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Out-of-equilibrium properties of the semi-infinite kinetic spherical model

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Abstract
We study the ageing properties of the semi-infinite kinetic spherical model at the critical point and in the ordered low-temperature phase for both Dirichlet and Neumann boundary conditions. The surface fluctuation–dissipation ratio and the scaling functions of two-time surface correlation and response functions are determined explicitly in the dynamical scaling regime. In the low-temperature phase, our results show that for the case of Dirichlet boundary conditions the value of the non-equilibrium surface exponent b_1 differs from the usual bulk value of systems undergoing phase ordering.

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1. Introduction

Ageing phenomena encountered in systems with slow degrees of freedom are due to relaxation processes that depend on the thermal history of the sample. Ageing is found in various systems, ranging from structural glasses and spin glasses to colloids and polymers [1–3]. In addition, ageing phenomena are also observed in ferromagnets quenched to or below their critical point [4–7].

Ageing processes are best revealed through the study of two-time quantities such as dynamical correlation and response functions. Well-known examples are given by the autocorrelation and autoresponse functions:

$$C(t,s) = \langle \phi(t)\phi(s)\rangle\,, \qquad R(t,s) = \left.\frac{\delta\langle\phi(t)\rangle}{\delta h(s)}\right|_{h=0} \quad (t > s), \tag{1}$$

where $\phi(t)$ is the time-dependent order parameter and h is the field conjugate to ϕ. The time t elapsed since the quench is usually called the observation time and s is the waiting time. In out-of-equilibrium systems, one often observes in the regime $t, s, t - s \gg t_{\text{micro}}$ (t_{micro} being a microscopical time scale) the following dynamical scaling behaviour [3]:

$$C(t, s) = s^{-b} f_C(t/s), \qquad R(t, s) = s^{-1-a} f_R(t/s). \tag{2}$$

Here a and b are non-equilibrium exponents, whereas $f_C(y)$ and $f_R(y)$ are scaling functions which for $y \gg 1$ show the power-law behaviours:

$$f_C(y) \sim y^{-\lambda_C/z}, \qquad f_R(y) \sim y^{-\lambda_R/z}, \tag{3}$$

where λ_C and λ_R are called autocorrelation [8, 9] and autoresponse exponents [10], and z is the dynamical exponent. These simple scaling forms are observed in systems which are characterized by the existence of a time-dependent length scale $\xi \sim t^{1/z}$.

Specifically, for ferromagnets we distinguish between physically very different situations. Below T_c phase ordering takes place, and the slow degrees of freedom are provided by the moving interfaces separating different ordered domains. We then commonly have $b = 0$, whereas a takes on the value $1/z$ or $(d-2+\eta)/z$, depending on whether the static correlations decay exponentially or whether they follow a power law with an exponent $d - 2 + \eta$ [11, 12], where d is the number of space dimensions. At the critical point, general scaling arguments lead to the relation $a = b = (d - 2 + \eta)/z$, where η is the well-known static critical exponent. Furthermore, the autocorrelation exponent λ_C can be related to the initial slip exponent [13] describing the relaxation of the order parameter in the short-time regime [14]. For initial states with short-range correlations and purely relaxational dynamics, one finds[3] $\lambda_C = \lambda_R$, but this relation may be broken when starting from long-range correlated initial states [10] or when some randomness is present [16].

The phenomenology just briefly described has been found to be valid in many bulk systems. It has only been realized recently [17] 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:

$$C_1(t, s) = \langle \phi_1(t)\phi_1(s) \rangle, \qquad R_1(t, s) = \left.\frac{\delta\langle \phi_1(t) \rangle}{\delta h_1(s)}\right|_{h_1=0} \quad (t > s), \tag{4}$$

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 $t, s, t - s \gg t_{\text{micro}}$, we expect simple scaling forms:

$$C_1(t, s) = s^{-b_1} f_{C_1}(t/s), \tag{5}$$

$$R_1(t, s) = s^{-1-a_1} f_{R_1}(t/s), \tag{6}$$

and the scaling functions $f_{C_1}(y)$ and $f_{R_1}(y)$ should display a power-law behaviour in the limit $y \longrightarrow \infty$:

$$f_{C_1}(y) \sim y^{-\lambda_{C_1}/z}, \qquad f_{R_1}(y) \sim y^{-\lambda_{R_1}/z}. \tag{7}$$

Equations (5)–(7) 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 [18, 19]. Relations between the different non-equilibrium exponents can again be derived from general scaling arguments [7, 17]. Thus, we obtain

$$a_1 = b_1 = (d - 2 + \eta_\parallel)/z, \tag{8}$$

[3] For Kawasaki dynamics, i.e. dynamics with a conserved order parameter, the relation $\lambda_C = \lambda_R$ does not hold at the critical point [7, 15].

where the static exponent $\eta_\parallel$ governs the decay of correlations parallel to the surface. For the surface autocorrelation exponent $\lambda_{C_1} = \lambda_{R_1}$, one finds [20, 21]

$$\lambda_{C_1} = \lambda_C + \eta_\parallel - \eta. \tag{9}$$

The scaling laws (5)–(7) and the different relations between the non-equilibrium critical exponents have been verified in [17] through Monte Carlo simulations of critical semi-infinite Ising models in two and three dimensions. In [7], 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 [18, 19]. In this paper, 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), is different from zero, the value encountered in bulk systems undergoing phase ordering [4].

The present work is on the one hand meant to close a gap in the study of kinetic spherical models [22–24], 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 [25–30]. 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 $N \longrightarrow \infty$ [27, 28], even so both models are strictly equivalent in the bulk system [31, 32].

The paper is organized in the following way. In section 2, we present the kinetic model in a quite general way, thus leaving open the possibility of considering different boundary conditions in the different space directions. In sections 3 and 4, we discuss the dynamical scaling behaviour of surface correlation and response functions, whereas in section 5 we compute the surface fluctuation–dissipation ratio. Finally, section 6 gives our conclusions.

