symmetries of a part of the Langevin equation in order to derive properties of the full stochastic non-equilibrium model. We also wanted to outline how a generalisation of LSI with $z = 2$ which includes also nonlinear models can be constructed. To this end, we have compared the known exact results for the two-time autoresponse

and autocorrelation functions in two specific models, see table 4.3, with the expressions derived from the standard field-theoretical actions which are habitually used to describe these systems. This is achieved through the same decomposition of the action we have already considered before. The action is decomposed into two parts $S = S_0 + S_b$ such that (i) S_0 is Schrödinger-invariant and the Bargmann superselection rules hold for the averages calculated with S_0 only and (ii) the remaining terms contained in S_b are such that a perturbative expansion terminates at a finite order, again due to the Bargmann superselection rules. The two models we considered, namely the bosonic variants of the critical contact and pair-contact processes, satisfy these requirements and are clearly in agreement with the predictions of local scale-invariance (LSI). In particular, our identification eq. (4.107) of the correct quasi-primary order-parameter and response fields is likely to be useful in more general systems.

Specifically, we have seen the following.

1. In the bosonic contact process, the symmetries of the noiseless part S_0 of the action is described in terms of the representation of the Schrödinger-group relevant for the *free* diffusion equation.

In consequence, the form of the two-time response function is completely fixed by LSI and in agreement with the known exact result. The connected autocorrelator is exactly reducible to certain noiseless three- and four-point functions. Schrödinger-invariance alone cannot determine these but the remaining free scaling functions can be chosen such that the known exact results can be reproduced.

2. For the bosonic pair-contact process, the symmetries of the partial action S_0 are described in terms of a new representation pertinent to a *non-linear* Schrödinger equation. This new representation, which we have explicitly constructed [17], involves a dimensionful coupling constant g . Therefore even the response function is no longer fully determined. As for the autocorrelation function, which again can be exactly reduced to certain three- and four-point functions calculable from the action S_0 , the remaining free scaling functions can be chosen as to fully reproduce the known exact results.

The consistency of the predictions of LSI with the exact results of these models furnishes further evidence in favour of an extension of the well-known dynamical scaling towards a (hidden) local scale-invariance which influences the long-time behaviour of slowly relaxing systems. An essential ingredient were the Bargmann superselection rules for which a generalisation for the case $z \neq 2$ was given. It would be interesting to generalise also the case $z \neq 2$ to include nonlinear models. This work is left for the future.

Chapter 5

Ageing at surfaces in semi-infinite systems

All systems considered up to now were translationally invariant. Obviously, this is not a realistic scenario as every physical system will have surfaces and corners which might influence the physical behaviour. As a first step towards a more realistic setup, we consider in this chapter semi-infinite systems: The systems stays infinitely extended in all but the first direction. In this special direction we introduce a surface at $x_1 = 0$, keeping the systems extended over the whole half-space $V = [0, \infty) \times \mathbb{R}^{d-1}$ (for a continuous system) or $V = \mathbb{Z}_{>0} \times \mathbb{Z}^{d-1}$ (for a system on a lattice where the lattice spacing was set to unity). We ask the question if and to what extent the ageing behaviour is changed by the presence of the surface. We will restrict ourselves here to the case of magnetic systems.

The investigation of out-of-equilibrium phenomena in semi-infinite systems has been started fairly recently in a numerical work by Pleimling [195] and a subsequent publication by Calabrese and Gambassi [45]. In this chapter we first want to add some exact results to this by considering the semi-infinite spherical model. This will then lead to some interesting new questions, which will be address in the second section.

The content of this chapter can be found in the following papers

- F. Baumann and M. Pleimling, J. Phys. A: Math. Gen. **39**, 1981 (2006).
- F. Baumann and M. Pleimling, Phys. Rev. **B 76**, 104422 (2007).

5.1 An exactly solvable model

5.1.1 Introduction

The phenomenology briefly described in chapter 1, in particular the scaling forms (1.11) and (1.12), has been found to be valid in many bulk systems. It has only been realised recently [195] that in semi-infinite critical systems similar dynamical scaling is also observed for surface quantities. At the surface we can define, in complete analogy with a bulk system, surface autocorrelation and autoresponse functions:

$$C_1(t, s) = \langle \phi_1(t) \phi_1(s) \rangle \quad , \quad R_1(t, s) = \left. \frac{\delta \langle \phi_1(t) \rangle}{\delta h_1(s)} \right|_{h_1=0} \quad (t > s) \quad (5.1)$$

where $\phi_1(t)$ is now the surface order parameter and h_1 is a field acting solely on the surface layer. In the regime $t, s, t - s \gg t_{micro}$ we expect simple scaling forms:

$$C_1(t, s) = s^{-b_1} f_{C_1}(t/s) \quad (5.2)$$

$$R_1(t, s) = s^{-1-a_1} f_{R_1}(t/s) \quad (5.3)$$

and the scaling functions $f_{C_1}(y)$ and $f_{R_1}(y)$ should display a power-law behaviour in the limit $y \rightarrow \infty$:

$$f_{C_1}(y) \sim y^{-\lambda_{C_1}/z} \quad , \quad f_{R_1}(y) \sim y^{-\lambda_{R_1}/z}. \quad (5.4)$$

Equations (5.2) - (5.4) define the surface exponents a_1 , b_1 , λ_{C_1} and λ_{R_1} . In general these surface non-equilibrium exponents may take on values that differ from their bulk counterparts. This is similar to what is known for static critical exponents where the surface values differ from the bulk ones [71, 196]. Relations between the different non-equilibrium exponents can again be derived from general scaling arguments [195, 45]. Thus we obtain

$$a_1 = b_1 = (d - 2 + \eta_{\parallel})/z \quad (5.5)$$

where the static exponent η_{\parallel} governs the decay of correlations parallel to the surface. For the surface autocorrelation exponent $\lambda_{C_1} = \lambda_{R_1}$ one finds [205, 197]

$$\lambda_{C_1} = \lambda_C + \eta_{\parallel} - \eta. \quad (5.6)$$

The scaling laws (5.2) - (5.4) and the different relations between the non-equilibrium critical exponents have been verified in [195] through Monte Carlo simulations of critical semi-infinite Ising models in two and three dimensions. In [45] the scaling forms in the presence of a surface have been discussed in more detail and calculations within the Gaussian model have been presented.

One of the most intriguing aspects of surface critical phenomena is the presence of different surface universality classes for a given bulk universality class [71, 196]. In this section we study ageing phenomena in semi-infinite spherical models with Dirichlet boundary conditions (corresponding at the critical point to the so-called ordinary transition where the bulk alone is critical) and with Neumann boundary conditions. Besides investigating the surface out-of-equilibrium dynamics at the critical point we also analyse the dynamical behaviour close to a surface in the ordered phase. To our knowledge this is the first study of surface ageing phenomena in systems where phase ordering takes place. As we shall see we thereby obtain for Dirichlet boundary conditions the unexpected result that

the value of the non-equilibrium exponent b_1 , describing the dynamical scaling of the surface autocorrelation (5.2), is different from zero, the value encountered in bulk systems undergoing phase ordering [37].

The present section is on the one hand meant to close a gap in the study of kinetic spherical models [59, 93, 5], which up to now have been restricted to systems with periodic boundary conditions. On the other hand our intention is also to extend towards dynamics earlier investigations of the surface criticality of the spherical model [149, 9, 10, 219, 61, 62]. It has to be noted in this context that the static properties of the critical semi-infinite spherical model with one spherical field (which means that all the spins are subject to the same spherical constraint) have been shown to differ from those of the $O(N)$ model with $N \rightarrow \infty$ [10, 219], even so both models are strictly equivalent in the bulk system [221, 143].

This section is organised in the following way. In subsection 5.1.2 we present the kinetic model in a quite general way, thus leaving open the possibility to consider different boundary conditions in the different space directions. In subsection 5.1.3 and 5.1.4 we discuss the dynamical scaling behaviour of surface correlation and response functions, whereas in subsection 5.1.5 we compute the surface fluctuation-dissipation ratio. Finally, subsection 5.1.6 gives our conclusions.

5.1.2 The model

General setting

We consider a finite hypercubic system Λ in d dimensions containing $\mathcal{N} = L_1 \times \dots \times L_d$ sites where L_ν denotes the length of the ν -th edge¹. To every lattice site $\mathbf{r}^T = (r_1, \dots, r_d)$ we associate a time-dependent real variable $S(\mathbf{r}, t)$ describing the spin on site \mathbf{r} . These variables are subject to the mean spherical constraint

$$\sum_{\mathbf{r} \in \Lambda} \langle S^2(\mathbf{r}, t) \rangle = \mathcal{N} \quad (5.7)$$

where the brackets indicate an average over the thermal noise. The Hamiltonian of the spherical model is given in a bulk system by

$$\mathcal{H} = -J \sum_{\langle \mathbf{r}, \mathbf{r}' \rangle} S(\mathbf{r})S(\mathbf{r}') \quad (5.8)$$

where the sum runs over pairs of neighbouring spins.

As we are interested in the d -dimensional slab geometry we impose periodic boundary conditions in all but one space direction. We then have in the ν -th direction (with $\nu = 2, \dots, d$)

$$S((r_1, \dots, r_\nu + m L_\nu, \dots, r_d), t) = S((r_1, \dots, r_\nu, \dots, r_d), t) \quad \text{for all } m \in \mathbb{Z}. \quad (5.9)$$

In the remaining direction we either consider Dirichlet boundary conditions or Neumann boundary conditions. For Dirichlet boundary conditions we impose that

$$S((0, r_2, \dots, r_d), t) = S((L_1 + 1, r_2, \dots, r_d), t) = 0. \quad (5.10)$$

¹We set the lattice spacing equal to one.

For Neumann boundary conditions, on the other hand, we have:

$$\begin{aligned} S((0, r_2, \dots, r_d), t) &= S((1, r_2, \dots, r_d), t) \\ S((L_1 + 1, r_2, \dots, r_d), t) &= S((L_1, r_2, \dots, r_d), t). \end{aligned} \quad (5.11)$$

In the following, quantities depending on the chosen boundary condition will be labelled by the superscript (p) , (d) , and (n) for periodic, Dirichlet, and Neumann boundary conditions, respectively.

The Hamiltonian can be written in the following general form

$$H = -\frac{1}{2} J \mathbf{S}_\Lambda^T \cdot \mathbf{Q}_\Lambda^{(\tau)} \cdot \mathbf{S}_\Lambda + \frac{1}{2} \lambda^{(\tau)}(t) \mathbf{S}_\Lambda^T \cdot \mathbf{S}_\Lambda - \mathbf{S}_\Lambda^T \cdot \mathbf{h}_\Lambda \quad (5.12)$$

where the vector $\mathbf{S}_\Lambda := \{S(\mathbf{r}) | \mathbf{r} \in \Lambda\}$ characterises the state of the system. $J > 0$ is the strength of the ferromagnetic nearest neighbour couplings and is chosen to be equal to one in the following. Furthermore, $\mathbf{h}_\Lambda := \{h(\mathbf{r}) | \mathbf{r} \in \Lambda\}$ where $h(\mathbf{r})$ is an external field acting on the spin at site \mathbf{r} , whereas $\lambda^{(\tau)}(t)$ is the Lagrange multiplier ensuring the constraint (5.7). Finally, the interaction matrix $\mathbf{Q}_\Lambda^{(\tau)}$ (with $\tau = (\tau_1, \dots, \tau_d)$ characterising the boundary conditions in the d different directions) is given by the tensor product [32]

$$\mathbf{Q}_\Lambda^{(\tau)} = \bigotimes_{\nu=1}^d (\Delta_\nu^{(\tau_\nu)} + 2\mathbf{E}_\nu). \quad (5.13)$$

Here \mathbf{E}_ν is the unit matrix of dimension L_ν , whereas $\Delta_\nu^{(\tau_\nu)}$ is the discrete Laplacian in the ν -direction which depends on the boundary condition.

It is convenient to parametrise the Lagrange multiplier in the following way [32]:

$$\lambda^{(\tau)}(t) = \mu_\Lambda^{(\tau)}(\boldsymbol{\kappa}) + z^{(\tau)}(t)$$

where $\mu_\Lambda^{(\tau)}(\boldsymbol{\kappa})$ is the largest eigenvalue of the interaction matrix $\mathbf{Q}_\Lambda^{(\tau)}$ and $\boldsymbol{\kappa}$ is the corresponding value of the vector \mathbf{k} (see Appendix A of [16]) which labels the different eigenvalues and eigenfunctions of $\mathbf{Q}_\Lambda^{(\tau)}$. In case of periodic boundary conditions in *all* directions we recover the usual expression

$$\lambda^{(p)}(t) = 2d + z^{(p)}(t).$$

Langevin equation

In order to study the out-of-equilibrium dynamical behaviour of the semi-infinite kinetic spherical model we prepare the system at time $t = 0$ in a fully disordered infinite temperature equilibrium state with vanishing magnetisation. We then bring the system in contact with a thermal bath at a given temperature T and monitor its temporal evolution. Assuming purely relaxational dynamics (i.e. model A dynamics), the dynamics of the system is given by the following stochastic Langevin equation:

$$\frac{d}{dt} \mathbf{S}_\Lambda(t) = (\mathbf{Q}_\Lambda^{(\tau)} - z^{(\tau)}(t) - \mu_\Lambda^{(\tau)}(\boldsymbol{\kappa})) \mathbf{S}_\Lambda(t) + \mathbf{h}_\Lambda(t) + \boldsymbol{\eta}_\Lambda(t) \quad (5.14)$$

where $\boldsymbol{\eta}_\Lambda(t) := \{\eta_{\mathbf{r}}(t) | \mathbf{r} \in \Lambda\}$ with $\eta_{\mathbf{r}}(t)$ being a Gaussian white noise:

$$\langle \eta_{\mathbf{r}}(t) \rangle = 0 \quad \text{and} \quad \langle \eta_{\mathbf{r}}(t) \eta_{\mathbf{r}'}(t') \rangle = 2T \delta_{\mathbf{r}, \mathbf{r}'} \delta(t - t').$$

We further assume that the external field \mathbf{h}_Λ is time-dependent. Equation (5.14) can easily be solved, yielding

$$\begin{aligned} \mathbf{S}_\Lambda(t) &= \exp\left(\int_0^t dt' (\mathbf{Q}_\Lambda^{(\tau)} - z^{(\tau)}(t') - \mu_\Lambda^{(\tau)}(\boldsymbol{\kappa}))\right) \times \left[\mathbf{S}_\Lambda(0) \right. \\ &\quad \left. + \int_0^t dt' \left(\exp\left(-\int_0^{t'} dt'' (\mathbf{Q}_\Lambda^{(\tau)} - z^{(\tau)}(t'') - \mu_\Lambda^{(\tau)}(\boldsymbol{\kappa}))\right) (\mathbf{h}_\Lambda(t') + \boldsymbol{\eta}_\Lambda(t'))\right)\right]. \end{aligned} \quad (5.15)$$

In order to proceed further we use a decomposition in an orthonormal basis of eigenfunctions of the interaction matrix $\mathbf{Q}_\Lambda^{(\tau)}$:

$$\tilde{S}(\mathbf{k}, t) := \sum_{\mathbf{r} \in \Lambda} \left(\prod_{\nu=1}^d u_{L_\nu}^{(\tau_\nu)}(r_\nu, k_\nu) \right) S(\mathbf{r}, t) \quad (5.16)$$

where the vectors $u_{L_\nu}^{(\tau_\nu)}(r_\nu, k_\nu)$ are given in Appendix A of [16]. We get the original vector back by the inverse transformation

$$S(\mathbf{r}, t) = \sum_{\mathbf{k} \in \Lambda} \left(\prod_{\nu=1}^d u_{L_\nu}^{(\tau_\nu)*}(r_\nu, k_\nu) \right) \tilde{S}(\mathbf{k}, t). \quad (5.17)$$

The transformation (5.16) diagonalizes the symmetric matrix $\mathbf{Q}_\Lambda^{(\tau)} - z(t) - \mu_\Lambda^{(\tau)}(\boldsymbol{\kappa})$, yielding

$$\tilde{S}(\mathbf{k}, t) = \frac{e^{-\omega^{(\tau)}(\mathbf{k})t}}{\sqrt{g^{(\tau)}(t)}} \left[\tilde{S}(\mathbf{k}, 0) + \int_0^t dt' \left(\sqrt{g^{(\tau)}(t')} e^{\omega^{(\tau)}(\mathbf{k})t'} (\tilde{h}(\mathbf{k}, t') + \tilde{\eta}(\mathbf{k}, t')) \right) \right] \quad (5.18)$$

with

$$g^{(\tau)}(t) := \exp\left(2 \int_0^t du z^{(\tau)}(u)\right) \quad (5.19)$$

and

$$\omega^{(\tau)}(\mathbf{k}) := -\mu_\Lambda^{(\tau)}(\mathbf{k}) + \mu_\Lambda^{(\tau)}(\boldsymbol{\kappa}). \quad (5.20)$$

We now take the limit of the semi-infinite system which extends from $-\infty$ to ∞ in the directions parallel to the surface, whereas in the remaining direction the coordinate r_1 takes on only positive values. In order to stress the existence of the special direction we set $\mathbf{r}^T = (r, \mathbf{x}^T)$ with $r := r_1$ and $\mathbf{x}^T := (r_2, \dots, r_d)$. The corresponding vector in reciprocal space is then written as $\mathbf{k}^T = (k, \mathbf{q}^T)$ with $k := k_1$ and $\mathbf{q}^T := (k_2, \dots, k_d)$. As a consequence of the semi-infinite volume limit sums have to be replaced by integrals in the following way [32]:

- $\frac{2}{L_1} \sum_{k_1=1}^{L_1} (\dots) \longrightarrow \frac{2}{\pi} \int_0^\pi dk (\dots)$ in the direction perpendicular to the surface,
- $\frac{1}{L_\nu} \sum_{k_\nu=1}^{L_\nu} (\dots) \longrightarrow \frac{1}{2\pi} \int_{-\pi}^\pi dk (\dots)$ in all other directions,

where the integration limits follow from Appendix A in [16]. It has to be noted that in the semi-infinite volume limit the largest eigenvalue of the interaction matrix (5.13) is

given by $\mu_\Lambda^{(\tau)}(\boldsymbol{\kappa}) = 2d$ irrespective of the chosen boundary condition. We therefore rewrite (5.20) in the following way:

$$\omega^{(\tau)}(\mathbf{k}) = \omega(k, \mathbf{q}) = \tilde{\omega}(k) + \hat{\omega}(\mathbf{q}) \quad (5.21)$$

with

$$\tilde{\omega}(k) = 2(1 - \cos k) \quad \text{and} \quad \hat{\omega}(\mathbf{q}) = 2 \sum_{\nu=2}^d (1 - \cos k_\nu). \quad (5.22)$$

where we used the explicit expressions for $\mu_\Lambda^{(\tau)}(\mathbf{k})$ (see Appendix A of [16]).

As usual we prepare the system at time $t = 0$ in a completely uncorrelated initial state with vanishing magnetisation. We then have at $t = 0$ in reciprocal space

$$\langle \tilde{S}(\mathbf{k}, 0) \tilde{S}(\mathbf{k}', 0) \rangle = (2\pi)^{d-1} \frac{\pi}{2} \delta^{d-1}(\mathbf{q} + \mathbf{q}') \tilde{C}^{(\tau)}(k, k') \quad (5.23)$$

where the quantity $\tilde{C}^{(\tau)}(k, k')$ is given by

$$\tilde{C}^{(\tau)}(k, k') = \begin{cases} \sum_{r=1}^{\infty} \sin(rk) \sin(rk') & \tau = d \\ \sum_{r=1}^{\infty} \cos((r - \frac{1}{2})k) \cos((r - \frac{1}{2})k') & \tau = n \end{cases} \quad (5.24)$$

When we transform this expression back into direct space it just gives a decorrelated initial correlator, as is easily checked.

Before deriving the scaling functions of dynamical two-point functions we have to pause briefly in order to discuss possible implementations of the mean spherical constraint in the semi-infinite geometry. Our starting point is Eq. (5.7) which should hold true at all times. However, in the semi-infinite geometry translation invariance in the direction perpendicular to the surface is broken. One can therefore not assume *a priori* that the spins in different layers should be treated on an equal footing. In the past, investigations of the static properties of the semi-infinite spherical model either considered one global spherical field [10, 61] (i.e. all the variable S are subject to the same spherical constraint) or introduced besides the bulk spherical field an additional spherical field for the surface layer [219, 62] (i.e. an additional spherical constraint for the variables in the surface layer). Both cases belong to universality classes which differ from that of the $O(N)$ model with $N \rightarrow \infty$. In studies of *static* quantities it has been proposed that the spherical constraint could be realised in the semi-infinite geometry by imposing in the Hamiltonian a different spherical field for every layer [149], thus yielding the universality class of the semi-infinite $O(N)$ model with $N \rightarrow \infty$. For dynamical quantities, however, this prescription leads to the unwanted effect that the matrices which then appear in the exponential in Eq. (5.15) do not commute, thus making an analytical treatment of the dynamical properties of the semi-infinite model prohibitively difficult. We therefore made the choice to retain only one spherical field, similar to what is done in the bulk system (see equation (5.36) below for a precise mathematical formulation). This then yields the Equations (5.18) - (5.20) that are at the centre of our considerations. It has to be stressed that this implementation of the mean spherical constraint is an integral part of the model studied in this section.

5.1.3 The surface autocorrelation function

The two-time spin-spin correlation function is defined by

$$C^{(\tau)}(\mathbf{r}, \mathbf{r}'; t, s) = \langle S(\mathbf{r}, t) S(\mathbf{r}', s) \rangle \quad (5.25)$$

with $\mathbf{r}^T = (r, \mathbf{x}^T)$ and $\mathbf{r}'^T = (r', \mathbf{x}'^T)$. Here (τ) again characterises the chosen boundary condition. In the semi-infinite system correlation functions are expected to behave differently close to the surface and inside the bulk. Of special interest is the surface autocorrelation

$$C_1^{(\tau)}(t, s) = C^{(\tau)}((1, \mathbf{x}), (1, \mathbf{x}); t, s) \quad (5.26)$$

where we follow the convention to attach a subscript 1 to surface related quantities.

From Eq. (5.18) we directly obtain the following expression for the correlation function in reciprocal space

$$\begin{aligned} \overline{C}^{(\tau)}(\mathbf{k}, \mathbf{k}'; t, s) &= \frac{e^{-\omega(\mathbf{k}, \mathbf{q})t - \omega(\mathbf{k}', \mathbf{q}')s}}{\sqrt{g^{(\tau)}(t)g^{(\tau)}(s)}} (2\pi)^{d-1} \frac{\pi}{2} \delta^{d-1}(\mathbf{q} + \mathbf{q}') \left[\tilde{C}^{(\tau)}(k, k') \right. \\ &\quad \left. + 2T \delta(k - k') \int_0^t dt' e^{2\omega(\mathbf{k}, \mathbf{q})t'} g^{(\tau)}(t') \right] \end{aligned} \quad (5.27)$$

where we have set the external field to zero. Transforming back to real space we obtain

$$\begin{aligned} C^{(\tau)}((r, \mathbf{x}), (r', \mathbf{x}); t, s) &= \frac{1}{\sqrt{g^{(\tau)}(t)g^{(\tau)}(s)}} \left[f^{(\tau)}\left(r, r'; \frac{t+s}{2}\right) \right. \\ &\quad \left. + 2T \int_0^s du f^{(\tau)}\left(r, r'; \frac{t+s}{2} - u\right) g^{(\tau)}(u) \right] \end{aligned} \quad (5.28)$$

where a boundary dependent function $f^{(\tau)}$ has been defined, with

$$f^{(d)}(r, r'; t) = \frac{2}{\pi} \int \frac{d^{d-1} \mathbf{q}}{(2\pi)^{(d-1)}} e^{-2\tilde{\omega}(\mathbf{q})t} \quad (5.29)$$

$$\begin{aligned} &\int_0^\pi dk \sin(r \cdot k) \sin(r' \cdot k) e^{-2\tilde{\omega}(k)t} \\ &= (e^{-4t} I_0(4t))^{d-1} \cdot e^{-4t} (I_{r-r'}(4t) - I_{r+r'}(4t)) \end{aligned} \quad (5.30)$$

and

$$\begin{aligned} f^{(n)}(r, r'; t) &= \frac{2}{\pi} \int \frac{d^{d-1} \mathbf{q}}{(2\pi)^{(d-1)}} e^{-2\tilde{\omega}(\mathbf{q})t} \\ &\int_0^\pi dk \cos((r - 1/2) \cdot k) \cos((r' - 1/2) \cdot k) e^{-2\tilde{\omega}(k)t} \\ &= (e^{-4t} I_0(4t))^{d-1} \cdot e^{-4t} (I_{r-r'}(4t) + I_{r+r'-1}(4t)) \end{aligned} \quad (5.31)$$

with the modified Bessel functions $I_\nu(u)$. In the long time limit $t \rightarrow \infty$ we get

$$f^{(d)}(r, r'; t) \stackrel{t \rightarrow \infty}{\approx} 4\pi (8\pi t)^{-\frac{d+2}{2}} r \cdot r' \quad (5.32)$$

$$f^{(n)}(r, r'; t) \stackrel{t \rightarrow \infty}{\approx} 2(8\pi t)^{-\frac{d}{2}} \quad (5.33)$$

where the well-known asymptotic expansion

$$I_\nu(u) \stackrel{u \rightarrow \infty}{\approx} \frac{e^u}{\sqrt{2\pi u}} \left(1 - \frac{\nu^2 - 1/4}{2u} + O(1/u^2) \right) \quad (5.34)$$

of the Bessel function has been used. The function $g^{(\tau)}(t)$ is obtained as the solution of a nonlinear Volterra equation

$$g^{(\tau)}(t) = \lim_{L \rightarrow \infty} \frac{1}{L} \sum_{r=1}^L \left(f^{(\tau)}(r, r; t) + 2T \int_0^t du f^{(\tau)}(r, r; t-u) g^{(\tau)}(u) \right) \quad (5.35)$$

that follows directly from the implementation of the mean spherical constraint through the requirement

$$\lim_{L \rightarrow \infty} \frac{1}{L} \sum_{r=1}^L C^{(\tau)}((r, \mathbf{0}), (r, \mathbf{0}); t, t) = 1 \quad (5.36)$$

for all times t . This provides an implicit equation for the Lagrange multiplier introduced earlier. Inserting the expressions (5.32) and (5.33) for $f^{(\tau)}$ into Eq. (5.35) we observe that we end up with the known bulk equation [59]

$$g(t) = \hat{f}(t) + 2T \int_0^t du \hat{f}(t-u) g(u) \quad (5.37)$$

with

$$\hat{f}(t) := \int_{-\pi}^{\pi} \frac{d^{d-1} \mathbf{q}}{(2\pi)^{d-1}} \int_{-\pi}^{\pi} \frac{dk}{2\pi} e^{-2\omega(k, \mathbf{q})t} = (e^{-4t} I_0(4t))^d, \quad (5.38)$$

independently of whether we choose Dirichlet or Neumann boundary conditions. We can therefore drop in the following the superscript (τ) when dealing with the function g . The asymptotic behaviour of g has been discussed in detail in [93].