2. The model

2.1. General setting

We consider a finite hypercubic system Λ in d dimensions containing $\mathcal{N} = L_1 \times \cdots \times L_d$ sites, where L_ν denotes the length of the νth edge[4]. With every lattice site $\boldsymbol{r}^T = (r_1, \ldots, r_d)$, we associate a time-dependent real variable $S(\boldsymbol{r}, t)$ describing the spin on site $\boldsymbol{r}$. These variables are subject to the mean spherical constraint

$$\sum_{\boldsymbol{r}\in\Lambda} \langle S^2(\boldsymbol{r}, t)\rangle = \mathcal{N}, \tag{10}$$

[4] We set the lattice spacing equal to 1.

where the angle brackets indicate an average over the thermal noise. The Hamiltonian of the spherical model is given in a bulk system by

$$\mathcal{H} = -J \sum_{\langle \boldsymbol{r}, \boldsymbol{r}' \rangle} S(\boldsymbol{r}) S(\boldsymbol{r}'), \tag{11}$$

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 νth direction (with $\nu = 2, \ldots, d$)

$$S((r_1, \ldots, r_\nu + mL_\nu, \ldots, r_d), t) = S((r_1, \ldots, r_\nu, \ldots, r_d), t) \qquad \text{for all } m \in \mathbb{Z}. \tag{12}$$

In the remaining direction, we either consider Dirichlet boundary conditions or Neumann boundary conditions. For Dirichlet boundary conditions, we impose that

$$S((0, r_2, \ldots, r_d), t) = S((L_1 + 1, r_2, \ldots, r_d), t) = 0. \tag{13}$$

For Neumann boundary conditions, on the other hand, we have

$$\begin{aligned} S((0, r_2, \ldots, r_d), t) &= S((1, r_2, \ldots, r_d), t), \\ S((L_1 + 1, r_2, \ldots, r_d), t) &= S((L_1, r_2, \ldots, r_d), t). \end{aligned} \tag{14}$$

In the following, quantities depending on the chosen boundary condition will be labelled by the superscripts (p), (d) and (n) for periodic, Dirichlet and Neumann boundary conditions, respectively.

The Hamiltonian can be written in the following general form:

$$H = -\tfrac{1}{2} J \boldsymbol{S}_\Lambda^T \cdot \mathbf{Q}_\Lambda^{(\tau)} \cdot \boldsymbol{S}_\Lambda + \tfrac{1}{2} \lambda^{(\tau)}(t) \boldsymbol{S}_\Lambda^T \cdot \boldsymbol{S}_\Lambda - \boldsymbol{S}_\Lambda^T \cdot \boldsymbol{h}_\Lambda, \tag{15}$$

where the vector $\boldsymbol{S}_\Lambda := \{S(\boldsymbol{r}) | \boldsymbol{r} \in \Lambda\}$ characterizes the state of the system. $J > 0$ is the strength of the ferromagnetic nearest-neighbour couplings and is chosen to be equal to 1 in the following. Furthermore, $\boldsymbol{h}_\Lambda := \{h(\boldsymbol{r}) | \boldsymbol{r} \in \Lambda\}$ where $h(\boldsymbol{r})$ is an external field acting on the spin at site $\boldsymbol{r}$, whereas $\lambda^{(\tau)}(t)$ is the Lagrange multiplier ensuring the constraint (10). Finally, the interaction matrix $\mathbf{Q}_\Lambda^{(\tau)}$ (with $\tau = (\tau_1, \ldots, \tau_d)$ characterizing the boundary conditions in the d different directions) is given by the tensor product [33]

$$\mathbf{Q}_\Lambda^{(\tau)} = \bigotimes_{\nu=1}^{d} \left(\Delta_\nu^{(\tau_\nu)} + 2\mathbf{E}_\nu \right). \tag{16}$$

Here $\mathbf{E}_\nu$ 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 parametrize the Lagrange multiplier in the following way [33]:

$$\lambda^{(\tau)}(t) = \mu_\Lambda^{(\tau)}(\boldsymbol{\kappa}) + z^{(\tau)}(t),$$

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 $\boldsymbol{k}$ (see appendix A) which labels the different eigenvalues and eigenfunctions of $\mathbf{Q}_\Lambda^{(\tau)}$. In the case of periodic boundary conditions in *all* directions, we recover the usual expression

$$\lambda^{(p)}(t) = 2d + z^{(p)}(t).$$

2.2. The 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 magnetization. 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:

$$\frac{\mathrm{d}}{\mathrm{d}t}\boldsymbol{S}_\Lambda(t) = \left(\mathbf{Q}_\Lambda^{(\tau)} - z^{(\tau)}(t) - \mu_\Lambda^{(\tau)}(\boldsymbol{\kappa})\right)\boldsymbol{S}_\Lambda(t) + \boldsymbol{h}_\Lambda(t) + \boldsymbol{\eta}_\Lambda(t), \tag{17}$$

where $\boldsymbol{\eta}_\Lambda(t) := \{\eta_{\boldsymbol{r}}(t)|\boldsymbol{r} \in \Lambda\}$ with $\eta_{\boldsymbol{r}}(t)$ being a Gaussian white noise:

$$\langle \eta_{\boldsymbol{r}}(t)\rangle = 0 \qquad \text{and} \qquad \langle \eta_{\boldsymbol{r}}(t)\eta_{\boldsymbol{r}'}(t')\rangle = 2T\delta_{\boldsymbol{r},\boldsymbol{r}'}\delta(t-t').$$

We further assume that the external field $\boldsymbol{h}_\Lambda$ is time dependent.

Equation (17) can easily be solved, yielding

$$\begin{aligned}\boldsymbol{S}_\Lambda(t) = {}& \exp\left(\int_0^t \mathrm{d}t'\left(\mathbf{Q}_\Lambda^{(\tau)} - z^{(\tau)}(t') - \mu_\Lambda^{(\tau)}(\boldsymbol{\kappa})\right)\right) \\ & \times\left[\boldsymbol{S}_\Lambda(0) + \int_0^t \mathrm{d}t'\left(\exp\left(-\int_0^{t'} \mathrm{d}t''\left(\mathbf{Q}_\Lambda^{(\tau)} - z^{(\tau)}(t'') - \mu_\Lambda^{(\tau)}(\boldsymbol{\kappa})\right)\right)\right)(\boldsymbol{h}_\Lambda(t') + \boldsymbol{\eta}_\Lambda(t'))\right].\end{aligned} \tag{18}$$

In order to proceed further, we use a decomposition in an orthonormal basis of eigenfunctions of the interaction matrix $\mathbf{Q}_\Lambda^{(\tau)}$:

$$\widetilde{S}(\boldsymbol{k},t) := \sum_{\boldsymbol{r}\in\Lambda}\left(\prod_{\nu=1}^{d} u_{L_\nu}^{(\tau_\nu)}(r_\nu,k_\nu)\right) S(\boldsymbol{r},t), \tag{19}$$

where the vectors $u_{L_\nu}^{(\tau_\nu)}(r_\nu,k_\nu)$ are given in appendix A. We get the original vector back by the inverse transformation

$$S(\boldsymbol{r},t) = \sum_{\boldsymbol{k}\in\Lambda}\left(\prod_{\nu=1}^{d} u_{L_\nu}^{(\tau_\nu)*}(r_\nu,k_\nu)\right)\widetilde{S}(\boldsymbol{k},t). \tag{20}$$

The transformation (19) diagonalizes the symmetric matrix $\mathbf{Q}_\Lambda^{(\tau)} - z(t) - \mu_\Lambda^{(\tau)}(\boldsymbol{\kappa})$, yielding

$$\widetilde{S}(\boldsymbol{k},t) = \frac{\mathrm{e}^{-\omega^{(\tau)}(\boldsymbol{k})t}}{\sqrt{g^{(\tau)}(t)}}\left[\widetilde{S}(\boldsymbol{k},0) + \int_0^t \mathrm{d}t'\left(\sqrt{g^{(\tau)}(t')}\mathrm{e}^{\omega^{(\tau)}(\boldsymbol{k})t'}(\widetilde{h}(\boldsymbol{k},t') + \widetilde{\eta}(\boldsymbol{k},t'))\right)\right] \tag{21}$$

with

$$g^{(\tau)}(t) := \exp\left(2\int_0^t \mathrm{d}u\, z^{(\tau)}(u)\right) \tag{22}$$

and

$$\omega^{(\tau)}(\boldsymbol{k}) := -\mu_\Lambda^{(\tau)}(\boldsymbol{k}) + \mu_\Lambda^{(\tau)}(\boldsymbol{\kappa}). \tag{23}$$

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 $\boldsymbol{r}^T = (r, \boldsymbol{x}^T)$ with $r := r_1$ and $\boldsymbol{x}^T := (r_2, \ldots, r_d)$. The corresponding vector in reciprocal space is then written as $\boldsymbol{k}^T = (k, \boldsymbol{q}^T)$ with $k := k_1$ and $\boldsymbol{q}^T := (k_2, \ldots, k_d)$. As a consequence of the semi-infinite volume limit, sums have to be replaced by integrals in the following way [33]:

- $\frac{2}{L_1}\sum_{k_1=1}^{L_1}(\cdots) \longrightarrow \frac{2}{\pi}\int_0^\pi \mathrm{d}k(\cdots)$ in the direction perpendicular to the surface,
- $\frac{1}{L_\nu}\sum_{k_\nu=1}^{L_\nu}(\cdots) \longrightarrow \frac{1}{2\pi}\int_{-\pi}^\pi \mathrm{d}k(\cdots)$ in all other directions,

where the integration limits follow from appendix A. It has to be noted that in the semi-infinite volume limit the largest eigenvalue of the interaction matrix (16) is given by $\mu_\Lambda^{(\tau)}(\boldsymbol{\kappa}) = 2d$ irrespective of the chosen boundary condition. We therefore rewrite (23) in the following way:

$$\omega^{(\tau)}(\boldsymbol{k}) = \omega(k, \boldsymbol{q}) = \widetilde{\omega}(k) + \hat{\omega}(\boldsymbol{q}) \tag{24}$$

with

$$\widetilde{\omega}(k) = 2\,(1 - \cos k) \qquad \text{and} \qquad \hat{\omega}(\boldsymbol{q}) = 2\sum_{\nu=2}^{d}(1 - \cos k_\nu)\,, \tag{25}$$

where we used the explicit expressions for $\mu_\Lambda^{(\tau)}(\boldsymbol{k})$ (see appendix A).

As usual, we prepare the system at time $t = 0$ in a completely uncorrelated initial state with vanishing magnetization. We then have at $t = 0$ in reciprocal space

$$\langle \widetilde{S}(\boldsymbol{k}, 0)\widetilde{S}(\boldsymbol{k}', 0)\rangle = (2\pi)^{d-1}\frac{\pi}{2}\delta^{d-1}(\boldsymbol{q} + \boldsymbol{q}')\tilde{C}^{(\tau)}(k, k'), \tag{26}$$

where the quantity $\tilde{C}^{(\tau)}(k, k')$ is given by

$$\tilde{C}^{(\tau)}(k, k') = \begin{cases} \sum_{r=1}^{\infty}\sin(rk)\sin(rk'), & \tau = d,\\ \sum_{r=1}^{\infty}\cos\left(\left(r - \frac{1}{2}\right)k\right)\cos\left(\left(r - \frac{1}{2}\right)k'\right), & \tau = n. \end{cases} \tag{27}$$

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 equation (10) 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 [27, 29] (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 [28, 30] (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 $N \longrightarrow \infty$. In studies of *static* quantities, it has been proposed that the spherical constraint could be realized in the semi-infinite geometry by imposing in the Hamiltonian a different spherical field for every layer [25], thus yielding the universality class of the semi-infinite $O(N)$ model with $N \longrightarrow \infty$. For dynamical quantities, however, this prescription leads to the unwanted effect that the matrices which then appear in the exponential in equation (18) 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 (39) for a precise mathematical formulation). This then yields equations (21)–(23) 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 paper.

3. The surface autocorrelation function

The two-time spin–spin correlation function is defined by

$$C^{(\tau)}(\boldsymbol{r}, \boldsymbol{r}'; t, s) = \langle S(\boldsymbol{r}, t)S(\boldsymbol{r}', s)\rangle \tag{28}$$

with $\boldsymbol{r}^T = (r, \boldsymbol{x}^T)$ and $\boldsymbol{r}'^T = (r', \boldsymbol{x}'^T)$. Here (τ) again characterizes 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

$$C_1^{(\tau)}(t, s) = C^{(\tau)}((1, \boldsymbol{x}), (1, \boldsymbol{x}); t, s), \tag{29}$$

where we follow the convention to attach a subscript 1 to surface-related quantities.