Everything is now in place for a discussion of the behaviour of the two-time correlations in the dynamical scaling regime $t, s, t-s \gg 1$. We shall in the following focus on the surface autocorrelation function. Other correlations (for example the correlation between surface and bulk spins) can be discussed along the same line. The surface autocorrelation function is readily obtained from Eq. (5.28) by setting $r = r' = 1$.

- $T < T_C$: From renormalisation group arguments we know that the asymptotic behaviour in that case corresponds to the $T = 0$ fixed point. Therefore the temperature can be set to zero and only the first term in (5.28) contributes in the scaling limit [93]. For both boundary conditions we obtain a dynamical scaling behaviour, as

$$C^{(d)}(t, s) = 2^{\frac{d}{2}} M_{eq}^2 s^{-1} \left(\frac{t}{s} \right)^{\frac{d}{4}} \left(\frac{t}{s} + 1 \right)^{-\left(\frac{d}{2}+1\right)}, \quad (5.39)$$

$$C^{(n)}(t, s) = 2^{\frac{d}{2}+1} M_{eq}^2 \left(\frac{t}{s} \right)^{\frac{d}{4}} \left(\frac{t}{s} + 1 \right)^{-\frac{d}{2}}. \quad (5.40)$$

where $M_{eq}^2 = 1 - T/T_C$ [25]. The non-equilibrium exponents can then be read off directly (recall $z = 2$):

$$b_1^{(d)} = 1, \quad b_1^{(n)} = 0, \quad \lambda_{C_1}^{(d)} = \frac{d}{2} + 2, \quad \lambda_{C_1}^{(n)} = \frac{d}{2}. \quad (5.41)$$

A few comments are now in order. When comparing the values (5.41) with those obtained for the bulk system [136, 93], see Table 3.3, we observe that for Neumann

boundary conditions the non-equilibrium exponents take on exactly the same values as in the bulk. This is not only observed for quenches to temperatures below the critical point but also for quenches to the critical point, see below, and also holds for the exponents related to the response function, as discussed in the next subsection. Interestingly, the agreement between the semi-infinite system with Neumann boundary conditions and the bulk system also extends to the scaling functions of two-time quantities which are identical, up to an unimportant numerical factor. ²

	bulk	Dirichlet ($\tau = d$)	Neumann ($\tau = n$)
$T < T_c, d > 2$			
$b_1^{(\tau)}$	0	1	0
$a_1^{(\tau)}$	$\frac{d}{2} - 1$	$\frac{d}{2}$	$\frac{d}{2} - 1$
$\lambda_{C_1}^{(\tau)} = \lambda_{R_1}^{(\tau)}$	$\frac{d}{2}$	$\frac{d}{2} + 2$	$\frac{d}{2}$
$X_\infty^{(\tau)}$	0	0	0
$T = T_c, 2 < d < 4$			
$b_1^{(\tau)}$	$\frac{d}{2} - 1$	$\frac{d}{2}$	$\frac{d}{2} - 1$
$a_1^{(\tau)}$	$\frac{d}{2} - 1$	$\frac{d}{2}$	$\frac{d}{2} - 1$
$\lambda_{C_1}^{(\tau)} = \lambda_{R_1}^{(\tau)}$	$\frac{3d}{2} - 2$	$\frac{3d}{2}$	$\frac{3d}{2} - 2$
$X_\infty^{(\tau)}$	$1 - \frac{2}{d}$	$1 - \frac{2}{d}$	$1 - \frac{2}{d}$
$T = T_c, d > 4$			
$b_1^{(\tau)}$	$\frac{d}{2} - 1$	$\frac{d}{2}$	$\frac{d}{2} - 1$
$a_1^{(\tau)}$	$\frac{d}{2} - 1$	$\frac{d}{2}$	$\frac{d}{2} - 1$
$\lambda_{C_1}^{(\tau)} = \lambda_{R_1}^{(\tau)}$	d	$d + 2$	d
$X_\infty^{(\tau)}$	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$

Table 5.1: Ageing exponents and fluctuation-dissipation ratio for the bulk system and for the semi-infinite systems with Dirichlet and Neumann boundary conditions.

The situation is different when considering free (i.e. Dirichlet) boundary conditions. The values of the non-equilibrium exponents are distinct from the values of their bulk counterparts and the scaling functions are different, too. The larger value of the surface autocorrelation exponent $\lambda_{C_1}^{(d)}$ thereby reflects the increased disorder at the surface due to the absence of neighbouring spins. Remarkably, the exponent $b_1^{(d)}$ is found to be different from zero, the value usually encountered when studying phase ordering in a bulk system. It is an open question whether this surprising observation is unique to the special situation of the spherical model or whether it is encountered in other systems as for example the semi-infinite Ising model quenched to temperatures below T_c .

The two types of dynamical scaling behaviour encountered in the semi-infinite spherical model quenched below the critical point are illustrated in Figure 5.1 in three

²This behaviour may be compared to that of the critical semi-infinite Ising model at the special transition point where the values of the non-equilibrium surface and bulk exponents and the surface and bulk scaling functions are found to disagree [195]. Similarly, the surface autocorrelation exponent λ_{C_1} for the $O(N)$ model in the limit $N \rightarrow \infty$ differs at the special transition point from the bulk autocorrelation exponent λ_C [167, 205].

dimensions. The analytical curves are given by the expressions (5.39) and (5.40) whereas the symbols, corresponding to different waiting times, are obtained from the direct numerical evaluation of Equation (5.28). It is obvious that we are well within the dynamical scaling regime even for the smallest waiting time considered. Furthermore this confirms *a posteriori* that it was justified to drop the second term in (5.28).

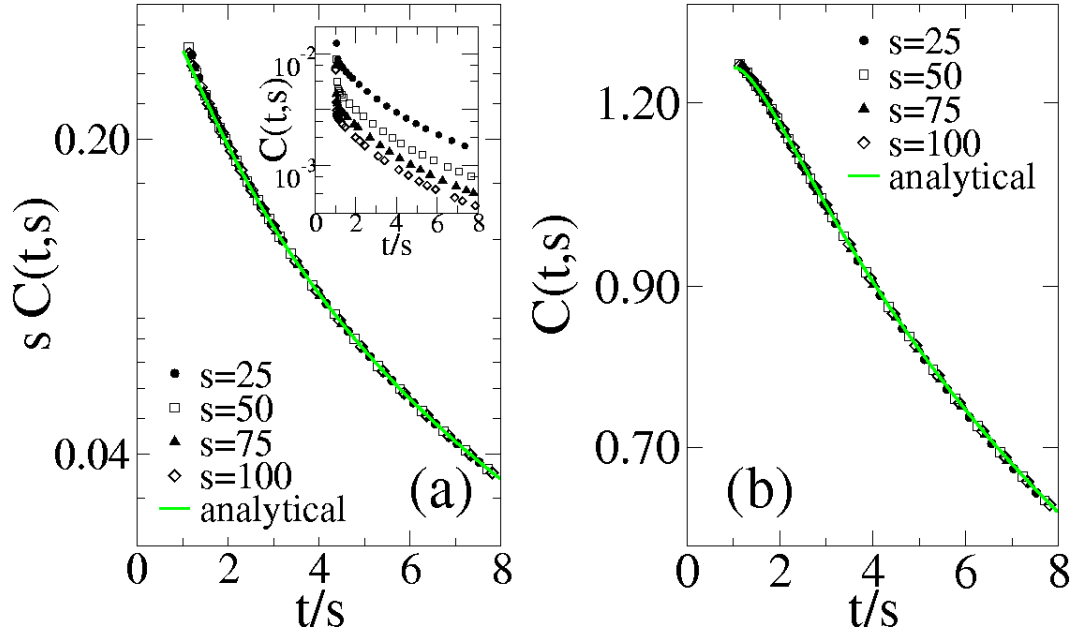


Figure 5.1: Scaling plots of the autocorrelation function for the case $T < T_C$ in three dimensions: (a) for Dirichlet boundary conditions with $b_1^{(d)} = 1$, (b) for Neumann boundary conditions with $b_1^{(n)} = 0$. The inset in (a) shows that no data collapse is observed for the unscaled data.

- $T = T_C$ and $2 < d < 4$: The behaviour of $C_1^{(\tau)}(t, s)$ in the regime $t, s, t - s \gg 1$ follows from the insertion of the asymptotic expressions for g and for $f^{(\tau)}$ into Eq. (5.28). One may wonder whether the use of the asymptotics for g in the integrand of Eq. (5.28) does not cause problems at the lower integration bound. As has been shown in [240] there exists for the spherical model a time scale $t_P \sim s^\zeta$ with $0 < \zeta < 1$ such that for times larger than t_P one is well within the ageing regime. Replacing g by its asymptotic value g_{age} for $u > t_P$, the integral of Eq. (5.28) can be written in the following way:

$$\begin{aligned}
 & \int_0^s du f^{(\tau)}(1, 1; (t+s)/2 - u) g(u) \\
 &= \int_0^{t_P} du g(u) f^{(\tau)}(1, 1; (t+s)/2 - u) + \int_{t_P}^s du g_{age}(u) f^{(\tau)}(1, 1; (t+s)/2 - u) \\
 &= W^{(\tau)}(t, s, t_P) + s \int_0^1 dv g_{age}(sv) f^{(\tau)}(1, 1; (t+s)/2 - sv) \tag{5.42}
 \end{aligned}$$

where in the last line we have assumed s to be large. An upper bound for the first

term $W^{(\tau)}(t, s, t_P) = \int_0^{t_P} du g(u) f^{(\tau)}(1, 1; (t+s)/2 - u)$ is given by

$$\begin{aligned} |W_P^{(\tau)}(t, s, t_P)| &\leq t_P \max_{\tau \in [0, t_P]} |g(\tau) f^{(\tau)}(1, 1; (t+s)/2 - \tau)| \\ &\stackrel{s \gg 1}{\approx} t_P \cdot \max_{\tau \in [0, t_P]} |g(\tau)| s^{-\frac{d}{2}} \left(4\pi \left(\frac{1}{2} \left(\frac{t}{s} + 1 \right) - \frac{t_P}{s} \right) \right)^{-\xi^{(\tau)}} \end{aligned} \quad (5.43)$$

where $\xi^{(d)} = \frac{d}{2} + 1$ and $\xi^{(n)} = \frac{d}{2}$. As $t_P \sim s^\zeta$, this upper bound disappears in the scaling limit faster than the second contribution in Eq. (5.42). We therefore drop $W^{(\tau)}(t, s, t_P)$ in the following and end up with the expression

$$\begin{aligned} C_1^{(\tau)}(t, s) &= \frac{1}{\sqrt{g_{age}(t)g_{age}(s)}} \left[f^{(\tau)} \left(1, 1; \frac{t+s}{2} \right) \right. \\ &\quad \left. + 2T \int_0^s du f^{(\tau)} \left(1, 1; \frac{t+s}{2} - u \right) g_{age}(u) du \right] \end{aligned} \quad (5.44)$$

in the asymptotic regime. It turns out that the thermal part of the expression (5.44) is the leading one at the critical points in any dimension, so that the first term can be disregarded. For $2 < d < 4$ we then obtain again dynamical scaling behaviour, as shown in Figure 5.2, as:

$$\begin{aligned} C^{(d)}(t, s) &= \frac{4T_C(4\pi)^{-\frac{d}{2}}}{d-2} s^{-\frac{d}{2}} \left(\frac{t}{s} \right)^{1-\frac{d}{4}} \left(\frac{t}{s} + 1 \right)^{-1} \left(\frac{t}{s} - 1 \right)^{-\frac{d}{2}} \\ &\quad \times \left[1 - \frac{4}{d} \left(\frac{t}{s} + 1 \right)^{-1} \right], \end{aligned} \quad (5.45)$$

$$C^{(n)}(t, s) = \frac{8(4\pi)^{-\frac{d}{2}} \cdot T_C}{(d-2)} s^{-(\frac{d}{2}-1)} \left(\frac{t}{s} \right)^{1-\frac{d}{4}} \left(\frac{t}{s} - 1 \right)^{1-\frac{d}{2}} \left(\frac{t}{s} + 1 \right)^{-1} \quad (5.46)$$

yielding the non-equilibrium critical exponents

$$b_1^{(d)} = \frac{d}{2}, \quad b_1^{(n)} = \frac{d}{2} - 1, \quad \lambda_{C_1}^{(d)} = \frac{3}{2}d, \quad \lambda_{C_1}^{(n)} = \frac{3}{2}d - 2. \quad (5.47)$$

The values $b_1^{(\tau)}$ agree with the expression

$$b_1^{(\tau)} = b + \frac{2(\beta_1^{(\tau)} - \beta)}{\nu z} \quad (5.48)$$

expected from general scaling considerations [45]. Eq. (5.48) is readily verified in three dimensions where $b = \frac{2\beta}{\nu z} = \frac{1}{2}$, whereas β and $\beta_1^{(\tau)}$, which are the usual static equilibrium critical exponents describing the vanishing of the bulk and surface magnetisations on approach to the critical point, take on the values $\beta = \frac{1}{2}$ and $\beta_1^{(d)} = \frac{3}{2}$, $\beta_1^{(n)} = \frac{1}{2}$. Finally, the static exponent $\nu = 1$ in three dimensions.

As a final remark, let us note that the tendency of the surface correlations to decay faster in time than the bulk correlations is mirrored at the ordinary transition by the larger value of the non-equilibrium autocorrelation exponent $\lambda_{C_1}^{(d)}$.

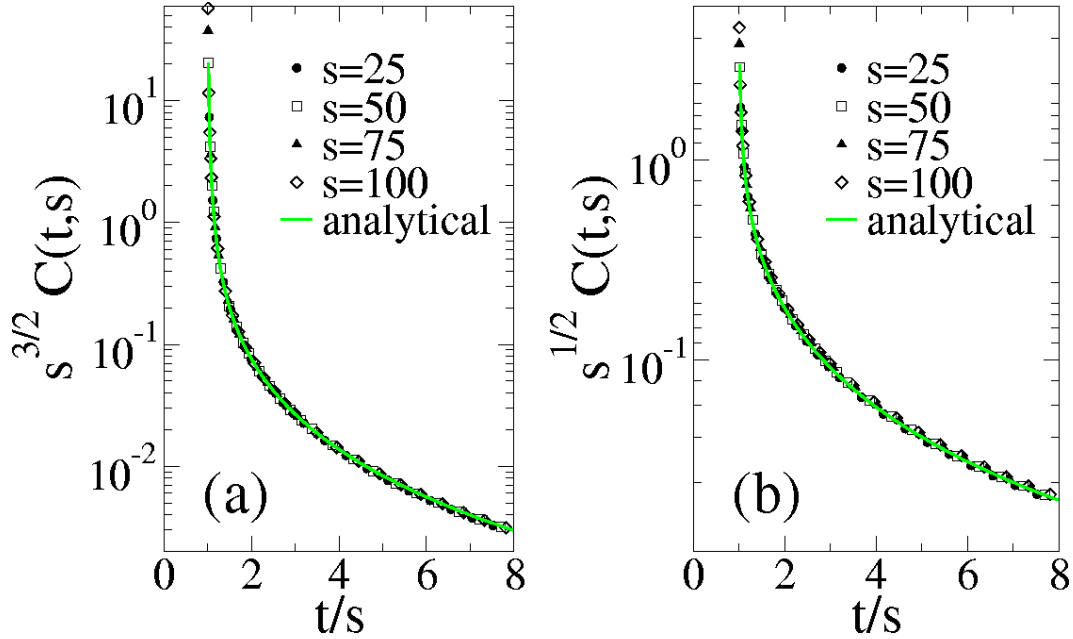


Figure 5.2: Scaling plots of the autocorrelation function for the case $T = T_C$ in three dimensions: (a) for Dirichlet boundary conditions, (b) for Neumann boundary conditions.

- $T = T_C$ and $d > 4$: In this case we obtain

$$C^{(d)}(t, s) = \frac{2(4\pi)^{-\frac{d}{2}}}{d} \cdot T_C \cdot s^{-\frac{d}{2}} \left(\left(\frac{t}{s} - 1 \right)^{-\frac{d}{2}} - \left(\frac{t}{s} + 1 \right)^{-\frac{d}{2}} \right) \quad (5.49)$$

$$C^{(n)}(t, s) = \frac{4(4\pi)^{-\frac{d}{2}}}{d-2} \cdot T_C \cdot s^{-(\frac{d}{2}-1)} \left(\left(\frac{t}{s} - 1 \right)^{1-\frac{d}{2}} - \left(\frac{t}{s} + 1 \right)^{1-\frac{d}{2}} \right). \quad (5.50)$$

Again dynamical scaling is found where the non-equilibrium critical exponents now take on the values

$$b_1^{(d)} = \frac{d}{2}, \quad b_1^{(n)} = \frac{d}{2} - 1, \quad \lambda_{C_1}^{(d)} = d + 2, \quad \lambda_{C_1}^{(n)} = d. \quad (5.51)$$

Also here (5.48) is verified with the values $b = \frac{d}{2} - 1$, $\beta_1^{(d)} = 1$, $\beta_1^{(n)} = \frac{1}{2}$, $\nu = \frac{1}{2}$ and $\beta = \frac{1}{2}$.

- $T > T_C$: We then have

$$C_1^{(\tau)}(t, s) = e^{-(t+s)/(2\tau_{eq})} \left[f^{(\tau)} \left(1, 1; \frac{t+s}{2} \right) + 2T \int_0^s du f^{(\tau)} \left(1, 1; \frac{t+s}{2} - u \right) g_{age}(u) \right]. \quad (5.52)$$

This amounts to an exponential decrease and the leading expression rapidly develops a dependence only on $t - s$ for $s \rightarrow \infty$ and $t - s$ fixed [93].

Inspection of Table 5.1 reveals the oddity that the values of a_1 and b_1 for Dirichlet and Neumann boundary conditions always exactly differ by one. This may again be compared to the critical semi-infinite Ising model (we are not aware of any study of ageing phenomena in the semi-infinite Ising model below T_c). We there have $a_1 = b_1 = 2\beta_1/(\nu z)$ [195, 45] with the values $\beta_1 = 0.80$ at the ordinary transition and $\beta_1 \approx 0.23$ at the special transition point [196], yielding different values for a_1 and b_1 in that case, too. However, the exact value one for the difference seems to be a property of the spherical model.

5.1.4 The response function

The response function is defined as usual:

$$R(\mathbf{r}, \mathbf{r}'; t, s) := \left. \frac{\delta \langle S(\mathbf{r}, t) \rangle}{\delta h(\mathbf{r}', s)} \right|_{h=0} ; \quad t > s \quad (5.53)$$

where $h(\mathbf{r}', s)$ is a magnetic field acting at time s on the spin located at lattice site \mathbf{r}' . Starting from expression (5.18) and assuming spatial translation invariance parallel to the surface, we find

$$R((k, \mathbf{q}), (k', \mathbf{q}); t, s) = \sqrt{\frac{g(s)}{g(t)}} e^{-\omega(k, \mathbf{q})(t-s)} \delta(k - k'). \quad (5.54)$$

The chosen boundary condition enters when transforming back to real space, yielding

$$\begin{aligned} R^{(d)}((r, \mathbf{x}), (r', \mathbf{y}); t, s) &= \sqrt{\frac{g(s)}{g(t)}} e^{-2(t-s)d} \prod_{i=1}^{d-1} I_{x_i - y_i}(2(t-s)) \\ &\times (I_{r' - r}(2(t-s)) - I_{r' + r}(2(t-s))) \end{aligned} \quad (5.55)$$

$$\begin{aligned} R^{(n)}((r, \mathbf{x}), (r', \mathbf{y}); t, s) &= \sqrt{\frac{g(s)}{g(t)}} e^{-2(t-s)d} \prod_{i=1}^{d-1} I_{x_i - y_i}(2(t-s)) \\ &\times (I_{r' - r}(2(t-s)) + I_{r' + r - 1}(2(t-s))). \end{aligned} \quad (5.56)$$

We refrain from giving a full discussion of the response function, but focus instead on the surface autoresponse function $R_1^{(\tau)}(t, s) = R^{(\tau)}((1, \mathbf{x}), (1, \mathbf{x}); t, s)$ that describes the answer of the surface at a certain position to a perturbation at the same site at an earlier time. With the large t behaviour (5.34) of the Bessel function we then find

$$R_1^{(d)}(t, s) = 4\pi \sqrt{\frac{g(s)}{g(t)}} (4\pi(t-s))^{-(\frac{d}{2}+1)} \quad (5.57)$$

$$R_1^{(n)}(t, s) = 2\sqrt{\frac{g(s)}{g(t)}} (4\pi(t-s))^{-\frac{d}{2}}. \quad (5.58)$$

It is evident from these expressions that the ageing behaviour of the surface autoresponse is again determined by the asymptotics g_{age} of the function g given in [93]. As for the autocorrelation function we have to distinguish four different cases:

- $T < T_C$: Here we have

$$R_1^{(d)}(t, s) = (4\pi)^{-\frac{d}{2}} \left(\frac{t}{s}\right)^{\frac{d}{4}} s^{-(\frac{d}{2}+1)} \left(\frac{t}{s} - 1\right)^{-(\frac{d}{2}+1)} \quad (5.59)$$

$$R_1^{(n)}(t, s) = 2(4\pi)^{-(\frac{d}{2})} \left(\frac{t}{s}\right)^{\frac{d}{4}} s^{-\frac{d}{2}} \left(\frac{t}{s} - 1\right)^{-\frac{d}{2}}. \quad (5.60)$$

For both choices of boundary conditions we observe dynamical scaling (see Figure 5.3) with the exponents

$$a_1^{(d)} = \frac{d}{2}, \quad a_1^{(n)} = \frac{d}{2} - 1, \quad \lambda_{R_1}^{(d)} = \frac{d}{2} + 2, \quad \lambda_{R_1}^{(n)} = \frac{d}{2}. \quad (5.61)$$

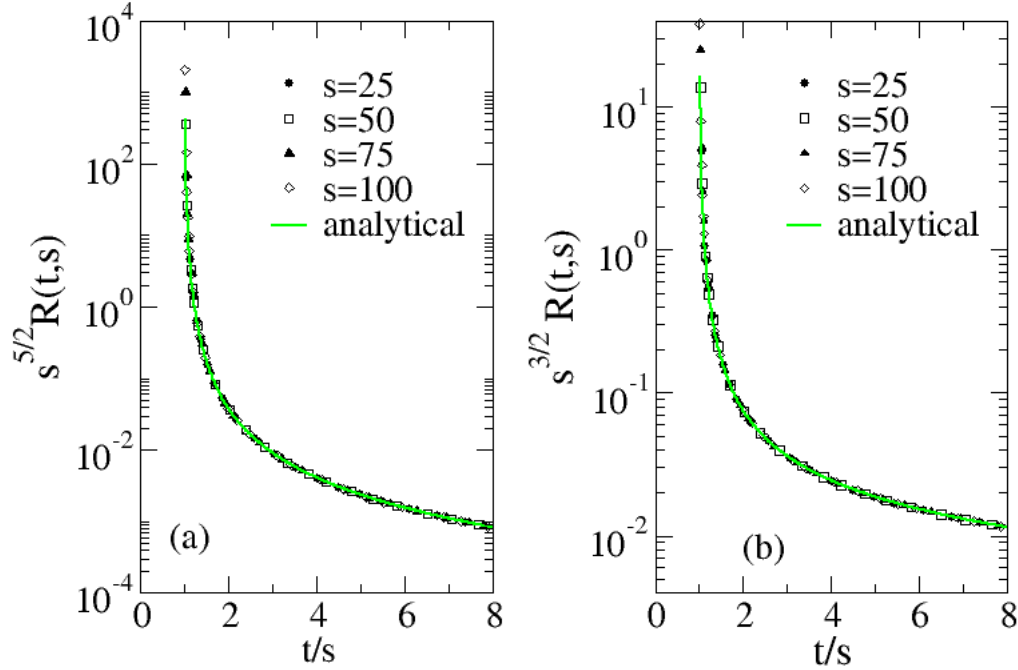


Figure 5.3: Scaling plots of the autoresponse function for the case $T < T_C$ in three dimensions: (a) for Dirichlet boundary conditions with $a_1^{(d)} = \frac{3}{2}$, (b) for Neumann boundary conditions with $a_1^{(n)} = \frac{1}{2}$.