From equation (21), we directly obtain the following expression for the correlation function in reciprocal space:

$$\begin{aligned} \overline{C}^{(\tau)}(\boldsymbol{k}, \boldsymbol{k}'; t, s) = \frac{\mathrm{e}^{-\omega(k,\boldsymbol{q})t-\omega(k',\boldsymbol{q}')s}}{\sqrt{g^{(\tau)}(t)g^{(\tau)}(s)}}(2\pi)^{d-1}\frac{\pi}{2}\delta^{d-1}(\boldsymbol{q}+\boldsymbol{q}')\Bigg[\tilde{C}^{(\tau)}(k, k') \\ +2T\delta(k-k')\int_0^t \mathrm{d}t'\, \mathrm{e}^{2\omega(k,\boldsymbol{q})t'}g^{(\tau)}(t')\Bigg], \end{aligned} \tag{30}$$

where we have set the external field to zero. Transforming back to real space, we obtain

$$\begin{aligned} C^{(\tau)}((r, \boldsymbol{x}), (r', \boldsymbol{x}); t, s) = \frac{1}{\sqrt{g^{(\tau)}(t)g^{(\tau)}(s)}}\Bigg[f^{(\tau)}\left(r, r'; \frac{t+s}{2}\right) \\ + 2T\int_0^s \mathrm{d}u\, f^{(\tau)}\left(r, r'; \frac{t+s}{2}-u\right)g^{(\tau)}(u)\Bigg], \end{aligned} \tag{31}$$

where a boundary-dependent function $f^{(\tau)}$ has been defined, with

$$f^{(\mathrm{d})}(r, r'; t) = \frac{2}{\pi}\int\frac{\mathrm{d}^{d-1}\boldsymbol{q}}{(2\pi)^{(d-1)}}\,\mathrm{e}^{-2\hat{\omega}(\boldsymbol{q})t}\int_0^\pi \mathrm{d}k\,\sin(r\cdot k)\sin(r'\cdot k)\,\mathrm{e}^{-2\widetilde{\omega}(k)t} \tag{32}$$

$$= (\mathrm{e}^{-4t}I_0(4t))^{d-1}\cdot\mathrm{e}^{-4t}(I_{r-r'}(4t) - I_{r+r'}(4t)) \tag{33}$$

and

$$\begin{aligned} f^{(\mathrm{n})}(r, r'; t) &= \frac{2}{\pi}\int\frac{\mathrm{d}^{d-1}\boldsymbol{q}}{(2\pi)^{(d-1)}}\,\mathrm{e}^{-2\hat{\omega}(\boldsymbol{q})t}\int_0^\pi \mathrm{d}k\,\cos((r-1/2)\cdot k)\cos((r'-1/2)\cdot k)\,\mathrm{e}^{-2\widetilde{\omega}(k)t} \\ &= (\mathrm{e}^{-4t}I_0(4t))^{d-1}\cdot\mathrm{e}^{-4t}(I_{r-r'}(4t) + I_{r+r'-1}(4t)) \end{aligned} \tag{34}$$

with the modified Bessel functions $I_\nu(u)$. In the long-time limit $t \longrightarrow \infty$, we get

$$f^{(\mathrm{d})}(r, r'; t) \overset{t\to\infty}{\approx} 4\pi(8\pi t)^{-\frac{d+2}{2}}r\cdot r', \tag{35}$$

$$f^{(\mathrm{n})}(r, r'; t) \overset{t\to\infty}{\approx} 2(8\pi t)^{-\frac{d}{2}}, \tag{36}$$

where the well-known asymptotic expansion

$$I_\nu(u) \overset{u\to\infty}{\approx} \frac{\mathrm{e}^u}{\sqrt{2\pi u}}\left(1 - \frac{\nu^2 - 1/4}{2u} + O(1/u^2)\right) \tag{37}$$

of the Bessel function has been used.

The function $g^{(\tau)}(t)$ is obtained as the solution of a nonlinear Volterra equation

$$g^{(\tau)}(t) = \lim_{L\to\infty}\frac{1}{L}\sum_{r=1}^{L}\left(f^{(\tau)}(r, r; t) + 2T\int_0^t \mathrm{d}u\, f^{(\tau)}(r, r; t-u)g^{(\tau)}(u)\right), \tag{38}$$

that follows directly from the implementation of the mean spherical constraint through the requirement

$$\lim_{L\to\infty} \frac{1}{L} \sum_{r=1}^{L} C^{(\tau)}((r,\mathbf{0}),(r,\mathbf{0});t,t) = 1 \tag{39}$$

for all times t. This provides an implicit equation for the Lagrange multiplier introduced earlier. Inserting expressions (35) and (36) for $f^{(\tau)}$ into equation (38), we observe that we end up with the known bulk equation [22]

$$g(t) = \hat{f}(t) + 2T \int_0^t \mathrm{d}u\, \hat{f}(t-u) g(u) \tag{40}$$

with

$$\hat{f}(t) := \int_{-\pi}^{\pi} \frac{\mathrm{d}^{d-1}\boldsymbol{q}}{(2\pi)^{d-1}} \int_{-\pi}^{\pi} \frac{\mathrm{d}k}{2\pi}\, \mathrm{e}^{-2\omega(k,\boldsymbol{q})t} = (\mathrm{e}^{-4t} I_0(4t))^d, \tag{41}$$

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 [23]. We recall these results in appendix B as they are needed in the following.

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 equation (31) by setting $r = r' = 1$.

- $T < T_c$: from renormalization 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 (31) contributes in the scaling limit [23]. For both boundary conditions, we obtain a dynamical scaling behaviour as

$$C^{(\mathrm{d})}(t,s) = 2^{\frac{d}{2}} M_{\mathrm{eq}}^2 s^{-1} \left(\frac{t}{s}\right)^{\frac{d}{4}} \left(\frac{t}{s}+1\right)^{-(\frac{d}{2}+1)}, \tag{42}$$

$$C^{(\mathrm{n})}(t,s) = 2^{\frac{d}{2}+1} M_{\mathrm{eq}}^2 \left(\frac{t}{s}\right)^{\frac{d}{4}} \left(\frac{t}{s}+1\right)^{-\frac{d}{2}}, \tag{43}$$

where $M_{\mathrm{eq}}^2 = 1 - T/T_c$ [34]. The non-equilibrium exponents can then be read off directly (recall $z = 2$) as

$$b_1^{(\mathrm{d})} = 1, \qquad b_1^{(\mathrm{n})} = 0, \qquad \lambda_{C_1}^{(\mathrm{d})} = \frac{d}{2} + 2, \qquad \lambda_{C_1}^{(\mathrm{n})} = \frac{d}{2}. \tag{44}$$

A few comments are now in order. When comparing the values (44) with those obtained for the bulk system [13, 23], see table 1, 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 section. Interestingly, the agreement between the semi-infinite system with Neumann boundary conditions and the bulk system also extends to

Table 1. Ageing exponents and fluctuation–dissipation ratio for the bulk system and for the semi-infinite systems with Dirichlet and Neumann boundary conditions.

	Bulk	Dirichlet (τ = d)	Neumann (τ = 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
$X_\infty^{(\tau)}$	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$

the scaling functions of two-time quantities which are identical, up to an unimportant numerical factor[5].

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 $\lambda_{C_1}^{(\mathrm{d})}$ thereby reflects the increased disorder at the surface due to the absence of neighbouring spins. Remarkably, the exponent $b_1^{(\mathrm{d})}$ 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 1 in three dimensions. The analytical curves are given by expressions (42) and (43) whereas the symbols, corresponding to different waiting times, are obtained from the direct numerical evaluation of equation (31). 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 (31).

- $T = T_c$ 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 equation (31). One may wonder whether the use of the asymptotics for g in the integrand of equation (31) does not cause problems at the lower integration bound. As has been shown in [36], there

[5] This 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 [17]. Similarly, the surface autocorrelation exponent λ_{C_1} for the $O(N)$ model in the limit $N \longrightarrow \infty$ differs at the special transition point from the bulk autocorrelation exponent λ_C [20, 35].

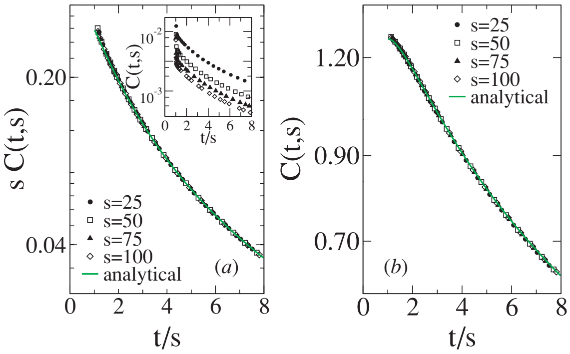

Figure 1. Scaling plots of the autocorrelation function for the case $T < T_c$ in three dimensions: (*a*) for Dirichlet boundary conditions with $b_1^{(d)} = 1$; (*b*) for Neumann boundary conditions with $b_1^{(n)} = 0$. The inset in (*a*) shows that no data collapse is observed for the unscaled data.

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 $g_{\rm age}$ for $u > t_P$, the integral of equation (31) can be written in the following way:

$$\int_0^s \mathrm{d}u\, f^{(\tau)}(1,1;(t+s)/2-u)g(u) = \int_0^{t_P} \mathrm{d}u g(u) f^{(\tau)}(1,1;(t+s)/2-u) + \int_{t_P}^s \mathrm{d}u\, g_{\rm age}(u) f^{(\tau)}(1,1;(t+s)/2-u) = W^{(\tau)}(t,s,t_P) + s\int_0^1 dv\, g_{\rm age}(sv) f^{(\tau)}(1,1;(t+s)/2-sv), \tag{45}$$

where in the last line we have assumed s to be large. An upper bound for the first term $W^{(\tau)}(t,s,t_P) = \int_0^{t_P}\mathrm{d}u\, g(u) f^{(\tau)}(1,1;(t+s)/2-u)$ is given by

$$\left|W_P^{(\tau)}(t,s,t_P)\right| \leqslant t_P \max_{\tau\in[0,t_P]} |g(\tau) f^{(\tau)}(1,1;(t+s)/2-\tau)| \overset{s\gg 1}{\approx} t_P \cdot \max_{\tau\in[0,t_P]} |g(\tau)| s^{-\frac{d}{2}} \left(4\pi\left(\frac{1}{2}\left(\frac{t}{s}+1\right) - \frac{t_P}{s}\right)\right)^{-\xi^{(\tau)}}, \tag{46}$$

where $\xi^{(\mathrm{d})} = \frac{d}{2}+1$ and $\xi^{(\mathrm{n})} = \frac{d}{2}$. As $t_P \sim s^\zeta$, this upper bound disappears in the scaling limit faster than the second contribution in equation (45). We therefore drop $W^{(\tau)}(t,s,t_P)$ in the following and end up with the expression

$$C_1^{(\tau)}(t,s) = \frac{1}{\sqrt{g_{\rm age}(t)g_{\rm age}(s)}}\left[f^{(\tau)}\left(1,1;\frac{t+s}{2}\right) + 2T\int_0^s \mathrm{d}u\, f^{(\tau)}\left(1,1;\frac{t+s}{2}-u\right) g_{\rm age}(u)\,\mathrm{d}u\right] \tag{47}$$

in the asymptotic regime. It turns out that the thermal part of expression (47) 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 again obtain dynamical scaling behaviour, as shown in figure 2, as

$$C^{(\mathrm{d})}(t,s) = \frac{4T_c(4\pi)^{-(\frac{d}{2})}}{d-2} s^{-\frac{d}{2}} \left(\frac{t}{s}\right)^{1-\frac{d}{4}} \left(\frac{t}{s}+1\right)^{-1} \left(\frac{t}{s}-1\right)^{-\frac{d}{2}} \times \left[1-\frac{4}{d}\left(\frac{t}{s}+1\right)^{-1}\right], \tag{48}$$

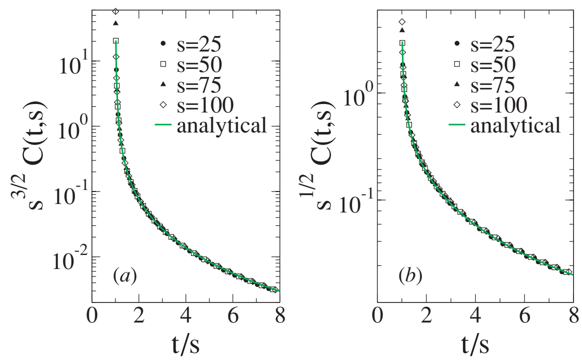

Figure 2. Scaling plots of the autocorrelation function for the case $T = T_c$ in three dimensions: (*a*) for Dirichlet boundary conditions; (*b*) for Neumann boundary conditions.

$$C^{(n)}(t,s) = \frac{8(4\pi)^{-\frac{d}{2}} \cdot T_c}{(d-2)} s^{-(\frac{d}{2}-1)} \left(\frac{t}{s}\right)^{1-\frac{d}{4}} \left(\frac{t}{s}-1\right)^{1-\frac{d}{2}} \left(\frac{t}{s}+1\right)^{-1}, \tag{49}$$

yielding the non-equilibrium critical exponents

$$b_1^{(d)} = \frac{d}{2}, \qquad b_1^{(n)} = \frac{d}{2} - 1, \qquad \lambda_{C_1}^{(d)} = \frac{3}{2}d, \qquad \lambda_{C_1}^{(n)} = \frac{3}{2}d - 2. \tag{50}$$

The values $b_1^{(\tau)}$ agree with the expression

$$b_1^{(\tau)} = b + \frac{2\big(\beta_1^{(\tau)} - \beta\big)}{\nu z} \tag{51}$$

expected from general scaling considerations [7]. Equation (51) 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 magnetizations on approaching 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 $\lambda_{C_1}^{(d)}$.