- $T = T_C$ and $2 < d < 4$: We find again dynamical scaling, as

$$R_1^{(d)}(t, s) = (4\pi)^{-\frac{d}{2}} \left(\frac{t}{s}\right)^{-\frac{d}{4}+1} s^{-(\frac{d}{2}+1)} \left(\frac{t}{s} - 1\right)^{-(\frac{d}{2}+1)} \quad (5.62)$$

$$R_1^{(n)}(t, s) = 2(4\pi)^{-\frac{d}{2}} \left(\frac{t}{s}\right)^{-\frac{d}{4}+1} s^{-\frac{d}{2}} \left(\frac{t}{s} - 1\right)^{-\frac{d}{2}} \quad (5.63)$$

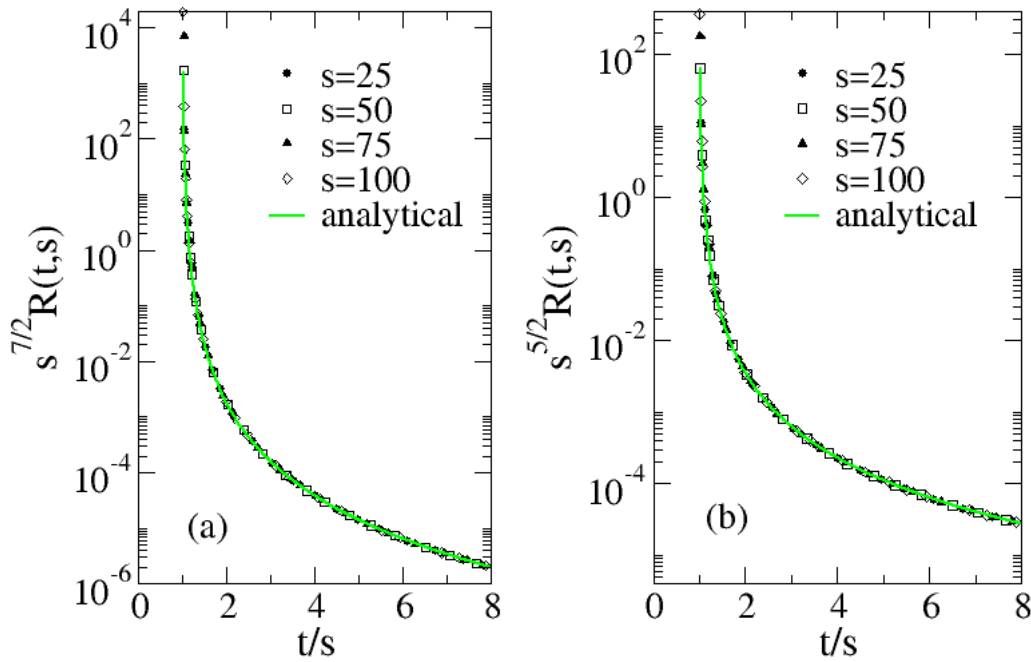


Figure 5.4: Scaling plots of the autoresponse function for the case $T = T_C$ in five dimensions: (a) for Dirichlet boundary conditions, (b) for Neumann boundary conditions.

with the following nonequilibrium critical exponents:

$$a_1^{(d)} = \frac{d}{2}, \quad a_1^{(n)} = \frac{d}{2} - 1, \quad \lambda_{R_1}^{(d)} = \frac{3}{2}d, \quad \lambda_{R_1}^{(n)} = \frac{3}{2}d - 2. \quad (5.64)$$

- $T = T_C$ and $d > 4$: This case yields the expressions

$$R_1^{(d)}(t, s) = (4\pi)^{-\frac{d}{2}} s^{-\left(\frac{d}{2}+1\right)} \left(\frac{t}{s} - 1\right)^{-\left(\frac{d}{2}+1\right)} \quad (5.65)$$

$$R_1^{(n)}(t, s) = 2(4\pi)^{-\frac{d}{2}} s^{-\frac{d}{2}} \left(\frac{t}{s} - 1\right)^{-\frac{d}{2}}. \quad (5.66)$$

Again dynamical scaling is found, the exponents now taking on the values

$$a_1^{(d)} = \frac{d}{2}, \quad a_1^{(n)} = \frac{d}{2} - 1, \quad \lambda_{R_1}^{(d)} = d + 2, \quad \lambda_{R_1}^{(n)} = d. \quad (5.67)$$

This dynamical scaling behaviour is illustrated in Figure 5.4 in five dimensions.

- $T > T_C$: Due to the exponential behaviour of $g_{age}(t)$, $R(t, s)$ disappears exponentially:

$$R_1^{(d)}(t, s) = 4\pi e^{-(t-s)/\tau_{eq}} (4\pi(t-s))^{-\left(\frac{d}{2}+1\right)} \quad (5.68)$$

$$R_1^{(n)}(t, s) = 2e^{-(t-s)/\tau_{eq}} (4\pi(t-s))^{-\frac{d}{2}} \quad (5.69)$$

and only a dependence on the time difference $t - s$ is observed.

Comparing the values of non-equilibrium exponents derived from the autoresponse with those obtained from the autocorrelation reveals that we have at criticality the identities $a_1^{(\tau)} = b_1^{(\tau)}$ and $\lambda_{R_1}^{(\tau)} = \lambda_{C_1}^{(\tau)}$ in agreement with the general scaling arguments given in the introduction.

We remark that there is an adaption of LSI to semi-infinite systems for the surface autoresponse function, which was given in [195]. The following prediction for the surface autoresponse function (with $t > s$):

$$R_1^{LSI}(t, s) = r_0 \left(\frac{t}{s}\right)^{\zeta_2 - \zeta_1} (t - s)^{\zeta_1 + \zeta_2} \quad (5.70)$$

where ζ_1 and ζ_2 are two exponents left undetermined by the theory, and r_0 is a non-universal normalisation constant. The values of ζ_1 and ζ_2 are fixed by comparing (5.70) with the expected scaling behaviour (see Equations (5.3) and (5.4)) yielding the result

$$R_1^{LSI}(t, s) = r_0 s^{-1 - a_1^{(\tau)}} \left(\frac{t}{s}\right)^{-1 - a_1^{(\tau)}} \left(\frac{t}{s} - 1\right)^{1 + a_1^{(\tau)} - \lambda_{R_1}^{(\tau)}/z}. \quad (5.71)$$

This prediction is in complete agreement with our exact results for $T \leq T_c$ both for Dirichlet and Neumann boundary conditions.

Finally, let us mention that it was shown in [106] that the dependence of the full response function (5.56) on r and r' can be deduced from the space-time symmetries in the case of Dirichlet boundary conditions.

5.1.5 The fluctuation-dissipation ratio

The fluctuation-dissipation ratio

$$X(t, s) := \frac{T R(t, s)}{\partial_s C(t, s)} \quad (5.72)$$

has been discussed extensively in recent years [56] as a possible way for attributing an effective temperature to an out-of-equilibrium system. Of importance in the following is the fact that a characteristic behaviour is expected for different physical situations. Thus in systems undergoing phase ordering one usually expects $X(t, s)$ to approach 0, whereas a different behaviour is observed for non-equilibrium critical systems. Indeed it has been realized [93, 45] that in the latter case the non-vanishing limit value

$$X^\infty := \lim_{s \rightarrow \infty} \lim_{t \rightarrow \infty} X(t, s) \quad (5.73)$$

is a universal quantity whose value characterises the given dynamical universality class. The concept of fluctuation-dissipation ratio, initially introduced for bulk systems, has been generalised in [195] to systems with surfaces. The surface fluctuation-dissipation ratio is thereby defined by

$$X_1(t, s) := \frac{T R_1(t, s)}{\partial_s C_1(t, s)}. \quad (5.74)$$

The asymptotic value $X_1^\infty := \lim_{s \rightarrow \infty} \lim_{t \rightarrow \infty} X_1(t, s)$ is in fact a ratio of two amplitudes and its value at the bulk critical point should be characteristic for a given surface universality class [45]. Recently, $X_1(t, s)$ has been determined numerically for the critical

two- and three-dimensional semi-infinite Ising models [195], with asymptotic values X_1^∞ differing from the values X^∞ obtained in the corresponding bulk systems. X_1^∞ has also been computed within the Gaussian model [45] yielding the value $\frac{1}{2}$.

Having already determined the surface autocorrelation and autoresponse functions in the previous subsection, we are in the position to compute $X_1(t, s)$ also for the semi-infinite spherical model. In doing so one immediately realizes that for Neumann boundary conditions $X_1^{(n)}(t, s)$ is identical to the bulk quantity $X(t, s)$ obtained in [93]. This follows from the fact that C_1 and R_1 for Neumann and periodic boundary conditions only differ by a numerical constant which drops out when the ratio is formed. For this reason we give here only the results obtained for Dirichlet boundary conditions:

- $T < T_C$:

$$X_1^{(d)}(t, s) = \frac{4(8\pi)^{-\frac{d}{2}}}{M_{eq}^2} s^{-\frac{d}{2}+1} \left(\frac{\frac{t}{s} + 1}{\frac{t}{s} - 1} \right)^{\frac{d}{2}+1} \frac{\frac{t}{s} + 1}{(4 + d)\frac{t}{s} - d} \quad (5.75)$$

yielding the limit value $X_1^\infty = 0$ as expected for ferromagnetic systems quenched below their critical point.

- $T = T_C$ and $2 < d < 4$: In this case a straightforward but somewhat tedious calculation yields

$$X_1^{(d)}(t, s) = \frac{d(d-2)\left(\frac{t}{s} + 1\right)^3}{(d^2 - 16) + (32 + d(3d - 8))\frac{t}{s} + (d-4)(4 + 3d)\left(\frac{t}{s}\right)^2 + d^2\left(\frac{t}{s}\right)^3} \quad (5.76)$$

with the limit value $X_1^\infty = \frac{d-2}{d}$.

- $T = T_C$ and $d > 4$: Here we obtain the same expressions as for Neumann and periodic boundary conditions:

$$X_1^{(d)}(t, s) = \frac{1}{1 + \left(\frac{\frac{t}{s} - 1}{\frac{t}{s} + 1} \right)^{\frac{d}{2}+1}} \quad (5.77)$$

with $X_1^\infty = \frac{1}{2}$.

In all cases the limit value turns out to be independent of the boundary condition, which is the reason why we have dropped the superscript (d). We therefore conclude that in the semi-infinite spherical model X_1^∞ equals X^∞ independently of the chosen boundary condition.

5.1.6 Conclusions of this section

In this section we have extended the study of out-of-equilibrium dynamical properties of the kinetic spherical model to the semi-infinite geometry with both Dirichlet and Neumann boundary conditions. The exact computation of two-time surface quantities (like the autocorrelation and the autoresponse functions) reveal that dynamical scaling is also observed close to a surface for quenches to temperatures below or equal to the critical temperature. Whereas for Neumann boundary conditions we find that the values of the non-equilibrium exponents and the scaling functions (up to a numerical factor) are identical to the bulk ones, the situation for Dirichlet boundary conditions is more interesting.

Indeed at the critical point we find that out-of-equilibrium dynamics is governed by universal exponents whose values differ from those of the corresponding bulk exponents. The values of these surface exponents are in complete agreement with predictions coming from general scaling considerations [195, 45]. Similarly, surface scaling functions are also found to differ from the bulk scaling functions. Interestingly, we find that in the ordered low-temperature phase the autocorrelation function scales in the ageing regime as

$$C_1(t, s) = s^{-1} f_{C_1}(t/s), \quad (5.78)$$

in strong contrast to the well-known bulk behaviour [37]

$$C(t, s) = f_C(t/s). \quad (5.79)$$

As this section is the first study of ageing phenomena close to a surface in an ordered phase, it is an interesting question whether this is only a special feature of the kinetic spherical model or whether this is a general property of semi-infinite systems undergoing phase ordering. We come back to this problem in section 5.2

5.2 Local ageing phenomena close to magnetic surfaces

5.2.1 Introduction

The previous section has left some question open. In particular the fact that $b_1 \neq 0$ in the case of phase ordering kinetics with Dirichlet boundary conditions requires further investigations. In this section we will provide on the one hand some additional results for the case of critical dynamics at surfaces. On the other hand we will consider the 2D Ising model for a quench below T_c . These simulations will help to clarify the question whether $b_1 \neq 0$ is really physical.

In order to discuss the expected ageing phenomenology close to a critical surface in more detail, let us establish some notations. We consider an idealised semi-infinite lattice in d dimensions where we write the position vector \mathbf{r} as $\mathbf{r} = (\mathbf{x}, y)$. Here \mathbf{x} is a $(d - 1)$ -dimensional vector parallel to the surface, whereas y labels the layers perpendicular to the surface (with $y = 1$ being the surface layer). With this we obtain the following generalisations for the correlation and response functions:

$$\begin{aligned} C(t, s; y, y', \mathbf{x} - \mathbf{x}') &= \langle \phi(\mathbf{x}, y; t) \phi(\mathbf{x}', y'; s) \rangle, \\ R(t, s; y, y', \mathbf{x} - \mathbf{x}') &= \left. \frac{\delta \langle \phi(\mathbf{x}, y; t) \rangle}{\delta h(\mathbf{x}', y'; s)} \right|_{h=0} \end{aligned}$$

where we assumed spatial translation invariance in the directions parallel to the surface. For $y, y' \rightarrow \infty$ we recover the bulk quantities, whereas $y = y' = 1$ yields the surface correlation and response functions. Of special interest are the surface autocorrelation and autoresponse functions with $\mathbf{x} = \mathbf{x}'$ that we write as $C_1(t, s) := C(t, s; 1, 1, \mathbf{0})$ and $R_1(t, s) := R(t, s; 1, 1, \mathbf{0})$. For these quantities, the simple scaling forms (5.2), (5.3) and (5.4) are expected [195, 45] and the surface exponents can be related to other known

exponents through (5.5) and (5.6).

We recall that like for bulk systems [56], surface autocorrelation and autoresponse functions can be combined to yield the surface fluctuation-dissipation ratio [195]

$$X_1(t, s) = \frac{T_c R_1(t, s)}{\partial_s C_1(t, s)}, \quad (5.80)$$

with a universal limit value

$$X_1^\infty = \lim_{s \rightarrow \infty} \left(\lim_{t \rightarrow \infty} X_1(t, s) \right) \quad (5.81)$$

that characterises the different dynamical surface universality classes [45]. The scaling picture (5.80) and the relations between the various nonequilibrium exponents have been verified by one of us through a numerical study of the out-of-equilibrium dynamics of various critical semi-infinite Ising models [195]. In addition, the critical semi-infinite Gaussian model [45] and the critical semi-infinite spherical model [16] (see also section 5.1) were also found to display this simple ageing scenario.

Whereas at least some knowledge has accumulated in recent years on the local ageing behaviour close to critical surfaces, almost nothing is known on surface ageing processes taking place in coarsening systems. In the last section we have looked at the out-of-equilibrium dynamical behaviour of the semi-infinite spherical model. For this special model we have verified the existence of dynamical scaling and simple ageing close to surfaces for quenches inside the ordered phase. Surprisingly, the nonequilibrium exponent b_1 , describing the scaling behaviour of the surface autocorrelation, was found to take on the value $b_1 = 1$, different from the standard value $b = 0$ of the corresponding exponent in bulk systems undergoing phase-ordering. This result calls for a thorough investigation of surface ageing phenomena in other semi-infinite systems with phase-ordering dynamics. In this section we continue our study of local ageing processes in bounded ferromagnets. On the one hand, we discuss various semi-infinite models (the short-range Ising model in the limit of high dimensions, the $O(N)$ model in the large N limit, and the Bray-Humayun approach to phase-ordering kinetics) which can be solved exactly. On the other hand, we present results of extensive Monte Carlo simulations of the standard two-dimensional semi-infinite Ising model prepared at high temperatures and then quenched inside the ordered phase. These numerical results yield new and interesting insights into the local processes taking place in coarsening systems close to surfaces. All the systems studied have in common that the dynamical exponent takes on the value $z = 2$.

This section is organised as follows. In subsection 5.2.2 we compute scaling functions and nonequilibrium exponents in the various exactly solvable semi-infinite models. Our numerical results obtained from simulations of the two-dimensional semi-infinite Ising model undergoing phase-ordering are then presented in subsection 5.2.3. Finally, in subsection 5.2.4 we draw our conclusions and summarise our results.

5.2.2 Quenching semi-infinite systems from high temperatures: exact results

We discuss in the following the nonequilibrium dynamical behaviour of various exactly solvable semi-infinite models prepared in an uncorrelated initial state and then quenched below or at the critical point. In Ref.[16] we studied the out-of-equilibrium dynamical

behaviour of the semi-infinite spherical model quenched to low temperatures. Some results obtained in that study can be found in the Tables 5.2 and 5.3 (see the concluding subsection) where they are compared with the results obtained in this work. The spherical model is a rather unrealistic model, due to the artificial spherical constraint which shapes to a large extent the properties of the model. It is therefore unclear whether the results we found in Ref.[16] are generic to semi-infinite systems or whether they are specific to the semi-infinite spherical model.

The Ising model in high dimensions

The out-of-equilibrium behaviour of the bulk Ising model with nearest neighbour ferromagnetic interactions has recently been studied in the limit of a large number d of space dimensions [89]. In this limit the model is mean-field like. Here we generalise the calculations of Garriga et al. to the semi-infinite case.

Using a semi-infinite hypercube with lattice constant 1, the Hamiltonian of our model can be written in the very general form

$$\mathcal{H} = -\frac{J_s}{2d} \sum_{(\mathbf{x}, \mathbf{x}')} \sigma_{\mathbf{x},1} \sigma_{\mathbf{x}',1} - \frac{J_b}{2d} \sum_{y \geq 2} \sum_{(\mathbf{x}, \mathbf{x}')} \sigma_{\mathbf{x},y} \sigma_{\mathbf{x}',y} - \frac{J_b}{2d} \sum_{y \geq 1} \sum_{\mathbf{x}} \sigma_{\mathbf{x},y} \sigma_{\mathbf{x},y+1} \quad (5.82)$$

where the sum over $(\mathbf{x}, \mathbf{x}')$ indicates a sum over all nearest neighbour pairs lying in the same layer. The spins can take on the values ± 1 , and an additional field term can be added if needed. In writing (5.82) we take into account the layered structure of the lattice and distinguish between nearest neighbour pairs lying in a layer parallel to the surface and nearest neighbour pairs belonging to different layers. As usual when dealing with semi-infinite systems [195], we have introduced a different coupling constant J_s for interactions between nearest neighbour spins located both in the surface layer. We will however restrict ourselves in the following to the special case $J_s = J_b = 1$. On the one hand this yields in the limit $d \rightarrow \infty$ the critical temperature $T_c = 1$ (where we set $k_B = 1$), on the other hand we then encounter at the critical temperature the so-called ordinary transition [195] where the bulk alone is critical.

The main difference between the present case and the model considered in Ref.[89] is of course the absence of spatial translation invariance in the direction perpendicular to the surface. Due to this, the time-dependent local fields that the spins experience are now layer-dependent, leading to the expressions

$$\begin{aligned} h_{\mathbf{x},y}(t) &= h_{\mathbf{x},y}^{ext}(t) + \frac{1}{2d} \left(\sigma_{\mathbf{x},y+1}(t) + \sum_{\mathbf{x}'(\mathbf{x})} \sigma_{\mathbf{x}',y}(t) \right) \quad \text{for } y = 1, \\ h_{\mathbf{x},y}(t) &= h_{\mathbf{x},y}^{ext}(t) + \frac{1}{2d} \left(\sigma_{\mathbf{x},y+1}(t) + \sigma_{\mathbf{x},y-1}(t) + \sum_{\mathbf{x}'(\mathbf{x})} \sigma_{\mathbf{x}',y}(t) \right) \quad \text{for } y \neq 1, \end{aligned} \quad (5.83)$$

where the sum over $\mathbf{x}'(\mathbf{x})$ is the sum over the in-plane nearest neighbour lattice sites \mathbf{x}' of \mathbf{x} . Note that we also added an external field $h_{\mathbf{x},y}^{ext}(t)$ needed for the computation of the response function. Using heat-bath dynamics, these local fields $h_{\mathbf{x},y}(t)$ appear in the flip rates, as each spin will flip independently with the rate $(1 - \sigma_{\mathbf{x},y}(t) \tanh(h_{\mathbf{x},y}(t)/T))/2$.

The correlation function:

In their paper [89] Garriga et al. derived very general equations of motion for the one- and the two-time correlation functions \mathcal{C} and C that can also be used in our case. Recalling that we still have invariance for spatial translations parallel to the surface, we can write the following equations [89]:

$$\begin{aligned} \partial_t \mathcal{C}(t; y, y', \mathbf{x} - \mathbf{x}') &= -2\mathcal{C}(t; y, y', \mathbf{x} - \mathbf{x}') + \langle \Delta t_{\mathbf{x},y}(t) \Delta \sigma_{\mathbf{x}',y'}(t) \rangle \\ &+ \langle \Delta \sigma_{\mathbf{x},y}(t) \Delta t_{\mathbf{x}',y'}(t) \rangle \end{aligned} \quad (5.84)$$

$$\partial_t C(t, s; y, y', \mathbf{x} - \mathbf{x}') = -C(t, s; y, y', \mathbf{x} - \mathbf{x}') + \langle \Delta t_{\mathbf{x},y}(t) \Delta \sigma_{\mathbf{x}',y'}(s) \rangle \quad (5.85)$$

where we use the notations $\Delta t_{\mathbf{x},y}(t) := \tanh(h_{\mathbf{x},y}(t)/T) - \langle \tanh(h_{\mathbf{x},y}(t)/T) \rangle$ and $\Delta \sigma_{\mathbf{x},y}(t) = \sigma_{\mathbf{x},y}(t) - \langle \sigma_{\mathbf{x},y}(t) \rangle$ for the deviations from the averages.

In the limit of large d we can develop $\tanh(h_{\mathbf{x},y}(t)/T)$ in $1/d$ which then yields the following expressions for the equations of motion:

$$\begin{aligned} \partial_t \mathcal{C}(t; y, y', \mathbf{x}) &= -2\mathcal{C}(t; y, y', \mathbf{x}) + \frac{\gamma}{2} \left(\mathcal{C}(t; y+1, y', \mathbf{x}) + \mathcal{C}(t; y-1, y', \mathbf{x}) \right. \\ &\left. + \mathcal{C}(t; y, y'+1, \mathbf{x}) + \mathcal{C}(t; y, y'-1, \mathbf{x}) + 2 \sum_{\mathbf{z}(\mathbf{x})} \mathcal{C}(t; y, y', \mathbf{z}) \right) + b(t; y, y', \mathbf{x}) \end{aligned} \quad (5.86)$$

$$\begin{aligned} \partial_t C(t, s; y, y', \mathbf{x}) &= -C(t, s; y, y', \mathbf{x}) + \frac{\gamma}{2} \left(C(t, s; y+1, y', \mathbf{x}) \right. \\ &\left. + C(t, s; y-1, y', \mathbf{x}) + \sum_{\mathbf{z}(\mathbf{x})} C(t, s; y, y', \mathbf{z}) \right). \end{aligned} \quad (5.87)$$

where we exploit the spatial translation invariance parallel to the surface by setting $\mathbf{x}' = \mathbf{0}$. The parameter γ is given by $\gamma := 1/(Td)$, whereas the sum over $\mathbf{z}(\mathbf{x})$ indicates a summation over the in-plane nearest neighbour lattice sites of \mathbf{x} . The quantity $b(t; y, y', \mathbf{x}) = \delta_{y,y'} \delta_{\mathbf{x},\mathbf{0}} \bar{b}(t; y)$, which is needed to enforce the condition $\mathcal{C}(t; y, y, \mathbf{0}) = 1$ for all times t , has to be determined self-consistently. In addition, the solution has to verify the boundary conditions

$$C(t, s; 0, y', \mathbf{x}) = 0 = C(t, s; y, 0, \mathbf{x}), \quad (5.88)$$

and the two-time correlator must yield the one-time correlator for $t = s$, i.e.

$$C(t, t; y, y', \mathbf{x}) = \mathcal{C}(t; y, y', \mathbf{x}). \quad (5.89)$$

The solution of these equations of motion is outlined in the appendix of [22]. For decorrelated initial conditions, our result is:

$$\begin{aligned} C(t, s; y, y', \mathbf{x}) &= e^{-(t+s)} \left(I_{y-y'}(\gamma(t+s)) - I_{y+y'}(\gamma(t+s)) \right) \prod_{i=1}^{d-1} I_{x_i}(\gamma(t+s)) \\ &+ \sum_{u \geq 1} \int_0^s d\tau \bar{b}(\tau, u) e^{-(t+s-2\tau)} \prod_{i=1}^{d-1} I_{x_i}(\gamma(t+s-2\tau)) \\ &\times \left(I_{u-y}(\gamma(t-\tau)) - I_{u+y}(\gamma(t-\tau)) \right) \left(I_{u-y'}(\gamma(s-\tau)) - I_{u+y'}(\gamma(s-\tau)) \right) \end{aligned}$$

where the functions I_ν are modified Bessel functions [97] and where we have taken into account the special form of $b(t; y, y', \mathbf{x})$ and the fact that [22]

$$\sum_{u \geq 0} (I_{u-y}(\gamma t) - I_{u+y}(\gamma t)) (I_{u-y'}(\gamma s) - I_{u+y'}(\gamma s)) = I_{y-y'}(\gamma(t+s)) - I_{y+y'}(\gamma(t+s)) \quad (5.90)$$

It remains to fix the parameter $\bar{b}(t, y)$, which we determine from the condition $\mathcal{C}(t; y, y; \mathbf{0}) = 1$. For large d the factor $\gamma = 1/(Td)$ becomes small, and we can use the following approximation

$$I_{y-y'}(\gamma(t-\tau)) \approx \delta_{y,y'} + O\left(\frac{1}{d}\right) \quad (5.91)$$

and similarly for other terms, see also Ref. [89]. This yields the equation

$$1 = e^{-2t} + \int_0^t d\tau e^{-2(t-\tau)} \bar{b}(\tau, y) \quad (5.92)$$

for all y and t . This equation can be solved by Laplace transform, yielding the result $\bar{b}(t, y) = 2$ for all y and t . It then follows that the correlation function in the semi-infinite model is given by Eq. (5.90) with $\bar{b}(t, x)$ set to 2. One can get rid of the sum over u by using $\sum_{m=-\infty}^{\infty} I_{m+k}(z_1) I_m(z_2) = I_k(z_1 + z_2)$ and $I_n(z) = I_{-n}(z)$. With this we obtain for the surface autocorrelation function the expression

$$C_1(t, s) = e^{-(t+s)} \left(I_0(\gamma(t+s)) \right)^{d-1} \left(I_0(\gamma(t+s)) - I_2(\gamma(t+s)) \right) \quad (5.93) \\ + 2 \int_0^s d\tau e^{-(t+s-2\tau)} \left(I_0(\gamma(t+s-2\tau)) \right)^{d-1} \left(I_0(\gamma(t+s-\tau)) - I_2(\gamma(t+s-2\tau)) \right).$$

We immediately remark that for a quench inside the ordered phase with $T < T_c = 1$ no simple scaling behaviour is observed, due to the extremely rapidly increasing Bessel functions. A similar absence of dynamical scaling is also seen in the bulk system quenched below the critical point [89]. At the critical point however, when $T = 1$ and therefore $\gamma = 1/d$, we can use the approximation $e^{-u} I_\nu(u) \approx (2\pi u)^{-1/2} \exp(-\nu^2/(2u))$. As the first term in (5.93) decreases more rapidly than the second one, we find in the scaling regime (with $Y = t/s$)

$$C_1(t, s) = 4 \left(\frac{2\pi}{d} \right)^{-d/2} s^{d/2} \left((Y-1)^{-d/2} - (Y+1)^{-d/2} \right). \quad (5.94)$$

This allows us to identify both the nonequilibrium exponents b_1 and λ_{C_1} and the scaling function $f_{C_1}(Y)$, see Eq. (5.2), (5.3) and (5.4):

$$b_1 = \frac{d}{2}, \quad \lambda_{C_1} = d + 2, \quad f_{C_1}(Y) = 4 \left(\frac{2\pi}{d} \right)^{-d/2} \left((Y-1)^{-d/2} - (Y+1)^{-d/2} \right) \quad (5.95)$$

where we used that in the limit of large d the critical dynamical exponent is equal to 2.