- $T = T_c$ and $d > 4$: in this case, we obtain

$$C^{(d)}(t,s) = \frac{2(4\pi)^{-\frac{d}{2}}}{d} \cdot T_c \cdot s^{-\frac{d}{2}} \left(\left(\frac{t}{s}-1\right)^{-\frac{d}{2}} - \left(\frac{t}{s}+1\right)^{-\frac{d}{2}} \right), \tag{52}$$

$$C^{(n)}(t,s) = \frac{4(4\pi)^{-\frac{d}{2}}}{d-2} \cdot T_c \cdot s^{-(\frac{d}{2}-1)} \left(\left(\frac{t}{s}-1\right)^{1-\frac{d}{2}} - \left(\frac{t}{s}+1\right)^{1-\frac{d}{2}} \right). \tag{53}$$

Again dynamical scaling is found where the non-equilibrium critical exponents now take on the values

$$b_1^{(d)} = \frac{d}{2}, \qquad b_1^{(n)} = \frac{d}{2} - 1, \qquad \lambda_{C_1}^{(d)} = d + 2, \qquad \lambda_{C_1}^{(n)} = d. \tag{54}$$

Also here (51) 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

$$C_1^{(\tau)}(t,s) = \mathrm{e}^{-(t+s)/(2\tau_{\mathrm{eq}})}\left[f^{(\tau)}\left(1,1;\frac{t+s}{2}\right) + 2T\int_0^s \mathrm{d}u\, f^{(\tau)}\left(1,1;\frac{t+s}{2}-u\right) g_{\mathrm{age}}(u)\right]. \tag{55}$$

This amounts to an exponential decrease and the leading expression rapidly develops a dependence only on $t-s$ for $s \to \infty$ and $t-s$ fixed [23].

Inspection of table 1 reveals the oddity that the values of a_1 and b_1 for Dirichlet and Neumann boundary conditions always exactly differ by 1. 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 $a_1 = b_1 = 2\beta_1/(\nu z)$ [7, 17] with the values $\beta_1 = 0.80$ at the ordinary transition and $\beta_1 \approx 0.23$ at the special transition point [19], yielding different values for a_1 and b_1 in that case, too. However, the exact value 1 for the difference seems to be a property of the spherical model.

4. The response function

The response function is defined as usual:

$$R(\boldsymbol{r},\boldsymbol{r}';t,s) := \left.\frac{\delta\langle S(\boldsymbol{r},t)\rangle}{\delta h(\boldsymbol{r}',s)}\right|_{h=0}, \qquad t > s, \tag{56}$$

where $h(\boldsymbol{r}',s)$ is a magnetic field acting at time s on the spin located at lattice site $\boldsymbol{r}'$. Starting from expression (21) and assuming spatial translation invariance parallel to the surface, we find

$$R((k,\boldsymbol{q}),(k',\boldsymbol{q});t,s) = \sqrt{\frac{g(s)}{g(t)}}\mathrm{e}^{-\omega(k,\boldsymbol{q})(t-s)}\delta(k-k'). \tag{57}$$

The chosen boundary condition enters when transforming back to real space, yielding

$$R^{(\mathrm{d})}((r,\boldsymbol{x}),(r',\boldsymbol{y});t,s) = \sqrt{\frac{g(s)}{g(t)}}\,\mathrm{e}^{-2(t-s)d}\prod_{i=1}^{d-1} I_{x_i-y_i}(2(t-s)) \times (I_{r'-r}(2(t-s)) - I_{r'+r}(2(t-s))), \tag{58}$$

$$R^{(\mathrm{n})}((r,\boldsymbol{x}),(r',\boldsymbol{y});t,s) = \sqrt{\frac{g(s)}{g(t)}}\,\mathrm{e}^{-2(t-s)d}\prod_{i=1}^{d-1} I_{x_i-y_i}(2(t-s)) \times (I_{r'-r}(2(t-s)) + I_{r'+r-1}(2(t-s))). \tag{59}$$

We refrain from giving a full discussion of the response function, but focus instead on the surface autoresponse function $R_1^{(\tau)}(t,s) = R^{(\tau)}((1,\boldsymbol{x}),(1,\boldsymbol{x});t,s)$ 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 (37) of the Bessel function, we then find

$$R_1^{(\mathrm{d})}(t,s) = 4\pi\sqrt{\frac{g(s)}{g(t)}}(4\pi(t-s))^{-(\frac{d}{2}+1)}, \tag{60}$$

$$R_1^{(\mathrm{n})}(t,s) = 2\sqrt{\frac{g(s)}{g(t)}}(4\pi(t-s))^{-\frac{d}{2}}. \tag{61}$$

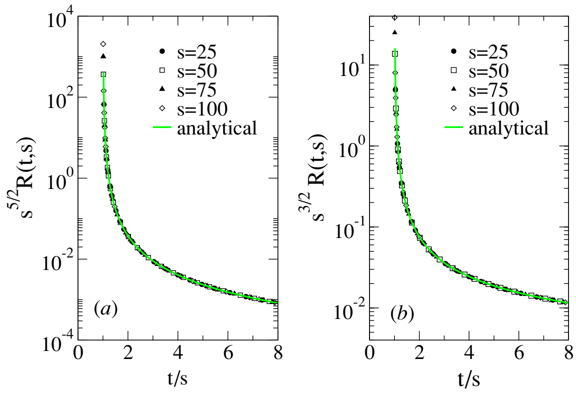

Figure 3. Scaling plots of the autoresponse function for the case $T < T_c$ in three dimensions: (*a*) for Dirichlet boundary conditions with $a_1^{(d)} = \frac{3}{2}$; (*b*) for Neumann boundary conditions with $a_1^{(n)} = \frac{1}{2}$.

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 appendix B. As for the autocorrelation function, we have to distinguish four different cases:

- $T < T_c$: here we have

$$R_1^{(d)}(t,s) = (4\pi)^{-\frac{d}{2}} \left(\frac{t}{s}\right)^{\frac{d}{4}} s^{-(\frac{d}{2}+1)} \left(\frac{t}{s}-1\right)^{-(\frac{d}{2}+1)}, \tag{62}$$

$$R_1^{(n)}(t,s) = 2(4\pi)^{-(\frac{d}{2})} \left(\frac{t}{s}\right)^{\frac{d}{4}} s^{-\frac{d}{2}} \left(\frac{t}{s}-1\right)^{-\frac{d}{2}}. \tag{63}$$

  For both choices of boundary conditions, we observe dynamical scaling (see figure 3) with the exponents

$$a_1^{(d)} = \frac{d}{2}, \qquad a_1^{(n)} = \frac{d}{2} - 1, \qquad \lambda_{R_1}^{(d)} = \frac{d}{2} + 2, \qquad \lambda_{R_1}^{(n)} = \frac{d}{2}. \tag{64}$$

- $T = T_c$ and $2 < d < 4$: we again find dynamical scaling as

$$R_1^{(d)}(t,s) = (4\pi)^{-\frac{d}{2}} \left(\frac{t}{s}\right)^{-\frac{d}{4}+1} s^{-(\frac{d}{2}+1)} \left(\frac{t}{s}-1\right)^{-(\frac{d}{2}+1)}, \tag{65}$$

$$R_1^{(n)}(t,s) = 2(4\pi)^{-\frac{d}{2}} \left(\frac{t}{s}\right)^{-\frac{d}{4}+1} s^{-\frac{d}{2}} \left(\frac{t}{s}-1\right)^{-\frac{d}{2}} \tag{66}$$

  with the following non-equilibrium critical exponents:

$$a_1^{(d)} = \frac{d}{2}, \qquad a_1^{(n)} = \frac{d}{2} - 1, \qquad \lambda_{R_1}^{(d)} = \frac{3}{2}d, \qquad \lambda_{R_1}^{(n)} = \frac{3}{2}d - 2. \tag{67}$$

- $T = T_c$ and $d > 4$: this case yields the expressions

$$R_1^{(d)}(t,s) = (4\pi)^{-\frac{d}{2}} s^{-(\frac{d}{2}+1)} \left(\frac{t}{s}-1\right)^{-(\frac{d}{2}+1)}, \tag{68}$$

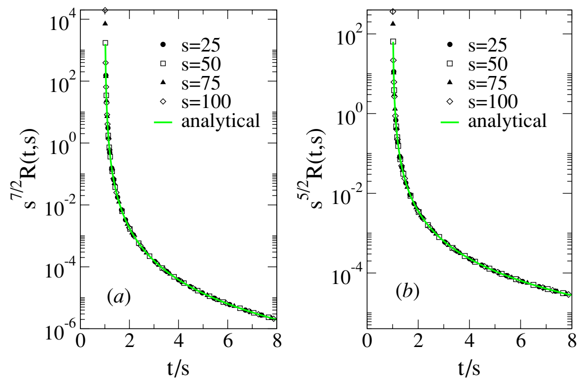

Figure 4. Scaling plots of the autoresponse function for the case $T = T_c$ in five dimensions: (*a*) for Dirichlet boundary conditions; (*b*) for Neumann boundary conditions.

$$R_1^{(n)}(t,s) = 2(4\pi)^{-\frac{d}{2}} s^{-\frac{d}{2}} \left(\frac{t}{s} - 1\right)^{-\frac{d}{2}}. \tag{69}$$

Again dynamical scaling is found, the exponents now taking on the values

$$a_1^{(d)} = \frac{d}{2}, \qquad a_1^{(n)} = \frac{d}{2} - 1, \qquad \lambda_{R_1}^{(d)} = d + 2, \qquad \lambda_{R_1}^{(n)} = d. \tag{70}$$

This dynamical scaling behaviour is illustrated in figure 4 in five dimensions.

- $T > T_c$: due to the exponential behaviour of $g_{\mathrm{age}}(t)$, $R(t,s)$ disappears exponentially:

$$R_1^{(d)}(t,s) = 4\pi\, \mathrm{e}^{-(t-s)/\tau_{\mathrm{eq}}} (4\pi(t-s))^{-(\frac{d}{2}+1)}, \tag{71}$$

$$R_1^{(n)}(t,s) = 2\, \mathrm{e}^{-(t-s)/\tau_{\mathrm{eq}}} (4\pi(t-s))^{-\frac{d}{2}} \tag{72}$$

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.

It has been argued [37] that in out-of-equilibrium dynamics the scaling functions of response functions can be derived from the spacetime symmetries of the corresponding noiseless Langevin equation. This has been checked for a series of exactly solvable systems (see [5, 6] and references therein), among them the spherical model in the bulk system[6]. In [17], local scale invariance was used to derive the following prediction for the surface autoresponse function (with $t > s$):

$$R_1^{\mathrm{LSI}}(t,s) = r_0 \left(\frac{t}{s}\right)^{\zeta_2 - \zeta_1} (t-s)^{-\zeta_1 - \zeta_2}, \tag{73}$$

[6] Note, however, that in critical systems with $z \neq 2$, as for example in the critical two- and three-dimensional Ising models, corrections to the prediction of local scale invariance (LSI) have been shown to exist [38–40]. But even in that case the scaling function coming from the theory of local scale invariance [41] yields an excellent description of the numerically determined autoresponse function.

where ζ_1 and ζ_2 are two exponents left undetermined by the theory and r_0 is a non-universal normalization constant. The values of ζ_1 and ζ_2 are fixed by comparing (73) with the expected scaling behaviour (see equations (6) and (7)) yielding the result

$$R_1^{\rm LSI}(t,s) = r_0\, s^{-1-a_1^{(\tau)}} \left(\frac{t}{s}\right)^{-1-a_1^{(\tau)}} \left(\frac{t}{s}-1\right)^{1+a_1^{(\tau)}-\lambda_{R_1}^{(\tau)}/z}. \tag{74}$$

This prediction is in complete agreement with our exact results for $T \leqslant T_{\rm c}$ for both Dirichlet and Neumann boundary conditions.

Finally, let us mention that it was shown in [42] that the dependence of the full response function (59) on r and r' can be deduced from the spacetime symmetries in the case of Dirichlet boundary conditions.

5. The fluctuation–dissipation ratio

The fluctuation–dissipation ratio

$$X(t,s) := \frac{T R(t,s)}{\partial_s C(t,s)} \tag{75}$$

has been discussed extensively in recent years [43] 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 [7, 23] that in the latter case the non-vanishing limit value

$$X^\infty := \lim_{s\to\infty}\lim_{t\to\infty} X(t,s) \tag{76}$$

is a universal quantity whose value characterizes the given dynamical universality class.

The concept of fluctuation–dissipation ratio, initially introduced for bulk systems, has been generalized in [17] to systems with surfaces. The surface fluctuation–dissipation ratio is thereby defined by

$$X_1(t,s) := \frac{T R_1(t,s)}{\partial_s C_1(t,s)}. \tag{77}$$

The asymptotic value $X_1^\infty := \lim_{s\to\infty}\lim_{t\to\infty} X_1(t,s)$ 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 [7]. Recently, $X_1(t,s)$ has been determined numerically for the critical two- and three-dimensional semi-infinite Ising models [17], 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 [7] yielding the value $\frac{1}{2}$.