The response function:

In order to compute the response function we start from the differential equation

$$\partial_t \langle \sigma_{\mathbf{x},y}(t) \rangle = -\langle \sigma_{\mathbf{x},y}(t) \rangle + \langle \Delta t_{\mathbf{x},y}(t) \Delta \sigma_{\mathbf{x},y}(t) \rangle \quad (5.96)$$

for $\langle \sigma_{\mathbf{x},y}(t) \rangle$ [89] in the presence of a small external magnetic field $h_{\mathbf{x},y}^{ext}$. As both $h_{\mathbf{x},y}^{ext}$ and $1/d$ are small we can develop the tanh to first order in both quantities:

$$\tanh(h_{\mathbf{x},y}(t)/T) \approx \frac{1}{T} h_{\mathbf{x},y}^{ext}(t) + \frac{\gamma}{2} \left(\sigma_{\mathbf{x},y+1}(t) + \sigma_{\mathbf{x},y-1}(t) + \sum_{\mathbf{z}(\mathbf{x})} \sigma_{\mathbf{z},y}(t) \right). \quad (5.97)$$

The definition

$$R(t, s; y, y'; \mathbf{x} - \mathbf{x}') := \frac{\delta \langle \sigma_{\mathbf{x},y}(t) \rangle}{\delta h_{\mathbf{x}',y'}^{ext}(s)} \quad (5.98)$$

of the response function now directly yields the differential equation (where we set again $\mathbf{x}' = \mathbf{0}$)

$$\begin{aligned} \partial_t R(t, s; y, y', \mathbf{x}) &= -R(t, s; y, y', \mathbf{x}) + \frac{\gamma}{2} \left(R(t, s; y+1, y', \mathbf{x}) + R(t, s; y-1, y', \mathbf{x}) \right. \\ &\quad \left. + \sum_{\mathbf{z}(\mathbf{x})} R(t, s; y, y', \mathbf{z}) \right) + \frac{1}{T} \delta(t-s) \delta_{y,y'} \delta_{\mathbf{x},\mathbf{0}} \end{aligned} \quad (5.99)$$

This equation is solved with similar methods as outlined in the Appendix of [22] for the correlation function. As a result we obtain

$$R(t, s; y, y', \mathbf{x}) = \frac{\Theta(t-s)}{T} e^{-(t-s)} \left(I_{y-y'}(\gamma(t-s)) - I_{y+y'}(\gamma(t-s)) \right) \prod_{i=1}^{d-1} I_{x_i}(\gamma(t-s)) \quad (5.100)$$

For the case $T = T_c = 1$ the surface autoresponse function can again be evaluated in the scaling regime, yielding (with $Y = t/s$)

$$R_1(t, s) = \frac{2d}{T_c} \left(\frac{2\pi}{d} \right)^{-d/2} s^{-\frac{d}{2}-1} (Y-1)^{-(d+2)/2} \quad (5.101)$$

and therefore

$$a_1 = \frac{d}{2}, \quad \lambda_{R_1} = d+2, \quad f_{R_1}(Y) = \frac{2d}{T_c} \left(\frac{2\pi}{d} \right)^{-d/2} (Y-1)^{-\frac{d}{2}-1}. \quad (5.102)$$

We can now also compute the surface fluctuation-dissipation ratio from the expressions (5.94) and (5.101) and obtain

$$\begin{aligned} X_1(t, s) &= \frac{T_c R_1(t, s)}{\partial_s C_1(t, s)} \\ &= \frac{(Y-1)^{-\frac{d}{2}-1}}{Y \left((Y-1)^{-\frac{d}{2}-1} - (Y+1)^{-\frac{d}{2}-1} \right) - \left((Y-1)^{-\frac{d}{2}} - (Y+1)^{-\frac{d}{2}} \right)} \end{aligned} \quad (5.103)$$

from which the limit value $X_1^\infty = 1/2$ follows.

Comparing with the results obtained for the spherical model, see Table 5.2, we note that the values of the nonequilibrium exponents in the critical short-range Ising model in the limit of high dimensions are in full agreement with the values obtained for the critical spherical model in dimensions $d > 4$ [16]. Even the scaling functions are identical up to a nonuniversal numerical prefactor. Both models are mean-field like in the limit of large dimensions, and the values of the universal quantities are identical to the values obtained within mean-field approximation. This demonstrates that universal nonequilibrium features are indeed encountered close to critical surfaces.

Semi-infinite models with continuous spins

In this subsection we consider continuum models described by the $O(N)$ -symmetric Landau-Ginzburg-Wilson Hamiltonian

$$H(\phi) = \frac{1}{2} \int d^d x \left[r_0 \phi^2 + (\nabla \phi)^2 + g_0 (\phi^2)^2 \right] \quad (5.104)$$

where $\phi = (\phi_1, \dots, \phi_N)$ is a N -component vector. In order to treat the semi-infinite case, this Hamiltonian has to be augmented by the appropriate boundary term [70, 71].

Critical dynamics:

The case of semi-infinite $O(N)$ models quenched to the critical point has already been discussed in Ref. [45]. For completeness, we shall here briefly summarise their results which we cast in a slightly different form.

The general scaling forms of the space- and time-dependent surface response and correlation functions are easily obtained close to the surface, yielding the results [45]

$$\begin{aligned} R(t, s; y, y', \mathbf{x}) &= \mathcal{A}_R s^{-a_1-1} \left(\frac{t}{s} - 1 \right)^{-a_1-1} \left(\frac{t}{s} \right)^{-\lambda_{R_1}/z+1+a_1} (y \cdot y')^{(\beta_1-\beta)/\nu} \\ &\times \mathcal{F}_R \left(y (t-s)^{-1/z}, y' (t-s)^{-1/z}, \mathbf{x} (t-s)^{-1/z}, \frac{s}{t} \right), \end{aligned} \quad (5.105)$$

$$\begin{aligned} C(t, s; y, y', \mathbf{x}) &= \mathcal{A}_C s^{-b_1} \left(\frac{t}{s} - 1 \right)^{-b_1} \left(\frac{t}{s} \right)^{-\lambda_{C_1}/z+b_1} (y \cdot y')^{(\beta_1-\beta)/\nu} \\ &\times \mathcal{F}_C \left(y (t-s)^{-1/z}, y' (t-s)^{-1/z}, \mathbf{x} (t-s)^{-1/z}, \frac{s}{t} \right). \end{aligned} \quad (5.106)$$

where the amplitudes \mathcal{A}_R and \mathcal{A}_C are fixed by requiring $\mathcal{F}_R(0, 0, \mathbf{0}, 0) = 1$ and $\mathcal{F}_C(0, 0, \mathbf{0}, 0) = 1$. In addition, one finds that the surface critical exponents a_1 and b_1 are equal and are related to known critical exponents by [195, 45]

$$a_1 = a + \frac{2(\beta_1 - \beta)}{\nu z} \quad \text{and} \quad b_1 = b + \frac{2(\beta_1 - \beta)}{\nu z}. \quad (5.107)$$

In the Gaussian approximation (for which one sets $g_0 = 0$ in Equation (5.104)) two-time quantities can be computed exactly [45], yielding in the dynamical scaling regime the

expressions (with $t > s$)

$$R(t, s; y, y', \mathbf{x}) = (4\pi(t-s))^{-\frac{d}{2}} \exp\left(-\frac{\mathbf{x}^2}{4(t-s)}\right) \times \left[\exp\left(-\frac{(y-y')^2}{4(t-s)}\right) - \exp\left(-\frac{(y+y')^2}{4(t-s)}\right) \right], \quad (5.108)$$

$$C(t, s; y, y', \mathbf{x}) = \int_{t-s}^{\infty} du R(u, 0; y, y', \mathbf{x}) - \int_{t+s}^{\infty} du R(u, 0; y, y', \mathbf{x}). \quad (5.109)$$

from which critical exponents and the fluctuation-dissipation ratio can be inferred. For example, for Dirichlet boundary conditions one has in the scaling regime the expressions[45]

$$R_1(t, s) = (4\pi)^{-\frac{d}{2}} s^{-\frac{d}{2}-1} \left(\frac{t}{s} - 1\right)^{-\frac{d}{2}-1}$$

$$C_1(t, s) = \frac{2(4\pi)^{-\frac{d}{2}}}{d} s^{-\frac{d}{2}} \left(\left(\frac{t}{s} - 1\right)^{-\frac{d}{2}} - \left(\frac{t}{s} + 1\right)^{-\frac{d}{2}} \right) \quad (5.110)$$

at the surface, yielding $a_1 = b_1 = \frac{d}{2}$, $\lambda_{R_1} = \lambda_{C_1} = d + 2$ (where we used that $z = 2$), whereas X_1^∞ is equal to $1/2$. Therefore, the Gaussian model in high dimensions is in the same dynamical surface universality class as the critical lattice model with Ising spins considered in the last subsection.

Phase-ordering kinetics:

Below the critical temperature the factor r_0 in the Hamiltonian (5.104) is not vanishing any more. In order to make progress in this case, we consider for the bulk system the equation of motion [37] of the i -th component ϕ_i ,

$$\partial_t \phi_i = -\frac{\delta H}{\delta \phi_i} = (r_0 + \nabla^2) \phi_i - 2g_0(\phi^2) \phi_i. \quad (5.111)$$

Replacing g_0 by $\frac{u}{2N}$ (with the new coupling constant u), we can substitute in the limit of large N the term $\frac{1}{N} \phi^2(\mathbf{r}, t)$ by the correlator $\mathcal{C}(t; \mathbf{r}, \mathbf{r}) = \langle \phi_i(\mathbf{r}, t) \phi_i(\mathbf{r}, t) \rangle$ (for any i), which leads to the following differential equations for the one and two-time correlation functions:

$$\begin{aligned} \partial_t \mathcal{C}(t; \mathbf{r}, \mathbf{r}') &= (r_0 + \nabla_{\mathbf{r}}^2) \mathcal{C}(t; \mathbf{r}, \mathbf{r}') - u \mathcal{C}(t; \mathbf{r}, \mathbf{r}) \mathcal{C}(t; \mathbf{r}, \mathbf{r}') \\ &\quad + (r_0 + \nabla_{\mathbf{r}'}^2) \mathcal{C}(t; \mathbf{r}, \mathbf{r}') - u \mathcal{C}(t; \mathbf{r}', \mathbf{r}') \mathcal{C}(t; \mathbf{r}, \mathbf{r}'), \end{aligned} \quad (5.112)$$

$$\partial_t C(t, s; \mathbf{r}, \mathbf{r}') = (r_0 + \nabla_{\mathbf{r}}^2) C(t, s; \mathbf{r}, \mathbf{r}') - u C(t; \mathbf{r}, \mathbf{r}) C(t, s; \mathbf{r}, \mathbf{r}'). \quad (5.113)$$

As we are for the moment discussing the bulk system, translation invariance holds, and $\tilde{a}(t) := \mathcal{C}(t; \mathbf{r}, \mathbf{r})$ merely depends on time and not on the spatial coordinates. This allows for a self-consistent solution that yields eventually critical exponents and a fluctuation-dissipation ratio that are identical to those known from the bulk spherical model.

In the semi-infinite geometry, where spatial translation invariance is broken, one has, in principle, to solve the full non-linear diffusion equations (5.112) and (5.113) with the boundary condition $C(t, s; 0, 0, \mathbf{x}) = 0$. The general solutions to these equations are not

known. We shall therefore further simplify the problem: Instead of replacing $\frac{1}{N}\phi^2$ by a simple (local) average, we perform a spatial average over the direction perpendicular to the surface. We can do this in the following two ways:

- We can give the same weight to every layer, i.e. $\mathbf{a}_1(t) := \lim_{L \rightarrow \infty} \int_0^L \mathcal{C}(t; y, y, \mathbf{0}) dy$, thus treating all the layers on the same footing. This approach corresponds in fact to the treatment done in our study of the semi-infinite spherical model [16]. We call this the "case 1".
- We can take the weighted average $\mathbf{a}_2(t) := \int_0^\infty w(y) \mathcal{C}(t; y, y, \mathbf{0}) dy$ where $w(y)$ is a positive function with $\int_0^\infty w(y) dy = 1$. In order to fulfil this latter condition, the function $w(y)$ must vanish for $y \rightarrow \infty$. We call this the "case 2".

Introducing the average into the equations of motion obtained in the semi-infinite system yields the equations (with $i = 1, 2$)

$$\partial_t \mathcal{C}(t; y, y', \mathbf{x}) = (2r_0 + 2\nabla_{\mathbf{x}}^2 + \partial_y^2 + \partial_{y'}^2 - 2u\mathbf{a}_i(t))\mathcal{C}(t; y, y', \mathbf{x}), \quad (5.114)$$

$$\partial_t C(t, s; y, y', \mathbf{x}) = (r_0 + \nabla_{\mathbf{x}}^2 + \partial_y^2 - u\mathbf{a}_i(t))C(t, s; y, y', \mathbf{x}). \quad (5.115)$$

These equations can be solved by standard methods, similar to those outlined in Ref. [16] and above, whereby a Fourier-Sine transformation is performed in the direction perpendicular to the surface, whereas in all other directions an ordinary Fourier transformation is used. The solution of equation (5.114) in Fourier space is then given by

$$\widehat{C}(t; k, k', \mathbf{q}) = \exp((2r_0 - 2\mathbf{q}^2 - k^2 - k'^2)t - 2u\mathbf{b}_i(t)) \widehat{C}(0; k, k', \mathbf{q}) \quad (5.116)$$

with $\mathbf{b}_i(t) := \int_0^t \mathbf{a}_i(t') dt'$. For decorrelated initial conditions we have $\widehat{C}(0; k, k', \mathbf{q}) = (\pi/2) \delta(k - k')$, so that the back transformation to direct space yields

$$\begin{aligned} \mathcal{C}(t; y, y', \mathbf{x}) &:= e^{2r_0 t - 2u\mathbf{b}_i(t)} (8\pi t)^{-d/2} \exp\left(-\frac{\mathbf{x}^2}{8t}\right) \\ &\times \left(\exp\left(-\frac{(y - y')^2}{8t}\right) - \exp\left(-\frac{(y + y')^2}{8t}\right) \right). \end{aligned} \quad (5.117)$$

Using the definition of $\mathbf{a}_1(t)$, one can now write for case 1

$$\mathbf{a}_1(t) = \lim_{L \rightarrow \infty} \int_0^L \mathcal{C}(t; y, y, \mathbf{0}) dy \quad (5.118)$$

$$= e^{2r_0 t - 2u\mathbf{b}_1(t)} (8\pi t)^{-\frac{d}{2}} \underbrace{\lim_{L \rightarrow \infty} \int_0^L \left(1 - e^{-y^2/(2t)}\right) dy}_{=: g(t)}, \quad (5.119)$$

with

$$g(t) = \lim_{L \rightarrow \infty} \int_0^L \left(1 - e^{-y^2/(2t)}\right) dy = \lim_{L \rightarrow \infty} \frac{L - \sqrt{\pi/2t} \operatorname{erf}((L/(\sqrt{2t}))}{L} = 1 \quad (5.120)$$

for all times t . In the case 2, we find

$$g(t) = \int_0^\infty w(y) \left(1 - e^{-y^2/(2t)}\right) dy. \quad (5.121)$$

Provided $w(y)$ decreases rapidly for $y \rightarrow 0$, the factor $1 - e^{-y^2/(2t)}$ contributes mainly close to the surface, thus yielding the following asymptotic behaviour:

$$g(t) \stackrel{t \rightarrow \infty}{\sim} \int_0^\infty \frac{y^2 \cdot w(y)}{2t} dy \sim \frac{g_0}{t} \quad (5.122)$$

with a constant g_0 . One can easily check this asymptotic behaviour for typical functions $w(x)$ (like for instance $w(x) = \exp(-x)$).

Altogether the asymptotic large time behaviour for both cases can be written as

$$g(t) \sim g_0 t^F, \quad \text{with } F = \begin{cases} 0 & \text{for case 1} \\ -1 & \text{for case 2} \end{cases}. \quad (5.123)$$

The behaviour of $\mathbf{b}(t)$ (from now on we suppress the subscript i) is then found similarly as in Ref.[147], with

$$\partial_t \mathbf{b}(t) = \mathbf{a}(t) = e^{2r_0 t - 2u\mathbf{b}(t)} (8\pi t)^{-\frac{d}{2}} g_0 t^F. \quad (5.124)$$

In terms of the variable $\tilde{\mathbf{b}}(t) := 2r_0 t - 2u\mathbf{b}(t)$, this equation is given by

$$\partial_t \tilde{\mathbf{b}}(t) = 2r_0 - 2u g_0 (8\pi)^{-\frac{d}{2}} e^{\tilde{\mathbf{b}}(t)} t^{F-\frac{d}{2}}. \quad (5.125)$$

Admitting that for large times $\partial_t \tilde{\mathbf{b}} = 0$ [147, 37], we find in that limit the behaviour

$$e^{\tilde{\mathbf{b}}(t)} \sim \frac{r_0 (8\pi)^{\frac{d}{2}}}{u g_0} t^{\frac{d}{2}-F}. \quad (5.126)$$

Inserting this expression into Equation (5.117) yields the asymptotic expression for the one-time correlator.

The equation for the two-time correlator can be treated along the same lines as that for the one-time correlator, yielding the asymptotic expression we were looking for:

$$\begin{aligned} C(t, s; y, y'; \mathbf{x}) &= \left(e^{\tilde{\mathbf{b}}(t)} \right)^{\frac{1}{2}} \left(e^{\tilde{\mathbf{b}}(s)} \right)^{\frac{1}{2}} (4\pi(t+s))^{-\frac{d}{2}} \exp\left(\frac{\mathbf{x}^2}{4(t+s)}\right) \\ &\times \left(\exp\left(-\frac{(y-y')^2}{4(t+s)}\right) - \exp\left(-\frac{(y+y')^2}{4(t+s)}\right) \right) \end{aligned} \quad (5.127)$$

$$\begin{aligned} &= \frac{r_0 (4\pi)^{-\frac{d}{2}}}{u g_0 (8\pi)^{-\frac{d}{2}}} (t \cdot s)^{\frac{d}{4}-\frac{F}{2}} (t+s)^{-\frac{d}{2}} \exp\left(\frac{\mathbf{x}^2}{4(t+s)}\right) \\ &\times \left(\exp\left(-\frac{(y-y')^2}{4(t+s)}\right) - \exp\left(-\frac{(y+y')^2}{4(t+s)}\right) \right). \end{aligned} \quad (5.128)$$

For the surface correlation function we obtain

$$C_1(t, s) \sim c_1 s^{-1-F} \left(\frac{t}{s}\right)^{\frac{d}{4}-\frac{F}{2}} \left(\frac{t}{s} + 1\right)^{-\frac{d}{2}-1} \quad (5.129)$$

which yields the critical exponents (as $z = 2$)

$$b_1 = F + 1 \quad \text{and} \quad \lambda_{C_1} = \frac{d}{2} + 2 + F. \quad (5.130)$$

The response function is rapidly found from the equation

$$\partial_t \widehat{\phi}(t; k, \mathbf{q}) = (r_0 - \mathbf{q}^2 - k^2) \widehat{\phi}(t; k, \mathbf{q}) - a(t) \widehat{\phi}(t; k, \mathbf{q}) + \widehat{h}(t; k, \mathbf{q}), \quad (5.131)$$

with the result

$$\begin{aligned} R(t, s; y, y', \mathbf{x}) &= \theta(t-s) \left(e^{\tilde{b}(t)} e^{-\tilde{b}(s)} \right)^{\frac{1}{2}} (8\pi(t-s))^{-\frac{d}{2}} \exp\left(-\frac{\mathbf{x}^2}{8(t-s)}\right) \\ &\quad \left(\exp\left(-\frac{(y-y')^2}{8(t-s)}\right) - \exp\left(-\frac{(y+y')^2}{8(t-s)}\right) \right) \end{aligned} \quad (5.132)$$

for the space-time response and

$$R_1(t, s) = r_1 s^{-\frac{d}{2}-1} \left(\frac{t}{s}\right)^{\frac{d}{4}-\frac{F}{2}} \left(\frac{t}{s} - 1\right)^{-\frac{d}{2}-1} \quad (5.133)$$

for the surface autoresponse function. The corresponding critical exponents are then

$$a_1 = \frac{d}{2} \quad \text{and} \quad \lambda_{R_1} = \frac{d}{2} + 2 + F + 1 = \lambda_{C_1}. \quad (5.134)$$

It is interesting to compare these results with those obtained in our previous study of the semi-infinite spherical model quenched below the critical point [16], see Table II in the concluding subsection. We first remark that for the case 1, where all layers enter into the average with the same weight, we recover the results from the spherical model. Especially, we also obtain that the exponent b_1 , which governs the scaling behaviour of the autocorrelation, is different from zero for the $O(N \rightarrow \infty)$ model undergoing phase-ordering. For the case 2, however, we see that the weighted average leads to $b_1 = 0$, which is the same value as that obtained for the corresponding exponent in the bulk system. This indicates that for the considered models the way we treat the influence of the bulk on the surface has a deep effect on the out-of-equilibrium dynamical behaviour close to the surface.

A different approach for phase-ordering kinetics

We conclude this subsection on exactly solvable models by generalising to the semi-infinite geometry an approach to phase-ordering kinetics due to Bray and Humayun [36]. Following the basic idea introduced by Ohta, Jasnow and Kawasaki [181], the order parameter field $\phi(t, \mathbf{r})$, which at $T = 0$ is ± 1 everywhere except at domain walls, is replaced by an auxiliary and smoothly varying field $m(t, \mathbf{r})$, with the interfaces given by $m = 0$. For this auxiliary field, Bray and Humayun derived for the bulk the equation of motion [36, 37]

$$\partial_t m = \nabla^2 m + (1 - |\nabla m|^2) m \quad (5.135)$$

as a starting point for a systematic calculation of scaling functions.

For the semi-infinite system we are interested in, we replace the term $(1 - |\nabla m|^2)$ by an average $\mathbf{a}(t)$ over the direction perpendicular to the surface. After the average, we have the following equation of motion for the auxiliary field m :

$$\partial_t m = \nabla^2 m + \mathbf{a}(t) m \quad (5.136)$$

where $\mathbf{a}(t)$ is given by

$$\mathbf{a}(t) = \lim_{L \rightarrow \infty} \int_0^L (1 - |\nabla m|^2) dy \quad \text{case 1,} \quad (5.137)$$

$$\mathbf{a}(t) = \int_0^\infty w(y)(1 - |\nabla m|^2) dy \quad \text{case 2,} \quad (5.138)$$

where we distinguish the same two averages as before. Equation (5.136) can be solved in exactly the same way as before, yielding

$$\widehat{m}(t; k, \mathbf{q}) = \widehat{m}(0; k, \mathbf{q}) \exp(-(\mathbf{q}^2 + k^2)t + \mathbf{b}(t)) \quad (5.139)$$

with $\mathbf{b}(t) = \int_0^t dt' \mathbf{a}(t')$. Using in Fourier space the initial correlations ($\Delta > 0$)

$$\langle m(0; k, \mathbf{q}) m(0; k', \mathbf{q}') \rangle = \Delta(\pi/2)(2\pi)^{d-1}, \quad (5.140)$$

corresponding to initial short-range spatial correlations [36], as well as the equations (5.137) and (5.138), we obtain again a self-consistent equation with the long-time solution

$$\exp(2\mathbf{b}(t)) \sim g_0 t^{\frac{d}{2}-F} \quad (5.141)$$

with a constant g_0 that will drop out in the end. The values of the exponent F are the same as those encountered in the previous subsection. With this, we obtain for the two-time correlation function the expression

$$\begin{aligned} \langle m(t; y, \mathbf{x}) m(s; y, \mathbf{0}) \rangle &= \left(g_0 t^{\frac{d}{2}-F} \right)^{\frac{1}{2}} \left(g_0 s^{\frac{d}{2}-F} \right)^{\frac{1}{2}} \frac{\Delta}{16} (4\pi)^{-\frac{d}{2}} (t+s)^{-\frac{d}{2}} \\ &\times \exp\left(-\frac{\mathbf{x}^2}{4(t+s)}\right) \left(\exp\left(-\frac{(y-y')^2}{4(t+s)}\right) - \exp\left(-\frac{(y+y')^2}{4(t+s)}\right) \right). \end{aligned} \quad (5.142)$$

We note that this quantity behaves close to the surface and for $\mathbf{x} = 0$ and $y = y'$ as

$$\langle m(t; y, \mathbf{0}) m(s; y, \mathbf{0}) \rangle = y^2 \left(g_0 t^{\frac{d}{2}-F} \right)^{\frac{1}{2}} \left(g_0 s^{\frac{d}{2}-F} \right)^{\frac{1}{2}} \frac{\Delta}{16} (4\pi)^{-\frac{d}{2}} (t+s)^{-\frac{d}{2}-1}. \quad (5.143)$$

In order to come back to the original fields, the joint probability distribution of the fields $m(t; y, \mathbf{x})$ [36, 37] is used, with the result

$$C(t, s; y, y', \mathbf{x}) = \frac{2}{\pi} \arcsin(\xi(t, s; y, y', \mathbf{x})) \quad (5.144)$$

where $\xi(t, s; y, y', \mathbf{x})$ is given by [36, 37]

$$\xi(t, s; y, y', \mathbf{x}) = \frac{\langle m(t; y, \mathbf{x}) m(s; y', \mathbf{0}) \rangle}{\sqrt{\langle m^2(t; y, \mathbf{0}) \rangle \langle m^2(s; y', \mathbf{0}) \rangle}}. \quad (5.145)$$

It has to be noted that due to the normalisation the terms involving the exponent F drop out, so that in this approach the final result for the correlation function is independent on the chosen way of making the average in the direction perpendicular to the surface. If we restrict ourselves to the surface-autocorrelator in the scaling regime, we can evaluate the

expression (5.145) with the help of Eq. (5.143). This gives us the following expression in the scaling regime with $t \gg s$:

$$\xi(t, s; y, y, \mathbf{0}) \sim \left(\frac{t}{s}\right)^{\frac{d}{4} + \frac{1}{2}} \left(\frac{t}{s} + 1\right)^{-\frac{d}{2} - 1} \quad (5.146)$$

Finally, in the same regime the surface autocorrelation is given by

$$C_1(t, s) \sim \xi(t, s; y, y, \mathbf{0}) \quad (5.147)$$

so that $b_1 = 0$ and $\lambda_{C_1} = \frac{d}{2} + 1$. These are exactly the same exponents as those obtained in the previous subsection for the $O(N)$ model with a weighted average perpendicular to the surface. Especially, it has to be noticed that the Bray/Humayun approach, generalised to semi-infinite systems, always yields the value 0 for the exponent b_1 .

Response functions in bulk systems with phase-ordering kinetics have been studied recently within a perturbative theory approach [170]. We did, however, not attempt to generalise this rather involved approach to the semi-infinite geometry.

5.2.3 Quenching semi-infinite systems from high temperatures: numerical results

The exactly solvable models discussed in 5.2.2 are all to some extent artificial. It is therefore unclear whether results derived from these models apply to more realistic cases. This is especially true for the case of semi-infinite systems undergoing phase-ordering as here some exactly solvable models (as, e.g., the spherical model [16]) yield $b_1 \neq 0$ for the exponent governing the scaling of the correlation function. As discussed in the last subsection, however, this does not seem to be a generic feature as other approaches to phase-ordering kinetics, extended towards the semi-infinite geometry, yield $b_1 = 0$.

In the following we present the results of extensive numerical simulations of the standard two-dimensional semi-infinite Ising model with only nearest-neighbour interactions quenched inside the ordered phase. The Hamiltonian is given by the usual expression

$$\mathcal{H} = -J \sum_{\langle i, j \rangle} \sigma_i \sigma_j, \quad (5.148)$$

where i and j label the sites of a semi-infinite lattice. The sum extends over nearest neighbour pairs, and we have the same coupling strength $J > 0$ for every bond connecting neighbouring spins. This system exhibits a continuous phase transition at the bulk critical point $T_c = 2/\ln(\sqrt{2} + 1) \approx 2.269$ (where the temperature is measured in units of J/k_B , with k_B being the Boltzmann constant).

Whereas surface ageing behaviour has already been studied in the past for Ising models quenched onto the critical point [195], this does not seem to be the case for quenches below the critical point. The following numerical study therefore allows us to close a gap in our understanding of the nonequilibrium dynamical behaviour of classical spin models. Especially, it yields new insights into the local dynamical behaviour of systems undergoing phase-ordering in the presence of surfaces.

For these simulations we use periodic boundary conditions in one direction and free boundary conditions in the other direction. We thereby consider square systems with $N = L \times L$

spins were L ranges from $L = 300$ to $L = 1000$, thus making sure that the data obtained at any one of the two surfaces are representative of the semi-infinite system. Only data free of finite-size effects are discussed in the following. Our focus lies on the surface autocorrelation function and on the surface autoresponse function. The surface autocorrelation function is given by the expression

$$C_1(t, s) = \frac{1}{2L} \sum_{i \in \text{surface}} \langle \sigma_i(t) \sigma_i(s) \rangle, \quad (5.149)$$

where the sum is over all the spins in the two surfaces. The data discussed in the following have been obtained after averaging over at least 5000 different runs with different realizations of the noise. In order to study the response to a magnetic field, we apply a weak binary random field between the time $t = 0$ (at which the quench takes place) and the time $t = s$ [13]. After the field has been switched off, we monitor the decay of the surface thermoremanent magnetisation given by the expression

$$M_1(t, s) = \frac{1}{2L} \sum_{i \in \text{surface}} \overline{\langle h_i \sigma_i(t) \rangle} / T, \quad (5.150)$$

where h_i is the strength of the binary random field at site i . In addition to averaging over the realizations of the noise we also average over the realizations of the random field as indicated by the bar. We discuss here data obtained with $|h_i| = 0.1$ (we checked that our conclusions remain the same when we slightly vary the value of $|h_i|$). As response functions are very noisy, we average over many more runs than for the autocorrelation. The thermoremanent magnetisation data discussed in this subsection have been obtained after averaging over typically 200,000 runs.

Autocorrelation function

Before discussing the surface autocorrelation function, let us briefly mention some results obtained for the autocorrelation function in the corresponding two-dimensional bulk system. The expected scaling form

$$C(t, s) = s^{-b} f_C(t/s) \quad \text{with} \quad f_C(t/s) \sim (t/s)^{-\lambda_C/z} \quad \text{for} \quad t/s \gg 1 \quad (5.151)$$

has been verified in various numerical studies. These studies showed that $b = 0$ and yielded the value $\lambda_C/z = 0.63(1)$ [85, 39, 110] (recall that $z = 2$) for the exponent governing the long-time decay of the scaling function. Numerous theoretical approaches have been proposed for computing the scaling function f_C [34, 35, 160, 210, 169], the most successful being the recent exploitation of space-time symmetries within the theory of local scale-invariance [114, 161, 126].

The main question we address here concerns the scaling behaviour of the surface autocorrelation function. Let us start by looking at the long-time decay of $C_1(t, s)$ with $s = 0$, as it is well known that this quantity is usually the most appropriate for the determination of λ_{C_1} . In Figure 5.5 we show this quantity for two different temperatures, $T = 1$ and $T = 1.5$, lower than the critical temperature. For comparison we also include the bulk autocorrelation function $C(t, s = 0)$ for the same two temperatures. Whereas at short times the surface autocorrelation (this is also true for the bulk quantity) is clearly temperature dependent, at longer times the two curves get identical. Interestingly, the decay

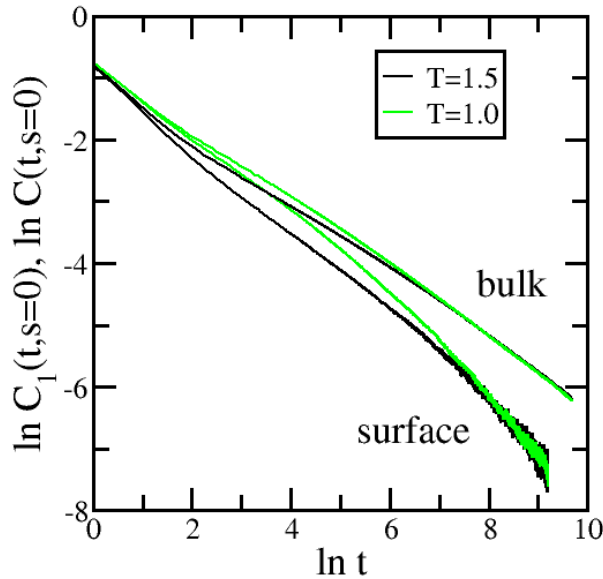


Figure 5.5: (Color online) The surface and bulk autocorrelation functions $C_1(t, s = 0)$ and $C(t, s = 0)$ for two different temperatures. At the surface the correlations decay much faster than inside the bulk, yielding the value $\lambda_{C_1}/z = 0.95(3)$ for the long-time power-law exponent, considerably larger than the value $\lambda_C/z = 0.63(1)$ in the bulk case.

of the surface correlations follow a power-law at late times. This power-law decay is faster at the surface than inside the bulk, yielding the value $\lambda_{C_1}/z = 0.95(3)$ which should be compared to the value $\lambda_C/z = 0.63(1)$ obtained inside the bulk. Obviously, this faster decay is due to the reduced coordination number at the surface.

In Figure 5.6 we discuss the behaviour of the surface autocorrelation function $C_1(t, s)$ with $s > 0$. When plotting $C_1(t, s)$ versus t/s , we do not observe a data collapse, see Figure 2a, in contrast to the data collapse observed when plotting the bulk autocorrelation as a function of t/s . The data shown in Figure 5.6a at first look suggest that the local exponent b_1 is different from zero at the surface. A more thorough analysis reveals however that a good scaling behaviour can not be achieved with a constant $b_1 > 0$. Figure 5.6b shows our best result obtained for $b_1 = 0.13$. A reasonable data collapse can be achieved this way for large values of t/s , but scaling breaks down for $t/s \leq 25$. Taken at face value, this would suggest for the surface autocorrelation function the existence of a large threshold value of t/s below which dynamical scaling is not observed. The possible physical mechanism responsible for this threshold is far from obvious. A better data collapse can be achieved by allowing the exponent b_1 to depend itself on t/s , but a non-constant exponent varying as a function of t/s is not supported by any theoretical approach.

We propose here another interpretation of the numerical data that is based on the recent observation that large finite-time corrections can to some extent mask the true scaling behaviour of the autocorrelation function in phase-ordering systems [125]. In order to take the existence of finite-time corrections into account, we try to describe our data by

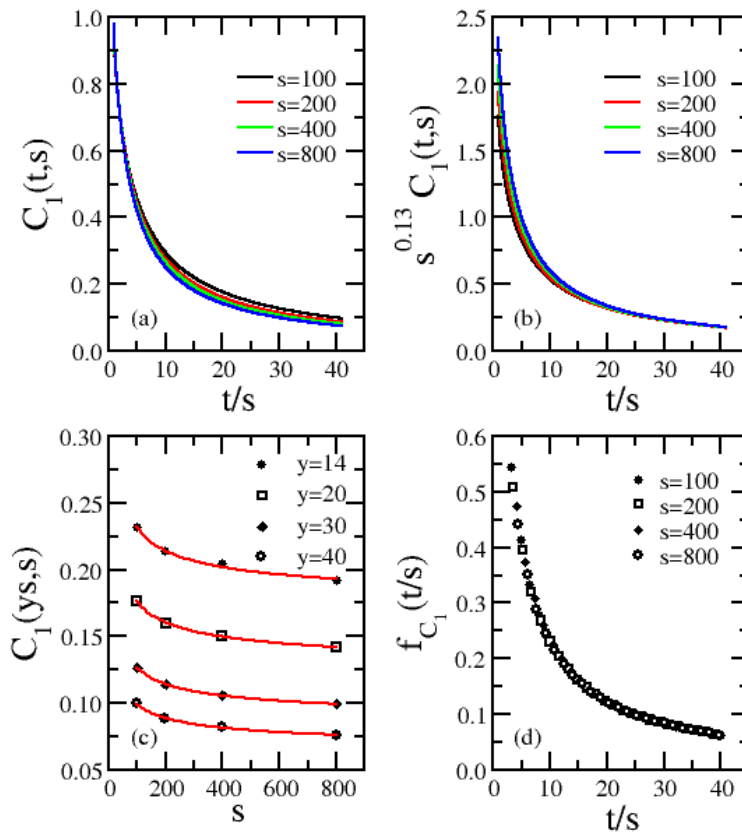


Figure 5.6: (Color online) Discussion of the surface autocorrelation $C_1(t, s)$ obtained after quenching the semi-infinite two-dimensional Ising model to $T = 1$. (a) Autocorrelation as a function of t/s . The expected data collapse with $b_1 = 0$ is not observed. (b) Plotting $s^{0.13}C_1(t, s)$ versus t/s leads to a collapse of data for large values of t/s , but no scaling is observed for smaller values of t/s . (c) Plot of $C_1(y, s)$ as a function of s for various values of $y = t/s$. The full lines are fits to the extended scaling form (5.152) with $b' = 0.49$. (d) Scaling function $f_{C_1}(t/s)$ obtained from the data shown in (a) after subtracting off the finite-time correction term. In (c) and (d) error bars are smaller than the symbol sizes.

the ansatz

$$C_1(t, s) = f_{C_1}(t/s) + s^{-b'} g_{C_1}(t/s) , \quad (5.152)$$

where the first term is the expected scaling behaviour with $b_1 = 0$, whereas the second term is the finite-time correction that is of decreasing importance for increasing values of the waiting time s . This ansatz has recently been used for the analysis of the autocorrelation functions in disordered ferromagnets quenched below their critical point [125, 121]. In Figure 5.6c we show $C_1(y, s)$ as a function of s for various values of the ratio $y = t/s$. The lines show that an excellent fitting of the data can be achieved with the extended scaling form (5.152) with a common value $b' = 0.49(1)$. The scaling function $f_{C_1}(t/s)$, obtained after subtracting off the correction term, is shown in Figure 5.6d. As the curves for the different values of s are not distinguishable on the scale of the Figure, we only show selected points as symbols. The data collapse shown in Figure 5.6d supports our interpretation that the true scaling behaviour of the surface autocorrelation function is masked by strong finite-time corrections. As a consistency check, we note that the data in

Figure 5.6d present for large values of t/s a power-law decay with an exponent 0.95(2), in full agreement with the value of λ_{C_1}/z obtained directly from $C_1(t, s = 0)$. Even though our data are perfectly described by Eq. (5.152), we must emphasise that we do not yet know why this finite-time correction shows up close to the surface but is not encountered inside the bulk.

Let us end the discussion of the surface autocorrelation function by noticing that the value $b' = 0.49(1)$ of the correction term exponent is compatible with $1/2 = 1/z$. However, we refrain from making the conjecture $b' = 1/z$ here without having studied other systems with surfaces (as for example semi-infinite Potts models).

Response function

Before discussing the surface thermoremanent magnetisation $M_1(t, s)$, let us again first recall the behaviour of the corresponding bulk quantity. The bulk thermoremanent magnetisation $M(t, s)$ is a temporally integrated response function that is related to the response function $R(t, s)$ by the integral

$$M(t, s) = \int_0^s du R(t, u) , \quad (5.153)$$

where the integration is over the whole time interval during which the magnetic field was acting on the system. From the scaling form (1.11) of $R(t, s)$, we therefore obtain the scaling behaviour

$$M(t, s) = s^{-a} f_M(t/s) \quad (5.154)$$

for the integrated response. Zippold, Kühn, and Horner [240] were the first to point out the existence of a subleading correction term which can be quite sizeable. For the thermoremanent magnetisation this leads to the following more complete scaling behaviour [112, 117],

$$M(t, s) = s^{-a} f_M(t/s) + s^{-\lambda_R/z} g_M(t/s) . \quad (5.155)$$

The second term in this equation is in fact the response of the system to fluctuations in the initial state, where the scaling function $g_M(t/s)$ is expected to be proportional to the power-law $(t/s)^{-\lambda_R/z}$ [131]. For the two-dimensional Ising model we have $a = 1/z = 1/2$ and $\lambda_R/z = 0.63$. Therefore this correction to scaling can not be neglected but must be included in order to obtain the correct description of the scaling behaviour of the bulk thermoremanent magnetisation [112, 117, 161].

In Figure 5.7 we summarise our findings for the surface thermoremanent magnetisation in the two-dimensional semi-infinite Ising model quenched below the critical point. Figure 5.7a shows the behaviour of this local response as a function of t/s for various values of the waiting time s . In a first attempt, we might try to achieve a scaling behaviour by assuming that

$$M_1(t, s) = s^{-a_1} f_{M_1}(t/s) , \quad (5.156)$$

thereby neglecting any possible corrections to scaling. A reasonable scaling behaviour is achieved this way for a value of $a_1 \approx 0.40$, slightly lower than the expected value $1/z = 1/2$. For a more thorough analysis we can fix $y = t/s$ and plot the response as a function of the waiting time in a log-log-plot. Fitting a straight line to the data, we obtain from the slope of that line a value of a_1 for every considered value of t/s . Thus,

we obtain $a_1 = 0.38$ for $t/s = 5$, $a_1 = 0.39$ for $t/s = 10$, $a_1 = 0.40$ for $t/s = 15$, and $a_1 = 0.42$ for $t/s = 20$. This points to the existence of a correction term that vanishes for increasing values of t/s . In Figure 5.7b we test the more complete scaling form

$$M_1(t, s) = s^{-a_1} f_{M_1}(t/s) + s^{-\lambda_{R_1}/z} g_{M_1}(t/s) \quad (5.157)$$

where the correction term with the scaling function $g_{M_1}(t/s) = r_1(t/s)^{-\lambda_{R_1}/z}$ describes the response of the surface to fluctuations in the initial state. Plugging in the value $\lambda_{R_1}/z = 0.95$ (where we assume that $\lambda_{R_1} = \lambda_{C_1}$ holds), we obtain a consistent description for any t/s with common values $r_1 = -0.106(1)$ for the amplitude of the correction term and $a_1 = 0.50(1)$ for the exponent of the leading term. The correction term being now completely fixed, we can subtract it off from the numerical data and obtain the data collapse shown in Figure 5.7c. Thus, as for the thermoremanent magnetisation in the bulk [112, 117, 161], we are able to identify the leading correction term and in addition obtain the value $a_1 = a = 1/z$.

We close this subsection by a brief discussion of the surface fluctuation-dissipation ratio. In Figure 5.7d we plot the ratio

$$Z_1(t, s) = \frac{TM_1(t, s)}{hC_1(t, s)} \quad (5.158)$$

as a function of s/t for various values of s . This ratio yields asymptotically the limit value X_1^∞ of the fluctuation-dissipation ratio (5.80), as

$$X_1^\infty = \lim_{s \rightarrow \infty} \left(\lim_{t \rightarrow \infty} Z_1(t, s) \right) . \quad (5.159)$$

For a given value of the waiting time, the ratio $Z_1(t, s)$ converges towards a constant finite value when $s/t \rightarrow 0$. At first look this might seem surprising as in coarsening systems one expects the limit value $X_1^\infty = 0$. However, this constant decreases for increasing values of s . Taking into consideration the leading scaling behaviours of $C_1(t, s) \sim f_{C_1}(t/s)$ and of $M_1(t, s) \sim s^{-1/2} f_{M_1}(t/s)$ found in our study as well as the fact that the scaling functions $f_{C_1}(t/s)$ and $f_{M_1}(t/s)$ display for large arguments a power-law behaviour with the same exponent 0.95, we find that the saturation value $\lim_{t \rightarrow \infty} Z_1(t, s)$ should vanish as $s^{-1/2}$. This is indeed verified in Figure 5.7e, where $s^{1/2} Z_1(t, s)$ leads to a collapse of the data onto a common curve for s/t small. This is also an *a posteriori* check that we have indeed correctly identified the leading scaling behaviours of both the surface autocorrelation and the surface integrated response functions.

5.2.4 Conclusions of this section

In this section we have extended the investigation of surface ageing phenomena to cases not studied previously. On the one hand we have computed nonequilibrium surface quantities in a series of exactly solvable models (short-range Ising model in the limit of a large number of space dimensions, two modifications of the $O(N)$ model quenched below the critical point, an extension to the semi-infinite geometry of the Bray/Humayun approach to phase-ordering kinetics), on the other hand we have presented numerical simulations of the standard semi-infinite Ising model quenched inside the ordered phase. Our study has yielded a fairly complete picture of surface ageing properties in magnetic systems.

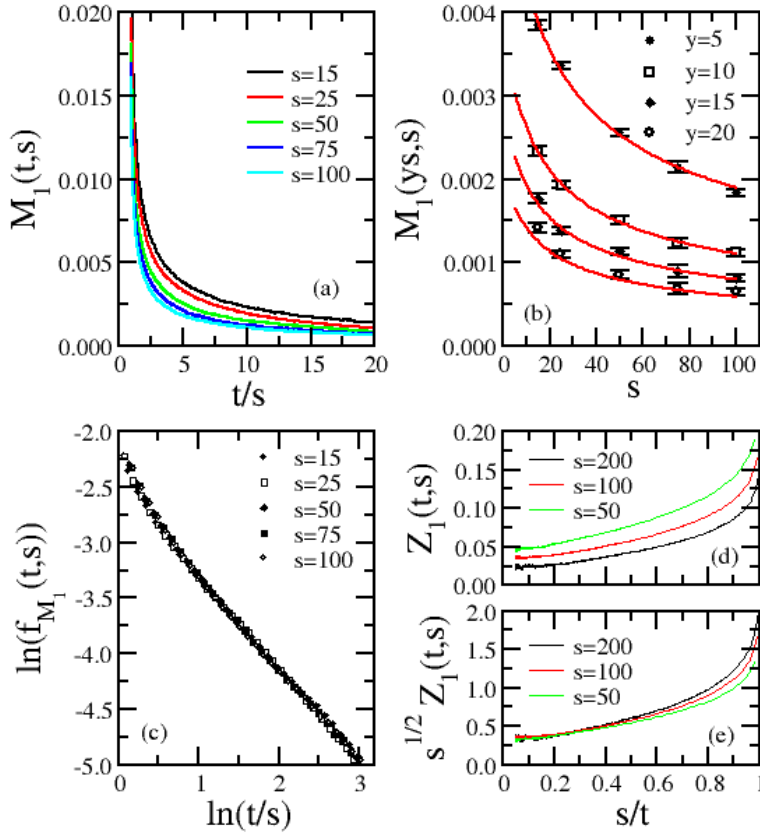


Figure 5.7: (Color online) Discussion of the surface thermoremanent magnetisation $M_1(t, s)$ obtained after quenching the semi-infinite two-dimensional Ising model to $T = 1$ where a random magnetic field of strength $h = 0.1$ is applied between $t = 0$ and $t = s$. (a) $M_1(t, s)$ plotted against t/s for various waiting times s . (b) Plot of $M_1(y s, s)$ as a function of s for various values of $y = t/s$. The full lines are fits to the extended scaling form (5.157). A consistent description of the data for any value of t/s is achieved for $\lambda_R/z = 0.95$, $a = 0.5$, and $r_1 = -0.106$, see main text. (c) Scaling function $f_{M_1}(t/s)$ obtained from the data shown in (a) after subtracting off the finite-time correction term. Error bars are smaller than the symbol sizes. (d) Plot of $Z_1(t, s)$, see Equation (5.158), versus s/t for different waiting times. (e) Plotting $s^{1/2} Z_1(t, s)$ versus s/t leads to a data collapse for small values of s/t .

For a quench to the critical point, we added the semi-infinite Ising model in high dimensions to the list of exactly solved models. The universal nonequilibrium surface quantities obtained in this study agree with those obtained for the critical semi-infinite spherical model [16], as expected for a mean-field like model. In Table I we summarise the known results for surface ageing phenomena in critical systems at the ordinary transition (the only situation studied in this section) by listing the values of the different universal nonequilibrium exponents as well as those of the asymptotic value of the fluctuation-dissipation ratio. It is worth mentioning that the existing numerical data for the semi-infinite Ising model [195] indicate a non-monotonous behaviour of the limit value of the surface fluctuation-dissipation ratio as a function of the dimensionality of the system (being $\frac{1}{2}$ for $d \geq 4$, then increasing to 0.59 in three dimensions, before decreasing to 0.31 in the two-dimensional

Table 5.2: Available values of nonequilibrium critical surface quantities at the ordinary transition determined in ageing systems quenched to the critical point.

model	$a_1 = b_1$	$\lambda_{R_1} = \lambda_{C_1}$	X_1^∞
spherical model ($2 < d < 4$) [16]	$\frac{d}{2}$	$\frac{3d}{2}$	$1 - \frac{2}{d}$
spherical model ($d > 4$)[16]	$\frac{d}{2}$	$d + 2$	$\frac{1}{2}$
Gaussian model[45]	$\frac{d}{2}$	$d + 2$	$\frac{1}{2}$
Ising model in large dimensions	$\frac{d}{2}$	$d + 2$	$\frac{1}{2}$
Ising model in $d = 3$, ordinary transition[195]	1.24(1)	2.10(1)	0.59(2)
Ising model in $d = 2$ [195]	0.46(1)	1.09(1)	0.31(1)

system). This behaviour is unexpected, and a satisfactory explanation is still lacking. Our emphasis in this section was on surface ageing phenomena in systems undergoing phase-ordering. Prior to this work, only the semi-infinite spherical model quenched below the critical point has been studied [16]. On the one hand we added in this section various exactly solvable models that display dynamical scaling when quenched inside the ordered phase, on the other hand we presented large-scale numerical simulations of the two-dimensional semi-infinite Ising model undergoing coarsening. From these results we conclude that the result $b_1 \neq 0$ for the spherical model [16] is not a generic one but can be traced back to the spatial average in the direction perpendicular to the surface that was introduced in [16] in order to make this model solvable. Introducing a weighted average already yields $b_1 = 0$, as demonstrated in this section for the $O(N)$ model in the limit $N \rightarrow \infty$. In addition, the Bray/Humayun approach to phase-ordering kinetics [36] as well as the numerical simulations of the two-dimensional Ising model yield $b_1 = 0$. This indicates that generically the exponent b_1 , that governs the scaling of the surface correlations, vanishes, similarly to what is observed inside the bulk.

One of the main conclusions of this section is that surface ageing phenomena in systems undergoing phase-ordering display the same general features as bulk ageing phenomena. Simple scaling forms prevail asymptotically for two-time quantities like the surface autoreponse and the surface autocorrelation functions, and universal nonequilibrium quantities, with values that differ from the bulk values, can also be identified in semi-infinite coarsening systems, see Table 5.3. For finite times, corrections to scaling can be rather important and might even mask the leading scaling behaviour. In our study of the two-dimensional semi-infinite Ising model we not only identified a sub-leading contribution to the thermoremanent surface magnetisation (a similar correction also appears inside the bulk), but we also showed the existence of corrections to scaling in the surface autocorrelation function. The physical origin of this last term is not yet clear. It is however worth noting that a similar correction term has recently been shown to exist for the random bond Ising model quenched below the critical point [125].

The semi-infinite geometry discussed in this chapter is of course only a special case of a more general wedge-shaped geometry. Wedges in critical systems have been studied quite intensively in the past [50, 133, 193, 196], as they lead to static critical quantities whose values depend on the opening angle of the wedge. However, the local critical dynamical behaviour in a wedge-shaped geometry has not yet been discussed in the literature. Phase-ordering in wedges can also be viewed as being one of the simplest cases of phase-ordering

Table 5.3: Available values of nonequilibrium surface quantities determined in ageing systems quenched below the critical point.

model	a_1	b_1	$\lambda_{R_1} = \lambda_{C_1}$
spherical model[16]	$\frac{d}{2}$	1	$\frac{d}{2} + 2$
$O(N \rightarrow \infty)$ model, case 1	$\frac{d}{2}$	1	$\frac{d}{2} + 2$
$O(N \rightarrow \infty)$ model, case 2	$\frac{d}{2}$	0	$\frac{d}{2} + 1$
Bray/Humayun approach	—	0	$\frac{d}{2} + 1$
Ising model in $d = 2$	$\frac{1}{2}$	0	1.90(6)

in confined geometries. The study of edge ageing phenomena is therefore the next logical step in the study of local nonequilibrium dynamical behaviour in confined geometries, and work along this line is in progress.

Chapter 6

Conclusions

The subject of this thesis have been systems far from thermal equilibrium undergoing ageing. We have contributed several results to the following aspects of this field:

- (1) The problem of a general description of out-of-equilibrium systems with an arbitrary dynamical exponent z in terms of a dynamical symmetry.
- (2) The ageing behaviour of systems without detailed balance and the differences occurring in comparison to magnetic systems.
- (3) The change of the out-of-equilibrium behaviour of the system when a surface is introduced.

In the following we sum up the results we have obtained for each one of these points.