Having already determined the surface autocorrelation and autoresponse functions in the previous sections, 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 $X_1^{(\rm n)}(t,s)$ is identical to the bulk quantity $X(t,s)$ obtained in [23]. 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:

- $T < T_{\rm c}$:

$$X_1^{(\rm d)}(t,s) = \frac{4(8\pi)^{-\frac{d}{2}}}{M_{\rm eq}^2} s^{-\frac{d}{2}+1} \left(\frac{\frac{t}{s}+1}{\frac{t}{s}-1}\right)^{\frac{d}{2}+1} \frac{\frac{t}{s}+1}{(4+d)\frac{t}{s}-d} \tag{78}$$

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

$$X_1^{(d)}(t,s) = \frac{d(d-2)\left(\frac{t}{s}+1\right)^3}{(d^2-16) + (32 + d(3d-8))\frac{t}{s} + (d-4)(4+3d)\left(\frac{t}{s}\right)^2 + d^2\left(\frac{t}{s}\right)^3} \quad (79)$$

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:

$$X_1^{(d)}(t,s) = \frac{1}{1 + \left(\frac{\frac{t}{s}-1}{\frac{t}{s}+1}\right)^{\frac{d}{2}+1}} \quad (80)$$

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.

6. Conclusion

In this paper, 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 (such as the autocorrelation and autoresponse functions) reveals 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 [7, 17]. 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

$$C_1(t,s) = s^{-1} f_{C_1}(t/s), \quad (81)$$

in strong contrast to the well-known bulk behaviour [4]

$$C(t,s) = f_C(t/s). \quad (82)$$

As this paper is the first study of ageing phenomena close to a surface in an ordered phase, it is an open and 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 intend to come back to this problem in the near future.

Acknowledgment

We acknowledge the support by the Deutsche Forschungsgemeinschaft through grant no PL 323/2.

Appendix A. Eigenvalues and eigenvectors of the interaction matrix $\mathbf{Q}_\Lambda^{(\tau)}$

The eigenvalues $\mu_\Lambda^{(\tau)}(\boldsymbol{k})$ of the interaction matrix $\mathbf{Q}_\Lambda^{(\tau)}$ depend on the boundary conditions and are given by [33]

$$\mu_\Lambda^{(\tau)}(\boldsymbol{k}) = 2\sum_{\nu=1}^{d} \cos\left(\varphi_{L_\nu}^{(\tau_\nu)}(k_\nu)\right), \qquad \boldsymbol{k} \in \Lambda, \tag{A.1}$$

where the functions $\varphi_L^{(\tau)}$ are

$$\varphi_L^{(\text{p})}(k) = \frac{2\pi k}{L} \quad \text{(periodic)}, \tag{A.2}$$

$$\varphi_L^{(\text{d})}(k) = \frac{\pi k}{L+1} \quad \text{(Dirichlet)}, \tag{A.3}$$

$$\varphi_L^{(\text{n})}(k) = \frac{\pi(k-1)}{L} \quad \text{(Neumann)}. \tag{A.4}$$

The (orthonormal) eigenvectors are given by the expressions

$$u_\Lambda^{(\tau)}(\boldsymbol{r}, \boldsymbol{k}) = \prod_{\nu=1}^{d} u_{L_\nu}^{(\tau_\nu)}(r_\nu, k_\nu) \tag{A.5}$$

with

$$u_L^{(\text{p})}(r,k) = L^{-\frac{1}{2}} \exp\left(-\text{i} r \varphi_L^{(\text{p})}(k)\right), \tag{A.6}$$

$$u_L^{(\text{d})}(r,k) = [2/(L+1)]^{\frac{1}{2}} \sin\left(r \varphi_L^{(\text{d})}(k)\right), \tag{A.7}$$

$$u_L^{(\text{n})}(r,k) = \begin{cases} L^{-\frac{1}{2}}, & k = 1, \\ (2/L)^{\frac{1}{2}} \cos\left(\left(r - \frac{1}{2}\right)\varphi_L^{(\text{n})}(k)\right), & k = 2, \ldots, L. \end{cases} \tag{A.8}$$

Appendix B. Asymptotic behaviour of *g*

In this appendix, we recall the asymptotic behaviour [23] of the function

$$g(t) = \hat{f}(t) + 2T \int_0^t \mathrm{d}u\, \hat{f}(t-u) g(u) \tag{B.1}$$

with

$$\hat{f}(t) := \int_{-\pi}^{\pi} \frac{\mathrm{d}^{d-1}\boldsymbol{q}}{(2\pi)^{d-1}} \int_{-\pi}^{\pi} \frac{\mathrm{d}k}{2\pi}\, \mathrm{e}^{-2\omega(k,\boldsymbol{q})t} = \left(\mathrm{e}^{-4t} I_0(4t)\right)^d. \tag{B.2}$$

Defining first the constants

$$A_j := \int \frac{\mathrm{d}^{d-1}\boldsymbol{q}}{(2\pi)^{d-1}} \int_{-\pi}^{\pi} \frac{\mathrm{d}k}{2\pi} \frac{1}{(2\omega(k,\boldsymbol{q}))^j}, \tag{B.3}$$

the critical temperature can be expressed as

$$T_\text{c} := \frac{1}{2A_1}. \tag{B.4}$$

The asymptotic behaviour of g for long times, denoted as g_age, is then given by

- $T > T_c$:

$$g_{age}(t) \overset{t\to\infty}{\sim} e^{t/\tau_{eq}}, \tag{B.5}$$

where the exact expression for the time scale τ_{eq} can be found in [23].

- $T < T_c$:

$$g_{age}(t) \overset{t\to\infty}{\sim} \frac{(8\pi t)^{-\frac{d}{2}}}{M_{eq}^2} \qquad \text{with} \qquad M_{eq}^2 = 1 - \frac{T}{T_c}. \tag{B.6}$$

- $T = T_c$ and $2 < d < 4$:

$$g_{age}(t) \overset{t\to\infty}{\sim} (d-2)(8\pi)^{\frac{d}{2}-1} \sin\left(\frac{(d-2)\pi}{2}\right) \frac{t^{-(2-\frac{d}{2})}}{T_c^2}. \tag{B.7}$$

- $T = T_c$ and $d > 4$:

$$g_{age}(t) \overset{t\to\infty}{\to} \frac{1}{4A_2 T_c^2}. \tag{B.8}$$

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