(1) At present, a general framework for the description of out-of-equilibrium systems is still lacking. By analogy with the description of two-dimensional equilibrium critical phenomena, it was proposed by Henkel [109] in 2002 to consider local extensions of dynamical scaling, which led to a first formulation of the principles of a theory of local scale-invariance (LSI). For the case $z = 2$ it was shown in [192] how also noisy systems can be described [192]. Here we have extended this theory to arbitrary values of z . This has been done by taking the same approach suggested by Henkel, but modifying the construction of the infinitesimal generators of LSI through a new kind of fractional derivative ∇_r^α . Using purely algebraic arguments we have arrived at a set of operators, which act as symmetry operators on certain linear *deterministic* dynamical equations. Due to the newly introduced fractional derivative ∇_r^α we have also been able to deduce a generalisation of the so-called Bargmann superselection rule and we discovered an interesting connection to integrable systems. This rule has allowed us to generalise the considerations of Picone et.al. [192], which reduce averages of the noisy theory to expressions which can be determined via the symmetries of the deterministic part of the theory. In this way, we have derived concrete expressions for the response and correlation functions. The response and correlation functions are particularly interesting as they show a fairly simple scaling behaviour in many situations, which allows the introduction of *ageing exponents* and *scaling functions*. They characterise the universality class of the system. LSI reproduced these scaling forms correctly, although the ageing exponents remain as undetermined parameters in this approach.

The predictions obtained have been thoroughly tested against concrete models. On the one hand, this was done for a certain number of relatively simple, exactly solvable models with linear Langevin equations like the spherical model with long-range interactions or the Mullins-Herring model for surface growth, for which perfect agreement has been found. On the other hand, the predictions were compared to numerical results in the diluted Ising model quenched into the ordered phase (where $z > 2$) and a good agreement with LSI was found. This suggests that the assumptions of LSI also hold in this highly nonlinear system and might be applicable to much wider range of models. In fact we are not aware of any other general theory for phase-ordering kinetics which yields such a good agreement. We stress however, that the applicability of LSI to nonlinear systems has not been proven yet. Only for the case $z = 2$ (see point **(2)**), a first step towards the inclusion of nonlinear models has been achieved [17].

Another interesting type of system, in which ageing has scarcely been considered in the past, are growing surfaces and interfaces. As a first step we have only looked at linearised models like the Edward-Wilkinson model or the Mullins-Herring model. The actual challenge in this field is however the **Kardar-Parisi-Zhang** equation [141] (KPZ-equation) which has an additional, quite complicated nonlinearity. We hope that LSI might become useful here in the future.

(2) In order to learn more about the ageing behaviour of systems without detailed balance, we have considered in detail several reaction-diffusion systems. The motivation for this have been numerical results obtained by Enss et. al [80] and Ramasco et. al [203] in the fermionic contact process, which is one representative of the paradigmatic directed percolation universality class. These results showed that for the autoresponse $R(t, s)$ function and the connected autocorrelation function $G(t, s)$ the scaling forms

$$R(t, s) = s^{-a-1} f_R \left(\frac{t}{s} \right), \quad G(t, s) = s^{-b} f_G \left(\frac{t}{s} \right)$$

$$f_R(y) \stackrel{y \rightarrow \infty}{\sim} y^{-\lambda_R/z}, \quad f_G(y) \stackrel{y \rightarrow \infty}{\sim} y^{-\lambda_G/z}$$

known from magnetic systems do hold at the critical point, but with $b = a + 1$, whereas $a = b$ holds for critical magnets. This has for instance consequences for the definition of a fluctuation-dissipation ratio (FDR), as $a = b$ is needed to obtain a nontrivial quantity in the limit $t \rightarrow \infty$ and then $s \rightarrow \infty$. It was already suggested by Enss et. al. to use the quantity $\Xi(t, s) = R(t, s)/G(t, s)$ instead of the usually defined FDR.

We have first investigated the directed percolation universality class via the field-theoretical renormalisation group. We have confirmed that indeed $b = a + 1$ at criticality and we have shown that this is a direct consequence of the so-called rapidity reversal symmetry, which is a special symmetry of the fermionic contact process. Also the equality $\lambda_G = \lambda_R = z + z\delta + d$ was proven, where δ is the critical exponent defined via the behaviour of the survival probability $P(t) \sim t^{-\delta}$. Further, we have suggested a concrete interpretation of the quantity $\Xi(t, s)^{-1} + 1$: it measures the distance of the system from its stationary state, in analogy to the usual fluctuation-dissipation ratio $X(t, s)$. We have also computed $\Xi(t, s)$ to first order in the epsilon-expansion and have found a good agreement with the numerical results.

On the other hand, we have realised, that the autoresponse function to first order in $\epsilon = 4 - d$ does not agree with the prediction of LSI. Probably one of the reasons for

this comes from the fact that in this system the average of the order parameter is non-vanishing, but LSI in its present formulation does require a vanishing average of the order parameter.

Two reaction-diffusion systems of a completely different type were also considered. The bosonic contact process with diffusion (BCPD) and the bosonic pair-contact process with diffusion (BPCPD). In these systems an arbitrary number of particles is allowed on each lattice site. In the BCPD scaling behaviour is found with $a = b$, if the particle creation and annihilation rate balance each other. In the BPCPD the situation is more involved: If particle creation and annihilation are equally strong, the model can be solved exactly. For $d \leq 2$, one never finds scaling behaviour. For $d > 2$, if diffusion is dominant compared to reactions the model behaves like the BCPD but if reactions dominate diffusion, one does not have scaling behaviour either. In between these two regimes, there is a multicritical point corresponding to a clustering transition, where scaling behaviour is found, but again with $a \neq b$. We have however *not* recovered the relation $b = a + 1$ found in the directed percolation universality class. This does not only provide further evidence that the equality $a = b$ does in general not hold in reaction-diffusion systems but also shows, that there is no apparent relation between the two exponents a and b .

Finally we have adapted the existing version of LSI for the case $z = 2$ to these two bosonic systems. These extended versions of LSI include also certain non-linear models. This work was based on previous results about nonlinear Schrödinger equations obtained by Stoimenov et. al. [222] in 2005.

(3) Finally, we have looked at ageing phenomena close to surfaces of semi-infinite system. This constitutes a first step towards more realistic systems, as every real physical system has surfaces, edges and corners. The understanding of this type of system will lead the way towards the investigation of the dynamics of more complicated geometries. One could think here about wedge- or cusp-shaped geometries. On the one hand, some results about the static behaviour of these systems are already available, on the other hand this type of system is already quite close to what turns up in an experimental situation, in particular in thin films or nanoobjects.

For the case of critical dynamics we have added two exactly solvable models to previously established results: The semi-infinite spherical model and the Ising model for large dimensionality. In both cases, surface ageing exponents, surface scaling functions and the surface fluctuation-dissipation ratio were exactly calculated. The results fit into the general scaling picture found in previous works, which is similar to the known bulk scaling behaviour. Previously established scaling relations between the critical exponents were also confirmed.

We have also considered for the first time phase-ordering kinetics close to surfaces. The solution of the spherical model suggest here, that the ageing exponent b_1 does not vanish for Dirichlet boundary conditions, which is markedly different from the situation in the bulk, where the corresponding bulk ageing exponent vanishes. We have also found this result in a modified version of the $O(N)$ model. To clarify this issue further we looked at other simply models like for instance a generalisation to semi-infinite geometries of the Bray and Humayun approach. In addition we have performed simulations in the 2D-Ising

model. The results clearly show that $b_1 = 0$ also in semi-infinite systems, which indicates that the result for the spherical model and of the modified version of the $O(N)$ model should rather be considered as an unphysical features of these simple systems.

In this way we have obtained a quite complete picture about the out-of-equilibrium dynamics at surfaces of semi-infinite magnetic systems. The general scaling behaviour is similar to what is known from the bulk, both in the case of critical dynamics and in the case of phase-ordering. However ageing exponents and scaling functions will in general be different from the corresponding bulk system. One reason which makes the numerical study of phase-ordering difficult is the fact, that there a strong finite time effects which can obscure the true behaviour.

Conclusions

Le sujet de cette thèse est l'étude des systèmes hors équilibre qui montrent un comportement de vieillissement. On a pu contribuer à de nouveaux résultats aux problèmes suivants.

- (1) Une description générale d'un système hors équilibre avec un exposant dynamique z arbitraire à l'aide de symétries dynamiques.
- (2) Le comportement de vieillissement dans des systèmes sans bilan détaillé et les différences qui apparaissent par rapport aux systèmes magnétiques.
- (3) Le changement du comportement hors équilibre du système quand une surface est introduite.

Résumons les résultats qu'on a obtenus pour ces différents points.

(1) A ce jour, il n'y a pas de théorie générale pour la description d'un système hors équilibre. Par analogie avec la description des phénomènes critiques à deux dimensions, il a été proposé par Henkel [109] en 2002 de considérer une généralisation du comportement d'échelle dynamique global vers un comportement d'échelle dynamique local. Cette démarche a abouti à une première formulation des principes de la théorie d'invariance d'échelle locale (LSI). Pour le cas $z = 2$ cette approche a même permis de décrire des systèmes avec du bruit. Dans ce travail on a élargi cette théorie à des valeurs arbitraires de z . Pour cela on a emprunté l'approche proposée par Henkel, tout en modifiant la construction des générateurs infinitésimaux de la LSI à travers l'utilisation d'une nouvelle forme de dérivée fractionnaire ∇_r^α . En utilisant des arguments purement algébriques on arrive à un ensemble d'opérateurs qui agissent comme des opérateurs de symétrie sur certaines équations dynamiques linéaires et *déterministes*. A l'aide de cette nouvelle forme de dérivées ∇_r^2 , une généralisation des règles de Bargmann a pu être déduite et un lien intéressant vers des systèmes intégrables est devenu apparent. Ces règles permettent de réduire les valeurs moyennes de la théorie incluant du bruit aux expressions qui peuvent être calculées en exploitant les symétries de la partie déterministe de la théorie. De cette façon, nous avons dérivé des expressions concrètes pour les fonctions de réponse et de corrélation. Les fonctions de corrélation et de réponse sont particulièrement intéressantes parce qu'elles montrent un comportement d'échelle plutôt simple dans de nombreuses situations. Ceci permet l'introduction d'*exposants de vieillissement* et de *fonctions d'échelle* qui caractérisent la classe d'universalité du système. Nous avons trouvé que la LSI reproduit ces fonctions d'échelles correctement, quoique les exposants de vieillissement restent des paramètres indéterminés dans cette approche.

Les prédictions obtenues ont été testées soigneusement dans des modèles concrets. Les premiers tests ont été faits dans un certain nombre de modèles relativement simples décrits par des équations de Langevin linéaires comme par exemple le modèle sphérique avec des interactions à longue portée ou le modèle de Mullins-Herring qui décrit la croissance d'une surface. Pour ces modèles on a trouvé un accord parfait avec la LSI. Les prédictions ont également été comparées aux résultats numériques dans le modèle d'Ising dilué, trempé dans la phase ordonnée (où $z > 2$). On constate un bon accord avec la LSI. Ceci suggère que l'hypothèse d'une invariance d'échelle locale est valide également dans ces systèmes fortement non-linéaires et qu'elle est peut-être applicable à une classe beaucoup plus vaste de modèles. A notre connaissance, il n'existe pas d'autre théorie générale qui donne un résultat aussi précis pour des phénomènes de cinétique de domaines dans la phase ordonnée. Nous précisons cependant que l'existence d'une symétrie dynamique locale dans des systèmes non-linéaires n'a pas encore été prouvée d'une façon rigoureuse. Pour le cas $z = 2$ (voir le point **(2)**), une première étape vers l'inclusion des systèmes non-linéaires a été réalisée [17].

Les modèles de croissance d'interfaces et de surfaces sont des systèmes dans lesquels les phénomènes de vieillissement n'ont guère été considérés. Dans ce travail on a considéré les modèles linéarisés comme le modèle de Edward-Wilkinson ou le modèle de Mullins-Herring. Le grand défi dans ce domaine est toutefois l'équation de Kardar-Parisi-Zhang (équation KPZ) qui a une non-linéarité compliquée. On espère que dans le futur la LSI pourrait également s'avérer utile dans ce domaine-ci.

(2) Pour apprendre plus sur le comportement de vieillissement des systèmes sans bilan détaillé, on a considéré en détail plusieurs systèmes de réaction-diffusion. Notre motivation est due aux travaux de Enss et. al. [80] et de Ramasco et. al. [203] sur le processus de contact fermionique, qui est un représentant de la classe d'universalité paradigmatique de la percolation dirigée. Les résultats montrent que pour la fonction d'autoréponse $R(t, s)$ et la fonction de corrélation connectée $G(t, s)$ les formes d'échelle

$$\begin{aligned} R(t, s) &= s^{-a-1} f_R \left(\frac{t}{s} \right), & G(t, s) &= s^{-b} f_G \left(\frac{t}{s} \right) \\ f_R(y) &\stackrel{y \rightarrow \infty}{\sim} y^{-\lambda_R/z}, & f_G(y) &\stackrel{y \rightarrow \infty}{\sim} y^{-\lambda_G/z} \end{aligned}$$

sont valides. Ces formes sont connues des systèmes magnétiques où $a = b$, tandis que pour le processus de contact fermionique on trouve $b = a + 1$. Or la condition $a = b$ est nécessaire pour que la définition habituelle d'un rapport fluctuation-dissipation (FDR) donne une quantité non-triviale dans la limite $t \rightarrow \infty$ puis $s \rightarrow \infty$. Il a déjà été suggéré par Enss et.al. d'utiliser pour le processus de contact fermionique la quantité $\Xi(t, s) = R(t, s)/G(t, s)$ au lieu du rapport FDR habituel.

Dans ce travail, on a d'abord considéré la percolation dirigée en utilisant le groupe de renormalisation dynamique. Nous avons confirmé que $b = a + 1$ au point critique et nous avons montré que cela est une conséquence directe de la symétrie de renversement de la rapidité qui est elle-même une symétrie spécifique du processus de contact fermionique. On a également montré l'égalité $\lambda_G = \lambda_R = z + z\delta + d$, où δ est un exposant critique défini à travers le comportement de la probabilité de survie $P(t) \sim t^{-\delta}$. On a également proposé une interprétation concrète de la quantité $\Xi^{-1}(t, s) + 1$: elle mesure la distance du système

par rapport à son état stationaire. Elle est l'analogie du rapport fluctuation-dissipation habituel $X(t, s)$. Nous avons aussi calculé $\Xi(t, s)$ au premier ordre dans l'expansion de epsilon et nous avons trouvé un bon accord avec les résultats numériques.

D'autre part on a aperçu que la fonction d'autoréponse au premier ordre en $\epsilon = 4 - d$ n'est pas en accord avec la prédiction de la LSI. Une raison probable de ce désaccord pourrait être la valeur moyenne du paramètre d'ordre qui ne s'annule. Or cette condition est nécessaire dans la LSI.

Deux systèmes de réaction-diffusion d'un type complètement différent ont aussi été considérés: le processus de contact bosonique (BCPD) et le processus de contact à paires bosoniques (BPCPD). Dans ces deux systèmes un nombre aléatoire de particules est permis sur chaque site. Dans le BCPD on trouve un comportement d'échelle avec $a = b$, si les taux d'annihilation et de création de particules sont égaux. Dans le BPCPD la situation est plus compliquée: si les processus de création et d'annihilation de particules sont égaux, le modèle peut être résolu exactement. Pour $d \leq 2$ on ne trouve pas de comportement d'échelle. Pour $d > 2$, si la diffusion est dominante comparée aux réactions, le système se comporte comme le BCPD et montre un comportement d'échelle dynamique. Dans le cas contraire quand les réactions dominent sur la diffusion, on ne trouve pas de comportement d'échelle. Entre ces deux régimes, il y a un point multicritique qui correspond à une transition d'agglomération, où on trouve un comportement d'échelle avec $a \neq b$. On n'obtient *pas* la relation $b = a + 1$ comme dans la classe d'universalité de la percolation dirigée. Ceci montre qu'il n'y a pas de relation apparente entre les exposants a et b dans les systèmes de réaction-diffusion.

Finalement on a adapté la version présente de la LSI pour le cas $z = 2$ à ces deux modèles bosoniques. Cette version adaptée de la LSI décrit aussi certains modèles non-linéaires. Ce travail est basé sur des résultats antérieurs sur l'équation de Schrödinger non-linéaire obtenu par Stoimenov et. al. [222] en 2005.

(3) Finalement, on a considéré des phénomènes de vieillissement proches des surfaces de systèmes magnétiques semi-infinis. Ces systèmes représentent un premier pas vers des systèmes plus réalistes, puisqu'un système réel présente des surfaces, des bords et des coins. La compréhension des systèmes de ce type est nécessaire pour l'investigation de la dynamique dans des géométries plus complexes. On pourrait penser ici aux géométries en forme de prisme ou de pointe. D'une part, on connaît déjà certaines choses sur le comportement statique dans ce type de systèmes, d'autre part ces systèmes sont plus proches des situations expérimentales, notamment quand on pense aux couches minces ou aux systèmes nanométriques.

Pour le cas d'une dynamique critique nous avons ajouté deux modèles exactement solubles aux résultats établis antérieurement : le modèle sphérique semi-infini et le modèle d'Ising à hautes dimensions. Dans les deux cas, les exposants de vieillissement de surface, les fonctions d'échelle de surface et le rapport fluctuation-dissipation de surface ont été calculés exactement. Les résultats sont en accord avec le comportement d'échelle général qui a été établi antérieurement et qui est similaire aux formes d'échelle dans le volume. Des relations d'échelle établies ont été confirmées également.

Nous avons également considéré pour la première fois la cinétique de domaine dans la phase ordonnée proche d'une surface. La solution du modèle sphérique suggère dans ce cas que l'exposant de vieillissement b_1 ne s'annule pas pour des conditions de bord de Dirichlet, contrairement à ce qu'on trouve dans le volume où l'exposant de volume correspondant est nul. Nous avons aussi rencontré ce phénomène dans une version modifiée du modèle $O(N)$. Pour rendre plus clair ce point on a aussi considéré d'autres modèles simples comme par exemple une généralisation aux géométries semi-infinies de l'approche de Bray et Humayun. De plus, on a effectué des simulations dans le modèle Ising en deux dimension. Les résultats montrent clairement que $b_1 = 0$ aussi dans des systèmes semi-infinis, ce qui indique que les résultats pour le modèle sphérique et pour la version modifiée du modèle $O(N)$ devraient être considérés plutôt comme des propriétés non-physique de ces modèles simples.

Nous avons pu obtenir ainsi une image assez claire de la dynamique hors-équilibre proche des surfaces pour des systèmes magnétiques semi-infinis. Le comportement d'échelle général est similaire à ce qu'on connaît des systèmes infinis, que ce soit dans le cas d'une dynamique critique ou dans le cas d'une cinétique de domaine dans la phase ordonnée. Il y a tout même des différences importantes au niveau des exposants de vieillissement et des fonctions d'échelle, qui sont en général différents de leur homologue de volume. Une raison pour laquelle l'étude numérique d'une cinétique de domaines dans la phase ordonnée proche d'une surface est difficile provient du fait qu'il y a des effets de temps fini très forts, qui peuvent cacher le vrai comportement d'échelle.

Schlußfolgerungen

Das Thema dieser Dissertation waren Systeme fern des thermischen Gleichgewichts, die Alterungsverhalten zeigen. Wir haben mehrere Ergebnisse zu den folgenden Aspekten dieses Themengebietes beigetragen:

- (1) Das Problem einer allgemeinen Beschreibung von Nichtgleichgewichtssystemen mit beliebigem dynamischen Exponenten z unter Zuhilfenahme dynamischer Symmetrien.
- (2) Das Alterungsverhalten von Systemen ohne detailliertes Gleichgewicht und die Unterschiede, die in diesen Systemen im Vergleich zu magnetischen Systemen auftreten.
- (3) Die Änderung des Nichtgleichgewichtverhaltens des Systems wenn eine Oberfläche eingefügt wird.

Im Folgenden fassen wir die Ergebnisse zu jedem dieser Punkte zusammen.

(1) Gegenwärtig existiert noch keine allgemeine Theorie zur Beschreibung von Nichtgleichgewichtssystemen. In Analogie zur Beschreibung von zweidimensionalen kritischen Phänomenen im Gleichgewicht wurde von Henkel [109] 2002 vorgeschlagen, lokale Erweiterungen von dynamischem Skalenverhalten zu betrachten, was zu einer ersten Formulierung einer Theorie lokaler Skaleninvarianzen (LSI) führte. Für den Fall $z = 2$ wurde diese Theorie weiterentwickelt, so daß sie auch verrauschte System beschreibt [192]. In dieser Arbeit haben wir diese Theorie auf beliebige Werte von z erweitert. Dies erfolgt durch den gleichen Zugang wie von Henkel vorgeschlagen, aber mit einer modifizierten Konstruktion der Massenterme der infinitesimalen Erzeuger von LSI, die eine neue Art von fraktionaler Ableitung ∇_r^α verwendet. Durch rein algebraische Argumente erhielten wir Operatoren, die als Symmetrieoperatoren für bestimmte (lineare) *deterministische* dynamische Gleichungen wirken. Durch die Einführung der neuen fraktionalen Ableitung ∇_r^α gelang es einerseits, Querverbindungen zu integrablen Systemen aufzuzeigen, andererseits, eine Verallgemeinerung der sogenannten Bargmannschen Überauswahlregel abzuleiten. Dies wiederum erlaubte es uns die Überlegungen von Picone et.al [192] zu verallgemeinern, welche Erwartungswerte der verrauschten Theorie auf Ausdrücke reduziert, die mit Hilfe der Symmetrien des deterministischen Anteils der Theorie bestimmt werden können. Auf diese Weise wurden konkrete Ausdrücke für die Antwort- und Korrelationsfunktionen abgeleitet. Diese beiden Funktionen sind besonders interessant, da sie in vielen Situationen ein relativ einfaches Skalenverhalten zeigen, welches die Einführung von *Alterungsexponenten* und *Skalenfunktionen* erlaubt. Sie charakterisieren die Universalitätsklasse des Systems und LSI reproduziert die Skalenformen korrekt, obwohl die Alterungsexponenten in diesem Zugang als unbestimmte Parameter verbleiben.

Die erhaltenen Vorhersagen wurden gründlich mit konkreten Modellen verglichen. Dabei haben wir zunächst einige exakt lösbare Modelle untersucht, die durch lineare Langevingleichungen beschrieben werden, wie das sphärische Modell mit langreichweitigen Wechselwirkungen oder mit erhaltenem Ordnungsparameter oder das Mullins-Herring Modell für Oberflächenwachstum, für die perfekte Übereinstimmung mit LSI gefunden wurde. Andererseits wurden die Vorhersagen verglichen mit numerischen Ergebnissen im verdünnten Isingmodell, das in die geordnete Phase abgeschreckt wurde (wo $z > 2$). Auch hier wurde eine gute Übereinstimmung erzielt. Dies legt nahe, daß die Voraussetzungen für LSI auch in stark nichtlinearen Systemen erfüllt sein könnte, so daß die Theorie auch auf eine sehr viel größere Klasse von Modellen als der hier betrachteten anwendbar sein könnte. Uns ist keine andere allgemeine Theorie für Phasenordnungskinetik bekannt, die eine solch gute Übereinstimmung liefert. Es sei aber an dieser Stelle angemerkt, daß die Gültigkeit von LSI für nichtlineare Theorien noch nicht streng bewiesen ist. Nur für den Fall $z = 2$ (siehe Punkt **(2)**) wurde ein erster Schritt hin zur Beschreibung von nichtlinearen Theorien bereits vollzogen [17].

Eine andere interessante Art von physikalischen Systemen, in dem Alterungsphänomene noch kaum betrachtet wurden, sind Oberflächenwachstumsmodelle. Als einen ersten Schritt betrachteten wir nur die linearisierten Modelle wie das Edward-Wilkinson Modell oder das Mullins-Herring Modell. Die eigentliche Herausforderung auf diesem Gebiet ist jedoch die **Kardar-Parisi-Zhang** Gleichung [141] (KPZ-Gleichung), welche eine zusätzliche, recht komplizierte Nichtlinearität aufweist. Wir hoffen, daß LSI hier in Zukunft nützlich werden könnte.

(2) Um mehr über das Alterungsverhalten von Systemen ohne detailliertes Gleichgewicht zu erfahren, betrachteten wir mehrere Reaktions-Diffusionssysteme genauer. Die Motivation hierfür waren numerische Ergebnisse von Enss et.al. [80] und Ramasco et.al. [203] im fermionischen Kontaktprozess, einem Repräsentanten der paradigmatischen Universalitätsklasse der gerichteten Perkolation. Diese Ergebnisse zeigen, daß für die Selbstantwort $R(t, s)$ und die zusammenhängende Autokorrelationsfunktion $G(t, s)$ die Skalenformen

$$R(t, s) = s^{-a-1} f_R \left(\frac{t}{s} \right), \quad G(t, s) = s^{-b} f_G \left(\frac{t}{s} \right)$$

$$f_R(y) \stackrel{y \rightarrow \infty}{\sim} y^{-\lambda_R/z}, \quad f_G(y) \stackrel{y \rightarrow \infty}{\sim} y^{-\lambda_G/z}$$

gültig sind, analog zu den bekannten von magnetischen Systemen. Für die gerichtete Perkolation wurde die Beziehung $b = a + 1$ gefunden, während für kritische Magneten $a = b$ gilt. Dies hat zum Beispiel Auswirkungen auf die Definition eines Fluktuations-Dissipationsverhältnisses (FDR), da die Eigenschaft $a = b$ notwendig ist, um eine nicht-triviale Größe im Limes zu erhalten wenn erst $t \rightarrow \infty$, dann $s \rightarrow \infty$. Es wurde bereits von Enss et. al. vorgeschlagen, die Größe $\Xi(t, s) = R(t, s)/G(t, s)$ statt des normalerweise verwendeten FDR zu benutzen.

Wir haben die Universalitätsklasse der gerichteten Perkolation unter Verwendung der feldtheoretischen dynamischen Renormierungsgruppe untersucht. Dabei wurde die Gleichung $b = a + 1$ bestätigt und es wurde gezeigt, daß dies eine direkte Konsequenz der sogenannten Rapiditäts-Inversions-Symmetrie ist, die eine spezielle Symmetrie des

fermionischen Kontaktprozesses darstellt. Es wurde auch die Gleichung $\lambda_G = \lambda_R = z + z\delta + d$ abgeleitet, wobei der kritische Exponent δ durch das Langzeitverhalten der Überlebenswahrscheinlichkeit $P(t) \sim t^{-\delta}$ definiert ist. Weiterhin wurde eine konkrete Interpretation der Größe $\Xi^{-1}(t, s) + 1$ vorgeschlagen: Sie mißt den Abstand des Systems von seinem stationären Zustand, in Analogie zu dem gewöhnlichen Fluktuations-Dissipationsverhältnis $X(t, s)$. Wir haben auch die den konkreten Wert von $\Xi(t, s)$ zur ersten Ordnung in der Epsilon-Entwicklung berechnet und fanden eine gute Übereinstimmung mit numerischen Ergebnissen.

Andererseits bemerkten wir, daß die Selbstantwort in der ersten Ordnung in $\epsilon = 4 - d$ nicht mit den LSI-Vorhersagen übereinstimmt. Ein vermutlicher Grund hierfür ist die Tatsache, daß in diesem System der Erwartungswert des Ordnungsparameters nicht verschwindet, während LSI in seiner aktuellen Formulierung einen verschwindenden Erwartungswert erfordert.

Zwei Reaktions-Diffusionssysteme vollkommen anderen Typs wurden auch untersucht. Der bosonische diffusive Kontaktprozess (BCPD) und der bosonische diffusive Paarkontaktprozess (BPCPD). In diesen Systemen kann sich eine beliebige Anzahl von Teilchen auf einem Gitterplatz aufhalten. Im BCPD tritt Skalenverhalten mit $a = b$ auf, falls die Teilchenerzeugungs- und die Teilchenvernichtungsprozesse sich gerade ausgleichen. Im BPCPD ist die Situation komplizierter: Falls Erzeugungs- und Vernichtungsprozesse gleich stark sind, kann das Modell exakt gelöst werden. Für $d \leq 2$ findet man ebenfalls kein Skalenverhalten. Für $d > 2$ und falls die Diffusion der dominante Prozess im Vergleich zu den Reaktionen ist, verhält sich das Modell so wie der BCPD. Falls aber die Reaktionsprozesse stärker sind als die Diffusion, findet man kein Skalenverhalten. Zwischen diesen beiden Bereichen befindet sich ein multikritischer Punkt, der einem Clusterübergang entspricht, an dem wieder Skalenverhalten mit $a \neq b$ auftritt. Wir fanden hier aber *nicht* die Beziehung $b = a + 1$, die in der gerichteten Perkolation auftrat. Dies ist nicht nur ein weiterer Beleg dafür, daß in Reaktion-Diffusionssystemen die Gleichheit $a = b$ im Allgemeinen nicht gilt, sondern zeigt auch, daß es keine offensichtliche simple Beziehung zwischen a und b gibt.

Schließlich wurde die existierende Version von LSI für den Fall $z = 2$ an diese beiden bosonischen Systeme angepasst. Diese erweiterte Version von LSI beinhaltet auch bestimmte nichtlineare Modelle. Diese Arbeit basierte auf Vorarbeiten über nichtlineare Schrödingergleichungen von Stoimenov et. al. [222] von 2005.

(3) Schließlich betrachteten wir Alterungsphänomene nahe der Oberfläche eines halbumendlichen Systems. Dies stellt einen ersten Schritt in Richtung realistischerer Systeme dar, da jedes reale physikalische System Oberflächen, Kanten und Ecken besitzt. Das Verständnis dieser Art von Systemen ist die Voraussetzung für das Verständnis der Dynamik in komplizierteren Geometrien. Hier könnte man an keilförmige Geometrien oder scharfe Spitzen denken. Einerseits sind über die Statik solcher Systeme schon einige Dinge bekannt, andererseits kommt diese Art von System experimentellen Systemen schon relativ nahe, vor allem in dünnen Schichten oder für Nanoobjecte.

Für den Fall der kritischen Dynamik konnten wir zwei exakt lösbare Modelle zu den bereits existierenden Lösungen hinzufügen: Das halbumendliche sphärische Modell und das Ising-

modell für hohe Dimensionen. In beiden Fällen wurden Oberflächen-Alterungsexponenten, Oberflächen-Skalenfunktionen und das Oberflächen Fluktuations-Dissipationsverhältnis wurden exakt berechnet. Die Ergebnisse paßten in das allgemeine Skalenverhalten, das in früheren Arbeiten gefunden wurde und das stark dem gewöhnlichen Skalenverhalten in translationsinvarianten Systemen ähnelt. Auch bereits bekannte Skalenbeziehungen zwischen den kritischen Exponenten wurden bestätigt.

Wir betrachteten auch den Fall von Phasenordnungskinetik nahe einer Oberfläche. Die Lösung des sphärischen Modells ergibt, daß der Alterungsexponent b_1 für Dirichletrandbedingungen nicht verschwindet, im Gegensatz zu der Situation, die man im Volumen vorfindet, wo der entsprechende Volumenexponent Null ist. Dieses Ergebnis erhielten wir auch in einer modifizierten version des $O(N)$ Modells. Um diesen Punkt zu klären, wurden auch noch andere Modelle betrachtet, zum Beispiel eine Verallgemeinerung eines Ansatzes von Bray und Humayun. Zusätzlich wurden Simulationen im zweidimensionalen Isingmodell durchgeführt. Die Ergebnisse zeigen klar, daß auch in halbunendlichen Systemen $b_1 = 0$ gilt, was dafür spricht, daß das Ergebnis im sphärischen Modell und im modifizierten $O(N)$ Modell eher als unphysikalische Besonderheiten dieser simplen Modelle betrachtet werden sollten.

Auf diese Weise konnte ein recht komplettes Bild über das Nichtgleichgewichtsverhalten an Oberflächen von halbunendlichen Systemen erstellt werden. Das allgemeine Skalenverhalten ist dem Skalenverhalten im Volumen sehr ähnlich, sowohl im Falle von kritischer Dynamik als auch für den Fall von Phasenordnungskinetik. Allerdings sind einige Alterungsexponenten und Skalenfunktionen verschieden von den entsprechenden Volumensystemen. Numerische Untersuchungen von Phasenordnungsphänomenen werden durch sehr starke Effekte endlicher Zeit erschwert, die das eigentliche Skalenverhalten überlagern.

Chapter 7

Appendices

A On fractional derivatives

This appendix is taken from [21]. We discuss the fractional derivative $\nabla_{\mathbf{r}}^{\alpha}$, applied on functions $f : \mathbb{R}^d \rightarrow \mathbb{C}$. To this end we use the Fourier representation of $f \in L^1(\mathbb{R}^d)$:

$$f(\mathbf{r}) = \int_{\mathbb{R}^d} \frac{d\mathbf{k}}{(2\pi)^d} e^{i\mathbf{r}\cdot\mathbf{k}} \widehat{f}(\mathbf{k}), \quad \widehat{f}(\mathbf{k}) = \int_{\mathbb{R}^d} d\mathbf{r} e^{-i\mathbf{r}\cdot\mathbf{k}} f(\mathbf{r}) \quad (\text{A.1})$$

with $\mathbf{r} = (r_1, \dots, r_d)$ and $\mathbf{k} = (k_1, \dots, k_d)$. We can then define $\nabla_{\mathbf{r}}^{\alpha}$ as a pseudodifferential operator.

Definition: *The action of the operator $\nabla_{\mathbf{r}}^{\alpha}$ with $\alpha \in \mathbb{R}$ on the function (A.1) is defined as*

$$\nabla_{\mathbf{r}}^{\alpha} f(\mathbf{r}) := i^{\alpha} \int_{\mathbb{R}^d} \frac{d\mathbf{k}}{(2\pi)^d} |\mathbf{k}|^{\alpha} e^{i\mathbf{r}\cdot\mathbf{k}} \widehat{f}(\mathbf{k}) \quad (\text{A.2})$$

where the righthand side of (A.2) is to be understood in a distributional sense [92].

With this definition at hand let us first give a simple example. We consider the case when $\nabla_{\mathbf{r}}^{\alpha}$ is applied to the function $f(\mathbf{r}) = \exp(i\mathbf{q} \cdot \mathbf{r})$ for a constant vector $\mathbf{q} \in \mathbb{R}^d$. Using the definition, we obtain

$$\nabla_{\mathbf{r}}^{\alpha} \exp(i\mathbf{q} \cdot \mathbf{r}) = i^{\alpha} \int_{\mathbb{R}^d} \frac{d\mathbf{k}}{(2\pi)^d} |\mathbf{k}|^{\alpha} \exp(i\mathbf{r} \cdot \mathbf{k}) \int_{\mathbb{R}^d} d\mathbf{s} \exp(-i\mathbf{s} \cdot \mathbf{k}) \exp(i\mathbf{q} \cdot \mathbf{s}) \quad (\text{A.3})$$

The inner integral gives $(2\pi)^d \delta(\mathbf{q} - \mathbf{k})$. Therefore

$$\nabla_{\mathbf{r}}^{\alpha} \exp(i\mathbf{q} \cdot \mathbf{r}) = i^{\alpha} |\mathbf{q}|^{\alpha} \exp(i\mathbf{q} \cdot \mathbf{r}) \quad (\text{A.4})$$

The exponential function is thus an eigenfunction of $\nabla_{\mathbf{r}}^{\alpha}$. Similar statements are true for $\sin(\mathbf{q} \cdot \mathbf{r})$ and $\cos(\mathbf{q} \cdot \mathbf{r})$:

$$\nabla_{\mathbf{r}}^{\alpha} \cos(\mathbf{q} \cdot \mathbf{r}) = i^{\alpha} |\mathbf{q}|^{\alpha} \cos(\mathbf{q} \cdot \mathbf{r}), \quad \nabla_{\mathbf{r}}^{\alpha} \sin(\mathbf{q} \cdot \mathbf{r}) = i^{\alpha} |\mathbf{q}|^{\alpha} \sin(\mathbf{q} \cdot \mathbf{r}) \quad (\text{A.5})$$

These results suggest that $\nabla_{\mathbf{r}}^{\alpha}$ might be viewed as a generalized Laplace operator to which it reduces for $\alpha = 2$, rather than a ‘true’ fractional derivative. The main calculational rules are as follows:

Lemma A1: *The linear operator $\nabla_{\mathbf{r}}^\alpha$ has the following properties*

$$\text{i.) } \nabla_{\mathbf{r}}^\alpha \nabla_{\mathbf{r}}^\beta = \nabla_{\mathbf{r}}^{\alpha+\beta} \quad (\text{A.6})$$

$$\text{ii.) } \sum_{i=1}^d \partial_{r_i}^2 = \nabla_{\mathbf{r}}^2 = \Delta_{\mathbf{r}} \quad (\text{A.7})$$

$$\text{iii.) } [\nabla_{\mathbf{r}}^\alpha, r_i] = \alpha \partial_{r_i} \nabla_{\mathbf{r}}^{\alpha-2} \quad (\text{A.8})$$

$$\text{iv.) } [\nabla_{\mathbf{r}}^\alpha, \mathbf{r}^2] = 2\alpha(\mathbf{r} \cdot \partial_{\mathbf{r}}) \nabla_{\mathbf{r}}^{\alpha-2} + \alpha(\alpha - 2 + d) \nabla_{\mathbf{r}}^{\alpha-2} \quad (\text{A.9})$$

$$\text{v.) } \nabla_{\mu\mathbf{r}}^\alpha f(\mu\mathbf{r}) = |\mu|^{-\alpha} \nabla_{\mathbf{r}}^\alpha f(\mu\mathbf{r}) \quad (\text{A.10})$$

$$\text{vi.) } \nabla_{\mu\mathbf{r}}^\alpha f(\mathbf{r}) = |\mu|^{-\alpha} \nabla_{\mathbf{r}}^\alpha f(\mathbf{r}) \quad (\text{A.11})$$

where $\Delta_{\mathbf{r}}$ is the Laplacian with respect to \mathbf{r} . We also use the shorthand $\mathbf{r} \cdot \partial_{\mathbf{r}} := \sum_{i=1}^d r_i \partial_{r_i}$ and $\partial_{r_i} = \frac{\partial}{\partial r_i}$ denotes the usual partial derivative into the i -th direction.

Proof:

i.) Let f be a function $\mathbb{R}^d \rightarrow \mathbb{C}$. Then according to the definition (A.2) $g(\mathbf{r}) := \nabla_{\mathbf{r}}^\beta f(\mathbf{r}) = i^\beta \int \frac{d\mathbf{k}}{(2\pi)^d} |\mathbf{k}|^\beta e^{i\mathbf{r} \cdot \mathbf{k}} \widehat{f}(\mathbf{k})$ and the Fourier transform of g is given by

$$\widehat{g}(\mathbf{k}) = i^\beta |\mathbf{k}|^\beta \widehat{f}(\mathbf{k}) \quad (\text{A.12})$$

Therefore, applying $\nabla_{\mathbf{r}}^\alpha$ on $g(\mathbf{r})$ we have

$$\nabla_{\mathbf{r}}^\alpha \cdot \nabla_{\mathbf{r}}^\beta f(\mathbf{r}) = i^{\alpha+\beta} \int_{\mathbb{R}^d} \frac{d\mathbf{k}}{(2\pi)^d} |\mathbf{k}|^{\alpha+\beta} e^{i\mathbf{r} \cdot \mathbf{k}} \widehat{f}(\mathbf{k}) = \nabla_{\mathbf{r}}^{\alpha+\beta} f(\mathbf{r}) \quad (\text{A.13})$$

ii.) follows trivially by applying the ordinary partial derivative to the Fourier representation (A.1) of a function f .

iii.) We prove this first for the case when $\alpha \notin \mathbb{Z}$. Let again f be a function $\mathbb{R}^d \rightarrow \mathbb{C}$. Denote also $g(\mathbf{r}) := r_i f(\mathbf{r})$. Then we find

$$\begin{aligned} \nabla_{\mathbf{r}}^\alpha r_i f(\mathbf{r}) &= i^\alpha \int_{\mathbb{R}^d} \frac{d\mathbf{k}}{(2\pi)^d} |\mathbf{k}|^\alpha \widehat{g}(\mathbf{k}) e^{i\mathbf{r} \cdot \mathbf{k}} \\ &= i^\alpha \int_{\mathbb{R}^d} \frac{d\mathbf{k}}{(2\pi)^d} |\mathbf{k}|^\alpha \int_{\mathbb{R}^d} d\mathbf{r}' r'_i f(\mathbf{r}') e^{i(\mathbf{r}-\mathbf{r}') \cdot \mathbf{k}} \end{aligned} \quad (\text{A.14})$$

At this point we use the following formula from [92] (p. 363, formula 4), which holds for $\frac{1}{2}(\alpha + d) \notin -\mathbb{N}$.

$$\int_{\mathbb{R}^d} d\mathbf{k} e^{-i\mathbf{r} \cdot \mathbf{k}} |\mathbf{k}|^\alpha = 2^{\alpha+d} \pi^{\frac{d}{2}} \frac{\Gamma((\alpha + d)/2)}{\Gamma(-\alpha/2)} |\mathbf{k}|^{-\alpha-d} \quad (\text{A.15})$$

and compute the left-hand side of (A.8)

$$\begin{aligned} [\nabla_{\mathbf{r}}^\alpha, r_i] f(\mathbf{r}) &= i^\alpha \int_{\mathbb{R}^d} d\mathbf{r}' (r'_i - r_i) f(\mathbf{r}') \int_{\mathbb{R}^d} \frac{d\mathbf{k}}{(2\pi)^d} |\mathbf{k}|^\alpha e^{i(\mathbf{r}-\mathbf{r}') \cdot \mathbf{k}} \\ &= 2^{\alpha+d} i^\alpha \pi^{\frac{d}{2}} \left(\frac{\Gamma((d + \alpha)/2)}{\Gamma(-\alpha/2)} \right) \int_{\mathbb{R}^d} d\mathbf{r}' f(\mathbf{r}') (r'_i - r_i) |\mathbf{r} - \mathbf{r}'|^{-\alpha-d} \end{aligned} \quad (\text{A.16})$$

On the other hand, the right-hand side of (A.8) gives

$$\begin{aligned} \alpha \partial_{r_i} \nabla_{\mathbf{r}}^{\alpha-2} f(\mathbf{r}) &= i^{\alpha-2} \alpha \partial_{r_i} \left(\int_{\mathbb{R}^d} d\mathbf{r}' f(\mathbf{r}') \int_{\mathbb{R}^d} \frac{d\mathbf{k}}{(2\pi)^d} |\mathbf{k}|^{\alpha-2} e^{i(\mathbf{r}-\mathbf{r}')\cdot\mathbf{k}} \right) \quad (\text{A.17}) \\ &= \alpha i^{\alpha-2} \left(2^{\alpha+d-2} \pi^{\frac{d}{2}} \frac{\Gamma((d+\alpha-2)/2)}{\Gamma(-(\alpha-2)/2)} \right) \partial_{r_i} \int_{\mathbb{R}^d} d\mathbf{r}' f(\mathbf{r}') |\mathbf{r}-\mathbf{r}'|^{-\alpha-d+2} \end{aligned}$$

Recall that for an arbitrary $\kappa \in \mathbb{R}$ the formula

$$\partial_{r_i} |\mathbf{r}-\mathbf{r}'|^{\kappa} = \kappa (r_i - r'_i) |\mathbf{r}-\mathbf{r}'|^{\kappa-2} \quad (\text{A.18})$$

holds true. It follows that (A.16) is equal to (A.17)

It remains to do the cases when $\alpha \in \mathbb{Z}$. As a matter of fact, it suffices to look at the three cases $\alpha \in \{-1, 0, 1\}$, as all the others follow then by induction with the help of property (A.6). The case $\alpha = 0$ is trivial and for the case $\alpha = 1$ the above argument goes through, as formula (A.15) still holds. The case $\alpha = -1$ can be obtained with the help of property (A.6) and the fact that we have already proven the claim for $\alpha \notin \mathbb{Z}$:

$$[\nabla_{\mathbf{r}}^{-1}, r_i] = \nabla_{\mathbf{r}}^{-1/2} [\nabla_{\mathbf{r}}^{-1/2}, r_i] + [\nabla_{\mathbf{r}}^{-1/2}, r_i] \nabla_{\mathbf{r}}^{-1/2} = -\partial_{r_i} \nabla_{\mathbf{r}}^{-3}. \quad (\text{A.19})$$

This completes the proof of property (A.8).

iv.) Using iii.), a straightforward evaluation of commutators gives the expression

$$[\nabla_{\mathbf{r}}^{\alpha}, r_i^2] = 2\alpha r_i \partial_{r_i} \nabla_{\mathbf{r}}^{\alpha-2} + \alpha(\alpha-2) \partial_{r_i}^2 \nabla_{\mathbf{r}}^{\alpha-4} + \alpha \nabla_{\mathbf{r}}^{\alpha-2} \quad (\text{A.20})$$

from which expression (A.9) follows immediately.

v.) We first write

$$\nabla_{\mu\mathbf{r}}^{\alpha} f(\mu\mathbf{r}) = (2\pi)^{-d} \int_{\mathbb{R}^d} d\mathbf{k} (i|\mathbf{k}|)^{\alpha} e^{i\mu\mathbf{r}\cdot\mathbf{k}} \int_{\mathbb{R}^d} d\mathbf{s} e^{-i\mathbf{k}\cdot\mathbf{s}} f(\mathbf{s}) \quad (\text{A.21})$$

Now one can transform this by rescaling the integration variables as $\mathbf{k} \rightarrow \mathbf{k}' = \mu\mathbf{k}$ and $\mathbf{s} \rightarrow \mathbf{s}' = \mu^{-1}\mathbf{s}$. This yields

$$\nabla_{\mu\mathbf{r}}^{\alpha} f(\mu\mathbf{r}) = (2\pi)^{-d} |\mu|^{-\alpha} \int_{\mathbb{R}^d} d\mathbf{s} f(\mu\mathbf{s}) \int_{\mathbb{R}^d} d\mathbf{k} (i\mathbf{k})^{\alpha} e^{i\mathbf{k}'\cdot(\mathbf{r}-\mathbf{s})} \quad (\text{A.22})$$

In the same way, one shows that the righthandside of (A.10) equals this expression, so that the equality is proven.

vi.) Follows from (A.10) as

$$\nabla_{\mu\mathbf{r}}^{\alpha} f(\mathbf{r}) = \nabla_{\boldsymbol{\rho}}^{\alpha} f(\mu^{-1}\boldsymbol{\rho}) = |\mu|^{-\alpha} \nabla_{\mu^{-1}\boldsymbol{\rho}}^{\alpha} f(\mu^{-1}\boldsymbol{\rho}) = |\mu|^{-\alpha} \nabla_{\mathbf{r}}^{\alpha} f(\mathbf{r}) \quad (\text{A.23})$$

q.e.d.

Before we proceed, let us compare the definition of $\nabla_{\mathbf{r}}^{\alpha}$ to other kinds of fractional derivatives which are known from the literature. We will restrict to the case $d = 1$ for simplicity.

- One of the most commonly used definitions is the Riemann-Liouville/Grünwald-Letnikov/Marchaud fractional derivative ${}_0D_r^\alpha$, see [211, 200, 174] for details. If e is *not* a negative integer, Hadamard gave the following definition

$${}_0D_r^\alpha r^e = \frac{\Gamma(e+1)}{\Gamma(e-\alpha+1)} r^{e-\alpha} \quad (\text{A.24})$$

The derivative of any function $f(r) = \sum_e f_e r^e$ is then found from the assumed linearity of ${}_0D_r^\alpha$. In particular, this reduces to the normal derivative d^n/dr^n when α is a positive integer n

$${}_0D_r^n f(r) = \frac{d^n}{dr^n} f(r) \quad \text{for } n \in \mathbb{N}. \quad (\text{A.25})$$

On the other hand, the exponential function is no longer an eigenfunction of ${}_0D_r^\alpha$ for generic α and one rather has the more complicated form [174]

$${}_0D_r^\alpha \exp(r) = r^{-\alpha} E_{1,1-\alpha}(r), \quad \text{with } E_{\eta,\delta}(r) := \sum_{k=0}^{\infty} \frac{z^k}{\Gamma(\eta k + \delta)} \quad (\text{A.26})$$

The Riemann-Liouville fractional derivative has the drawback that the property (A.6) does not hold true in general.

- The Riemann-Liouville derivative can be extended in a distributional sense such that the composition law (A.6) holds true [92, 109], along with several other handy formulæ such as a generalised Leibniz rule [109]. In consequence, the consideration of *sequential* fractional derivatives as required for the Riemann-Liouville derivative [174] is unnecessary. On the other hand, eq. (A.26) remains true if $\alpha \notin \mathbb{N}$ for the non-singular (non-distributional) part of this fractional derivative. This definition of a fractional derivative was used for the ‘old’ formulation of LSI.
- The Weyl fractional derivative W_r^α [174] does satisfy the composition law (A.6). It has the further nice property that the exponential function is an eigenfunction of W_r^α since

$$W_r^\alpha \exp(iqr) = i^\alpha q^\alpha \exp(iqr) \quad (\text{A.27})$$

but with respect to (A.4) there is no absolute value taken on q^α . It follows directly that [174]

$$W_r^\alpha \cos(qr) = q^\alpha \cos\left(qr - \frac{1}{2}\pi\alpha\right) \quad (\text{A.28})$$

which is quite distinct from (A.5).

- In [237] the following definition was used

$$\mathfrak{D}_r^\alpha f(\mathbf{r}) := \int_{\mathbb{R}^d} \frac{d\mathbf{k}}{(2\pi)^d} (i\mathbf{k})^\alpha e^{i\mathbf{r}\cdot\mathbf{k}} \widehat{f}(\mathbf{k}) \quad (\text{A.29})$$

which corresponds to our definition (A.2) but *without* the absolute values. It can be shown that both properties (A.6) and (A.25) hold true and furthermore, eqs. (A.27) and (A.28) remain valid, up to some prefactor [237]. This shows the importance of the absolute values in our definition (A.2).

This short review of some of the properties of several inequivalent fractional derivatives taken from the literature shows that the fractional derivative given in (A.2) is distinct to all of them. Apparently the absolute values in our definition (A.2) are essential for its distinct properties.

As we have shown, the property (A.6) holds for $\nabla_{\mathbf{r}}^\alpha$. We have however partially sacrificed property (A.25), which only holds for even n for $\nabla_{\mathbf{r}}^n$ (in $d = 1$). This is of course also a consequence of the absolute values used in the definition. The operator $\nabla_{\mathbf{r}}^\alpha$ should therefore be viewed as a generalisation of the Laplace operator $\nabla_{\mathbf{r}}^2 = \sum_{i=1}^d \partial_{r_i}^2$ rather than of the simple partial derivative.

Interestingly, we have (at least in one dimension) a kind of Cauchy formula for this derivative. More precisely:

Lemma A2: *For $d = 1$ and $\alpha \neq -1, -2, \dots$ and a holomorphic function $f(z)$, we have the following formula*

$$\nabla_z^\alpha f(z) = \frac{\Gamma(\alpha + 1)}{2\pi i} \oint_{C_z} dw \frac{f(w)}{(w - z)^{\alpha+1}} \tag{A.30}$$

where C_z is a contour containing z .

Proof: We first write the function $f(z)$ with the help of Cauchy's theorem as $f(z) = \frac{1}{2\pi i} \oint_{C_z} dw \frac{f(w)}{w - z}$, and apply then the definition of ∇_z^α . This yields

$$\nabla_z^\alpha f(z) = \frac{1}{4\pi^2 i} \oint_{C_z} dw f(w) \int_{\mathbb{R}} dy \frac{1}{w - y} \int_{\mathbb{R}} dk (i|k|)^\alpha e^{ik(z-y)} \tag{A.31}$$

The inner integral can be found in [92], so that we obtain finally

$$\nabla_z^\alpha f(z) = \frac{i^{\alpha-1} \sin(\pi\alpha/2)\Gamma(\alpha + 1)}{2\pi^2} \oint_{C_z} dw f(w) \int_{\mathbb{R}} dy \frac{1}{w - y} \frac{1}{|z - y|^{\alpha+1}} \tag{A.32}$$

We denote the integral over y by J and write it as a sum of two integrals in order to get rid of the absolute values

$$\begin{aligned} J &= \int_{\mathbb{R}} dy \frac{1}{w - y} \frac{1}{|z - y|^{\alpha+1}} \\ &= \int_{-\infty}^z dy \frac{1}{w - y} \frac{1}{(z - y)^{\alpha+1}} + \int_z^\infty dy \frac{1}{w - y} \frac{1}{(y - z)^{\alpha+1}} \end{aligned} \tag{A.33}$$

now the two integrals can be rewritten by a few standard integral transforms into

$$J = -2(w - z)^{-\alpha-1} \int_0^\infty du \frac{u^{-\alpha-1}}{u^2 - 1} \tag{A.34}$$

The principal value of this integral exists if $\alpha \in (-2, 0)$. The last step of the proof is to compute this integral, which we do in the following Proposition:

Proposition A1: If $\alpha \in (-2, 0)$ and $\beta \in \mathbb{R}$, one has

$$\int_0^\infty du \frac{u^{-\alpha-1}}{u^2 + \beta^2} = -\frac{\pi}{2} \frac{1}{\sin(\pi\alpha/2)} \beta^{-\alpha-2} \quad (\text{A.35})$$

This function is analytical in α and β , therefore one can continue it analytically provided one does not run over a singularity. In particular we can take the limit $\beta \rightarrow i$.

Proof of the proposition: We consider the following expression

$$J = \oint_C dz \frac{z^{-\alpha-1}}{z^2 + \beta^2} \quad (\text{A.36})$$

C denotes the contour shown in figure A.1, consisting of a small circle (radius r) and a big circle (radius R) around the origin, which are connected by straight lines along the positive real axis. We can then write J as

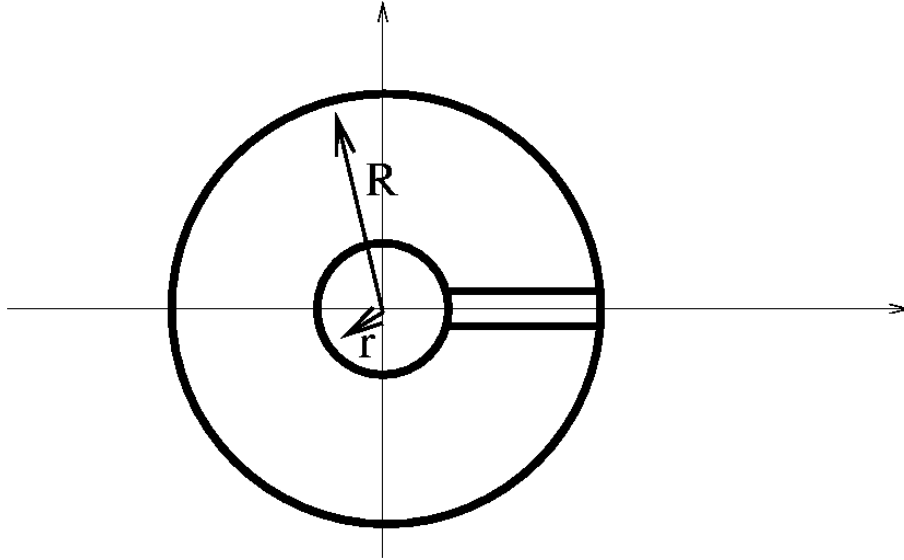


Figure A.1: Contour used for the integration in the proof of the proposition.

$$J = J_R + J_r + \int_0^\infty du \frac{u^{-\alpha-1}}{u^2 + \beta^2} + \int_0^\infty du \frac{(ue^{2\pi i})^{-\alpha-1}}{u^2 + \beta^2} \quad (\text{A.37})$$

where J_R and J_r denote the contributions of the two arcs. Then it is straightforward to show that the contribution of these two arcs vanishes for $R \rightarrow \infty$ and $r \rightarrow 0$ as

$$|J_R| \leq \text{const} \times R^{-\alpha-2}, \quad \text{and} \quad |J_r| \leq \text{const} \times r^{-\alpha} \quad (\text{A.38})$$

Therefore, in the limit $R \rightarrow \infty$ and $r \rightarrow 0$, we get

$$J = \int_0^\infty du \frac{u^{-\alpha-1}}{u^2 + \beta^2} (1 - e^{-2\pi i(\alpha+1)}) \quad (\text{A.39})$$

On the other hand the residue theorem yields that

$$J = 2\pi i \left(\frac{\beta^{-\alpha-1} e^{i\pi/2(-\alpha-1)}}{2\beta e^{i\pi/2}} + \frac{\beta^{-\alpha-1} e^{3\pi i/2(-\alpha-1)}}{2\beta e^{3\pi i/2}} \right) \quad (\text{A.40})$$

Therefore, from equating (A.39) and (A.40), we get the result of the lemma. q.e.d.

B Generalised representations of the ageing algebras for semi-linear Schrödinger equations

This appendix is taken from [17]. We discuss the Schrödinger-invariance of semi-linear Schrödinger equations of the form (4.154) and especially with non-linearities of the form (4.155). With respect to the well-known Schrödinger-invariance of the linear Schrödinger equation, the main difference comes from the presence of a dimensionful coupling constant g of the non-linear term.

It is enough to consider explicitly the one-dimensional case which simplifies the notation. In one spatial dimension, the Schrödinger algebra \mathfrak{sch}_1 is spanned by the following generators

$$\mathfrak{sch}_1 = \langle X_{-1}, X_0, X_1, Y_{-1/2}, Y_{1/2}, M_0 \rangle \tag{B.1}$$

while its subalgebra \mathfrak{age}_1 is spanned by

$$\mathfrak{age}_1 = \langle X_0, X_1, Y_{-1/2}, Y_{1/2}, M_0 \rangle \tag{B.2}$$

These generators for $g = 0$ are listed explicitly in eq. (4.117) and the non-vanishing commutators can be written compactly

$$\begin{aligned} [X_n, X_{n'}] &= (n - n')X_{n+n'} \\ [X_n, Y_m] &= (n/2 - m)Y_{n+m} \\ [Y_{\frac{1}{2}}, Y_{-\frac{1}{2}}] &= M_0 \end{aligned} \tag{B.3}$$

where $n, n' \in \{\pm 1, 0\}$ and $m \in \{\pm \frac{1}{2}\}$ (see [109] for generalizations to $d > 1$).

Following the procedure given in [222, 223], we now construct new representations of \mathfrak{age}_1 and of \mathfrak{sch}_1 which takes into account a dimensionful coupling g with scaling dimension \hat{y} as follows.

1. The generator of space-translations reads simply

$$Y_{-\frac{1}{2}} = -\partial_r. \tag{B.4}$$

2. The generator of scaling transformations is assumed to take the form

$$X_0 = -t\partial_t - \frac{1}{2}r\partial_r - \hat{y}g\partial_g - \frac{x}{2} \tag{B.5}$$

where \hat{y} is the scaling dimension of the coupling g .

3. For \mathfrak{sch}_1 we also keep the usual generator of time-translations

$$X_{-1} = -\partial_t. \tag{B.6}$$

4. The remaining generators we write in the most general form adding a possible g -dependence through yet unknown functions L, Q, P .

$$\begin{aligned} M_0 &= -\mathcal{M} - L(t, r, g)\partial_g \\ Y_{\frac{1}{2}} &= -t\partial_r - \mathcal{M}r - Q(t, r, g)\partial_g \\ X_1 &= -t^2\partial_t - tr\partial_r - \frac{\mathcal{M}}{2}r^2 - xt - P(t, r, g)\partial_g \end{aligned} \tag{B.7}$$

The representation given by eqs. (B.4,B.5,B.6,B.7) must satisfy the commutation relations (B.3) for \mathbf{age}_1 or \mathbf{sch}_1 . From these conditions the undetermined functions L, Q and P are derived. A straightforward but slightly longish calculation along the lines of [222] shows that for \mathbf{age}_1 , one has

$$L = 0 \quad , \quad Q = 0 \quad , \quad P = p_0(\mathcal{M}) t^{\widehat{y}+1} m(t/g) \quad (\text{B.8})$$

Here, $m(v)$ is an arbitrary differentiable function and $p_0(\mathcal{M})$ a \mathcal{M} -dependent constant. We shall use the shorthand $v = t^{\widehat{y}}/g$ in what follows.

In consequence, for \mathbf{age}_1 only the generator X_1 is modified with respect to the representation eq. (4.117) and this is described in by the function $m(v)$ and the constant $p_0(\mathcal{M})$. On the other hand, for \mathbf{sch}_1 the additional condition $[X_1, X_{-1}] = 2X_0$ leads to $p_0 = 2\widehat{y}, m(v) = v^{-1}$.

Hence, the new representations are still given by eq. (4.117) with the only exception of X_1 which reads

$$\begin{aligned} \mathbf{age}_1 \quad : \quad X_1 &= -t^2 \partial_t - tr \partial_r - p_0(\mathcal{M}) t^{\widehat{y}+1} m(t^{\widehat{y}}/g) \partial_g - \frac{\mathcal{M}r^2}{2} - xt \\ \mathbf{sch}_1 \quad : \quad X_1 &= -t^2 \partial_t - tr \partial_r - 2\widehat{y}tg \partial_g - \frac{\mathcal{M}r^2}{2} - xt \end{aligned} \quad (\text{B.9})$$

We require in addition the invariance of linear Schrödinger equation $(2\mathcal{M}\partial_t - \partial_r^2)\phi = 0$ with respect to this new representation. In terms of the Schrödinger operator \widehat{S} this means

$$[\widehat{S}, \mathcal{X}] = \lambda \widehat{S} \quad ; \quad \text{where} \quad \widehat{S} := 2M_0 X_{-1} - Y_{-1/2}^2 \quad (\text{B.10})$$

and \mathcal{X} is one of the generators of \mathbf{age}_1 eq. (B.2) or of \mathbf{sch}_1 eq. (B.1). Obviously, $\lambda = 0$ if $\mathcal{X} \in \langle X_{-1}, Y_{\pm 1/2}, M_0 \rangle$ and $\lambda = -1$ if $\mathcal{X} = X_0$. Finally, for X_1 we have from the definition of the Schrödinger operator \widehat{S}

$$\begin{aligned} [\widehat{S}, X_1] &= -4M_0 X_0 + (Y_{1/2} Y_{-1/2} + Y_{-1/2} Y_{1/2}) \\ &= -2t\widehat{S} + \mathcal{M}(1 - 2x - 4\widehat{y}g \partial_g) \end{aligned} \quad (\text{B.11})$$

where in the second line the explicit forms eqs. (B.4,B.5,B.6,B.7) were used. This also holds for all those representations of \mathbf{age}_1 for which there exists an operator $X_{-1} \notin \mathbf{age}_1$ such that $[X_1, X_{-1}] = 2X_0$ and we shall restrict our attention to those in what follows. On the other hand, the direct calculation of the same commutator with the explicit form (B.9) gives for \mathbf{age}_1

$$[\widehat{S}, X_1] = -2t\widehat{S} + \mathcal{M}(1 - 2x) - 2\mathcal{M}p_0(\mathcal{M})t^{\widehat{y}} [(\widehat{y} + 1)m(v) + \widehat{y}vm'(v)] \partial_g \quad (\text{B.12})$$

Besides $\lambda = -2t$, the consistency between these two implies for $m(v)$ the equation

$$v \left((\widehat{y} + 1)m(v) + \widehat{y}v \frac{dm(v)}{dv} \right) = \frac{2\widehat{y}}{p_0} \quad (\text{B.13})$$

with the general solution

$$m(v) = \frac{2\widehat{y}}{p_0} \frac{1}{v} + \frac{m_0}{p_0} v^{-1-1/\widehat{y}} \quad (\text{B.14})$$

where $m_0 = m_0(\mathcal{M})$ is an arbitrary constant. The larger algebra \mathfrak{sch}_1 is recovered from this if we set $p_0 = 2\hat{y}$ and $m_0 = 0$. Hence the final form for the generator X_1 in the special class of representations of the algebra \mathfrak{age}_1 defined above is

$$X_1 = -t^2\partial_t - tr\partial_r - 2\hat{y}tg\partial_g - m_0g^{1+1/\hat{y}}\partial_g - \frac{\mathcal{M}r^2}{2} - xt \tag{B.15}$$

Summarizing, this class of representations of \mathfrak{age}_1 we constructed is characterized by the triplet (x, \mathcal{M}, m_0) , whereas for \mathfrak{sch}_1 , the same triplet is $(x, \mathcal{M}, 0)$.

Finally, to make X_1 a dynamical symmetry on the solutions $\Phi = \Phi_g(t, r)$ of the Schrödinger equation $\hat{S}\Phi_g = 0$ we must impose the auxiliary condition $(1 - 2x - 4\hat{y}g\partial_g)\Phi_g = 0$ which leads to

$$\Phi_g(t, r) = g^{(1-2x)/(4\hat{y})}\Phi(t, r) \tag{B.16}$$

In particular, we see that if $x = 1/2$, we have a representation of \mathfrak{age}_1 without any further auxiliary condition.

We now look for those semi-linear Schrödinger equations of the form $\hat{S}\Phi = F(t, r, g, \Phi, \Phi^*)$ for which the representations of \mathfrak{age}_1 or \mathfrak{sch}_1 as given by eqs. (B.4,B.5,B.6,B.7) and with X_1 as in (B.15) act as a dynamical symmetry. The non-linear potential F is known to satisfy certain differential equations which can be found using standard methods, see [31],[222, eq. (2.8)]. In our case these equations read

$$X_{-1} : \partial_t F = 0 \tag{B.17}$$

$$Y_{-\frac{1}{2}} : \partial_r F = 0 \tag{B.18}$$

$$M_0 : (\Phi\partial_\Phi - \Phi^*\partial_{\Phi^*} - 1)F = 0 \tag{B.19}$$

$$Y_{\frac{1}{2}} : [t\partial_r F - \mathcal{M}r(\Phi\partial_\Phi - \Phi^*\partial_{\Phi^*} - 1)]F = 0 \tag{B.20}$$

$$X_0 : \left[t\partial_t + \frac{1}{2}r\partial_r + \hat{y}g\partial_g + 1 - \frac{x}{2}(\Phi\partial_\Phi + \Phi^*\partial_{\Phi^*} - 1) \right] F = 0 \tag{B.21}$$

$$X_1 : \left[t^2\partial_t + tr\partial_r + 2t(\hat{y}g\partial_g + 1) + m_0g^{1+1/\hat{y}}\partial_g - \frac{\mathcal{M}r^2}{2}(\Phi\partial_\Phi - \Phi^*\partial_{\Phi^*} - 1) - xt(\Phi\partial_\Phi + \Phi^*\partial_{\Phi^*} - 1) \right] F = 0 \tag{B.22}$$

We first solve these for \mathfrak{sch}_1 . From the conditions eqs. (B.17,B.18,B.19,B.20,B.21) we easily find

$$F = \Phi (\Phi\Phi^*)^{1/x} f \left(g^x (\Phi\Phi^*)^{\hat{y}} \right) \tag{B.23}$$

where f is an arbitrary differentiable function. Two comments are in order:

1. For a dimensionless coupling g , that is $\hat{y} = 0$, we have $x = 1/2$. Then the scaling function reduces to a g -dependent constant and we recover the standard form for the non-linear potential F as quoted ubiquitously in the mathematical literature, see e.g. [88].
2. Taking into account the generator X_1 from eq. (B.22) as well does not change the result. Hence in this case translation-, dilatation- and Galilei-invariance are indeed sufficient for the special Schrödinger-invariance generated by X_1 , see also [111]. We point out that traditionnally an analogous assertion holds for conformal field-theory, see e.g. [51], but counterexamples are known where in local theories scale- and translation-invariance are *not* sufficient for conformal invariance [199, 206].

Second, we now consider the representation of \mathfrak{age}_1 where X_1 is given by (B.15). We have the conditions eqs. (B.18,B.19,B.20,B.21,B.22). We write $F = \Phi\mathcal{F}(\omega, t, g)$ with $\omega = \Phi\Phi^*$ and the remaining equations coming from X_0 and X_1 are

$$\begin{aligned} (t\partial_t + \widehat{y}g\partial_g - xu\partial_u + 1)\mathcal{F} &= 0 \\ (t^2\partial_t + m_0g^{1+1/\widehat{y}}\partial_g)\mathcal{F} &= 0 \end{aligned} \quad (\text{B.24})$$

with the final result

$$F = \Phi(\Phi\Phi^*)^{1/x} f\left((\Phi\Phi^*)^{\widehat{y}} \left[g^{-1/\widehat{y}} - \frac{m_0}{\widehat{y}t}\right]^{-x\widehat{y}}\right) \quad (\text{B.25})$$

and where f is the *same* scaling function as encountered before for \mathfrak{sch}_1 . Finally, the result for the general representations of \mathfrak{age}_1 which depend on an arbitrary function $m(v)$ are not particularly inspiring and will not be detailed here. We observe

1. For $m_0 = 0$, this result is identical to the one found for \mathfrak{sch}_1 .
2. Even for $m_0 \neq 0$, the form of the non-linear potential reduces in the long-time limit $t \rightarrow \infty$ to the one found in eq. (B.23) for the larger algebra \mathfrak{sch}_1 .

We can summarize the main results of this appendix as follows.

Proposition. *Consider the following generators*

$$\begin{aligned} M_0 &= -\mathcal{M} \ , \ Y_{-1/2} = -\partial_r \ , \ Y_{1/2} = -t\partial_r - \mathcal{M}r \ , \ X_{-1} = -\partial_t \\ X_0 &= -t\partial_t - \frac{1}{2}r\partial_r - \widehat{y}g\partial_g - \frac{x}{2} \\ X_1 &= -t^2\partial_t - tr\partial_t - 2\widehat{y}tg\partial_g - m_0g^{1+1/\widehat{y}}\partial_g - \frac{\mathcal{M}r^2}{2} - xt \end{aligned} \quad (\text{B.26})$$

where x, \mathcal{M}, m_0 are parameters. Define the Schrödinger operator $\widehat{S} := 2M_0X_{-1} - Y_{-1/2}^2$. Then:

- (i) the generators $\langle X_{0,\pm 1}, Y_{\pm 1/2}, M_0 \rangle$ form a representation of the Lie algebra \mathfrak{age}_1 . If furthermore $m_0 = 0$, then $\langle X_{0,\pm 1}, Y_{\pm 1/2}, M_0 \rangle$ is a representation of the Lie algebra \mathfrak{sch}_1 .
- (ii) These representations are dynamical symmetries of the Schrödinger equation $\widehat{S}\Phi = 0$, under the auxiliary condition $(1 - 2x - 4\widehat{y}g\partial_g)\Phi = 0$.
- (iii) For the Schrödinger-algebra \mathfrak{sch}_1 and also in the asymptotic limit $t \rightarrow \infty$ for the ageing algebra \mathfrak{age}_1 , the semi-linear Schrödinger equation invariant under these representations has the form

$$\widehat{S}\Phi = \Phi(\Phi\Phi^*)^{1/x} f\left(g^x(\Phi\Phi^*)^{\widehat{y}}\right) \quad (\text{B.27})$$

where f is an arbitrary differentiable function.

This general form includes our potential (4.155) since the scaling dimension \widehat{y} is a remaining free parameter in our considerations

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Selbstständigkeitserklärung

Ich, Florian Baumann, versichere an Eides Statt, daß ich die vorliegende Dissertation selbstständig verfasst und keine anderen als die angegebenen Hilfsmittel und Quellen verwendet habe. Die Arbeit wird im Rahmen eines Doppelpromotionsverfahrens mit der Universität Henri Poincaré in Nancy auch der dortigen Prüfungskommission vorgelegt. Weiterhin versichere ich, daß ich mich nicht schon einmal ohne Erfolg an irgendeiner Hochschule einer Promotionsprüfung unterzogen oder zu promovieren versucht habe.

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Abstract

Ageing phenomena and dynamical scaling behaviour have been observed in many out-of-equilibrium systems, both in experiments, simulations and exactly solvable models. However a general framework for the description of such systems is still missing. Based on a Langevin equation, a first step in this direction is the theory of local scale-invariance (LSI), proposed some time ago, which attempts to identify generalised forms of spatio-temporal dynamical scaling. For systems with a dynamical exponent $z = 2$, it has already been known how to treat stochastic partial differential equations and the consequences for response and correlation functions have been verified in many explicit models.

In this thesis a reformulation and extension of LSI for systems with $z \neq 2$ is presented. Starting from the known axioms of LSI, our approach involves a reformulation on how to construct the mass terms in the generators of LSI. As a consequence, generalised Bargmann superselection rules can be derived for the first time. This permits the first discussion of extended dynamical symmetries of Langevin equations with $z \neq 2$ and we can establish a formalism for the calculation of non-equilibrium correlation -and response functions. The results are tested and confirmed in several new model calculations, both analytical and numerical. This includes as a new application of LSI the investigation of surface-growth models.

Secondly, the ageing behaviour in reaction-diffusion systems is investigated. Although the main features of ageing as seen previously in magnets are still valid, important differences in exponent relations are found which imply modifications of the definition of fluctuation-dissipation ratios. Explicitly, the contact process (directed percolation universality class) is studied through field-theoretical methods and two bosonic models are solved exactly. For the latter, we show how to extend LSI with $z = 2$ to nonlinear models.

Thirdly, the ageing behaviour in semi-infinite magnetic systems close to the surface is considered. The analytical and simulational results provide a fairly complete picture about this type of system. The general scaling picture known from infinite systems remains valid, but some ageing exponents and scaling functions differ from the bulk quantities.

keywords: systems far from equilibrium, field theory, conformal invariance, local scale-invariance, reaction-diffusion systems, semi-infinite systems

Zusammenfassung

Alterungsphänomene und dynamisches Skalenverhalten wurden in vielen Nichtgleichgewichtssystemen beobachtet, sowohl in Experimenten als auch in Simulationen und exakt lösbaren Modellen. Allerdings gibt es bis jetzt keine allgemeine Theorie, in deren Rahmen solche Systeme beschrieben werden können. Als erster Schritt zu einer solchen Theorie wurde, basierend auf einem Zugang über Langevin-Gleichungen, vor einiger Zeit die Theorie lokaler Skaleninvarianzen (LSI) vorgeschlagen, welche versucht, allgemeine Raumzeit-Skalenformen zu identifizieren. Für Systeme mit einem dynamischen Exponenten $z = 2$ ist bereits bekannt, wie partielle stochastische Differentialgleichungen behandelt werden können, und die Konsequenzen für Antwort- und Korrelationsfunktionen wurden in vielen expliziten Modellen verifiziert.

In dieser Dissertation wird eine Neuformulierung und Erweiterung von LSI für Systeme mit $z \neq 2$ präsentiert. Beginnend mit den bekannten LSI-Axiomen schlagen wir eine Reformulierung der Konstruktion der Massenterme vor. Als eine Konsequenz können zum ersten Mal verallgemeinerte Bargmannsche Überauswahlregeln abgeleitet werden. Dies wiederum erlaubt erstmalig die Diskussion von erweiterten dynamischen Symmetrien von Langevin-Gleichungen mit $z \neq 2$ und wir entwickeln einen Formalismus für die Berechnung von Nichtgleichgewichts Korrelations- und Antwortfunktionen fern des Gleichgewichts. Die Ergebnisse werden in mehreren neuen Modelrechnungen geprüft und bestätigt, sowohl analytisch als auch numerisch. Dazu gehört auch, als eine neue Anwendung von LSI, eine Untersuchung von Oberflächenwachstums-Modellen.

Zweitens wird das Alterungsverhalten von Reaktions-Diffusionssystemen untersucht. Obwohl die grundlegenden Alterungseigenschaften, wie sie in den vorher untersuchten magnetischen Systemen auftreten, erhalten bleiben, so treten doch wichtige Unterschiede bei Exponentenbeziehungen auf, welche Auswirkungen auf die Definition eines Fluktuations-Dissipationsverhältnisses haben. Explizit wird der Paarkontaktprozess (gerichtete Perkolations-Universalitätsklasse) mit feldtheoretischen Methoden untersucht, und zwei bosonische Modelle werden exakt gelöst. Für letztere zeigen wir, wie LSI mit $z = 2$ auf nichtlineare Modelle erweitert werden kann.

Drittens wird das Alterungsverhalten von halbbunendlichen magnetischen Systemen nahe der Oberfläche untersucht. Die Ergebnisse aus analytischen Rechnungen und Simulationen ergeben ein ziemlich vollständiges Bild über Systeme dieses Typs. Das grundlegende Skalenverhalten, das von unendlichen Systemen bekannt ist, bleibt erhalten, aber einige Alterungsexponenten und Skalenfunktionen unterscheiden sich von den entsprechenden Volumengrößen.

Stichworte: Systeme fern des Gleichgewichts, Feldtheorie, konforme Invarianz, lokale Skaleninvarianz, Reaktions-Diffusions-Systeme, halbbunendliche Systeme

Résumé

Les phénomènes de vieillissement et comportement d'échelle dynamique ont été observés dans le passé dans beaucoup de systèmes hors-équilibre : dans des expériences, des simulations numériques et dans des modèles exactement solubles. Toutefois il n'y a pas de théorie générale pour la description de ce type de système. Un premier pas a été réalisé avec la théorie d'invariance d'échelle locale (LSI) basée sur une équation de Langevin. Elle a été proposée il y a un certain temps et elle tente d'identifier une forme généralisée du comportement d'échelle dynamique spatio-temporelle. Pour des systèmes avec un exposant critique $z = 2$, il était déjà connu comment traiter des équations partielles stochastiques. Les conséquences pour la fonction de réponse et de corrélation ont été vérifiées explicitement dans beaucoup de modèles.

Dans cette thèse nous proposons une reformulation et un élargissement de la LSI aux systèmes avec $z \neq 2$. Comme point de départ on choisit les axiomes connus de la LSI, mais on reformule la construction des termes de masse. On en déduit pour la première fois des règles de Bargmann généralisées. Cela permet pour la première fois une discussion des symétries dynamiques élargies d'une équation de Langevin avec $z \neq 2$. Puis on établit un formalisme pour le calcul des fonctions de corrélations et de réponse hors équilibre. Les résultats sont testés et confirmés dans plusieurs nouveaux calculs dans des modèles concrets tant numériquement qu'analytiquement. Cela permet une nouvelle application de la LSI : l'investigation des modèles de croissance de surfaces.

En vue des applications nous étudions le comportement de vieillissement dans des systèmes de réaction-diffusion. Bien que les propriétés principales observées dans les systèmes magnétiques soient toujours valides, des différences importantes dans certaines relations des exposants apparaissent. Elles impliquent un changement dans la définition du rapport fluctuation-dissipation. Nous étudions explicitement le processus de contact (classe d'universalité de la percolation dirigée) par des méthodes du groupe de renormalisation dynamique. Puis deux modèles bosoniques sont résolus exactement. Nous montrons pour ces derniers comment élargir la LSI pour $z = 2$ afin d'inclure des modèles non-linéaires.

Finalement, nous considérons le comportement de vieillissement proche d'une surface dans un système magnétique. Les résultats analytiques et numériques fournissent une image presque complète de ce type de système. Les formes d'échelle qu'on trouve dans le volume restent valides, mais certains exposants et fonctions d'échelle sont différents des quantités de volume correspondantes.

Mots clés: systèmes hors équilibre, théorie de champs, invariance conforme, invariance d'échelle locale, systèmes de réaction-diffusion, systèmes semi-infinis