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Study of the dynamical approach to the interface localization–delocalization transition of the confined Ising model

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Abstract

Confined magnetic Ising films in a $L \times D$ geometry ($L \ll D$), with short-range competing magnetic fields (h) acting at opposite walls along the D-direction, exhibit a slightly rounded localization–delocalization transition of the interface between domains of different orientations that runs parallel to the walls. This transition is the precursor of a wetting transition that occurs in the limit of infinite film thickness ($L \to \infty$) at the critical curve $T_w(h)$. For $T < T_w(h)$ ($T > T_w(h)$) such an interface is bounded (unbounded) to the walls, while right at $T_w(h)$ the interface is freely fluctuating around the centre of the film.

Starting from disordered configurations, corresponding to $T = \infty$, we quench to the wetting critical temperature and study the dynamics of the approach to the stationary regime by means of extensive Monte Carlo simulations. It is found that for all layers parallel to the wall (rows), the row magnetizations exhibit a peak at a time $\tau_{max} \propto L^2$ and subsequently relax to the stationary, equilibrium behaviour. The characteristic time for such a relaxation scales as $\tau_R \propto L^4$, as expected from theoretical arguments, that are discussed in detail.

1. Introduction

The critical behaviour of confined materials is rather different from bulk criticality due to the subtle interplay between finite-size and surface effects. Within this context, the study of the critical properties of confined systems has attracted considerable attention over the last decades [1–13]. The interaction of a saturated gas in contact with a wall or a substrate may result in the occurrence of interesting wetting and capillary condensation phenomena, where a

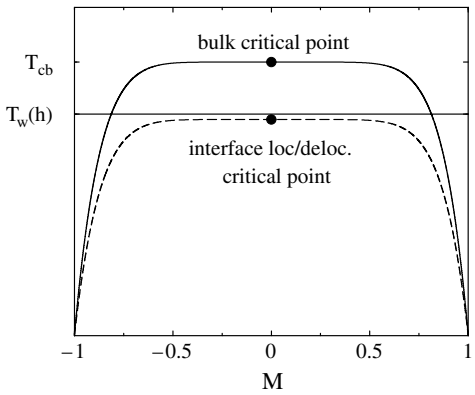

Figure 1. Sketch of the phase diagram of the bulk system (solid curve), which exhibits two-dimensional Ising behaviour at the critical temperature T_{cb}, and the behaviour of the confined system (dashed curve). The temperature T (ordinate) and the average magnetization M (abscissa) are chosen as independent variables. As the confined system is only quasi-one-dimensional, there is no true thermodynamic transition. The pseudo-critical point is located at $T_c(h, L)$ which differs from the well defined wetting transition temperature $T_w(h)$ only by a term which is very small for large film thickness L. The dashed curve describes phase separation on the length scale smaller than the equilibrium domain size that results in this system.

macroscopically thick liquid layer condenses at the wall, while the bulk fluid may remain in the gas phase [14–18]. The understanding of the wetting of solid surfaces by a fluid is of primary importance for many technological applications (lubrication, efficiency of detergents, oil recovery in porous material, stability of paint coatings, interaction of macromolecules with interfaces, etc [14, 19–21]).

Wetting transitions are also observed when a magnetic material is confined between parallel walls where competing surface magnetic fields act. We consider an Ising film [22, 23] which is confined between two competing walls a distance L apart from each other, such that the surface magnetic fields, h, are of the same magnitude but opposite directions [5, 6, 12, 13]. Close to the critical temperature T_{cb} of the bulk, domains of opposite magnetizations gradually build up at the corresponding walls and stabilize an interface which fluctuates around the centre of the film. Upon reducing the temperature further one encounters an interface localization–delocalization transition. Below the L-dependent transition temperature, $T_c(L, h)$, the system laterally phase separates into domains, in which the interface is localized either at the right- or the left-hand wall. This transition can be of second or first order, and we restrict ourselves here to a critical interface localization–delocalization transition. The qualitative behaviour is illustrated in figure 1. This interface localization–delocalization transition is a precursor of the true wetting transition $T_w(h)$ of the infinite system. In fact, the difference $T_w(h) - T_c(L, h)$ vanishes exponentially fast upon increasing the film thickness L for $d = 3$ dimensions.

Intriguingly, the universality class for the static critical behaviour of the interface localization–delocalization transition of a d-dimensional system corresponds to the $(d - 1)$-dimensional bulk system [24]. This behaviour has been confirmed for the static critical behaviour in three dimensions. In contrast to the considerable effort directed towards understanding their critical behaviour under equilibrium (stationary) conditions, little attention has been drawn to the study of the dynamical approach of films to their equilibrium states. In order to overcome this gap the aim of this manuscript is to present an extensive numerical study of quenching experiments close to the pseudo-critical point of the confined system that are

performed starting from fully disordered configurations ($T = \infty$). Does the relation between critical behaviour of the interface localization–delocalization transition in d dimensions and the bulk ordering in $d - 1$ dimension also hold for the kinetics?

The study of nonequilibrium relaxation right at the critical point is of great interest for several reasons: first of all, critical dynamics of bulk kinetic Ising models (with no conserved quantities) is a topic of longstanding discussion [25–32]. In particular, the value of the critical exponent z that describes the divergence of the relaxation time τ characterizing the asymptotic decay of order parameter fluctuations at criticality ($\tau \propto \xi^z$ where ξ is the correlation length of order parameter fluctuations) has been controversial for a long time [33]. One now believes that for the short-range two-dimensional Ising model z is known rather precisely [31], $z = 2.169 \pm 0.003$ for single-spin-flip dynamics—the same dynamics as we shall use in the following. Hence, one could expect this exponent also to ultimately describe the critical dynamics of the interface localization–delocalization transition in thin, three-dimensional Ising films with competing walls, since this phase transition belongs to the $d = 2$ Ising class.

The standard discussions of critical slowing down [34] all consider the dynamics of fluctuations in spatially homogeneous systems close to the bulk critical point at $T_{\rm cb}$. Here however, we consider a system at $T_{\rm c}(L, h) \approx T_{\rm w}(h) < T_{\rm cb}$ that is always spatially very inhomogeneous, containing regions of positive and negative magnetization separated by an interface (see snapshots in figure 4). While the universality of the static behaviour requires the type of the order parameter (i.e. a single scalar quantity, the average magnetization in a column perpendicular to the wall) to be identical, the universality of the dynamic behaviour poses additional requirements (e.g., a single-spin-flip algorithm has a different dynamic critical exponent z than a cluster algorithm). Hence, one could intuitively expect that the problem may be related to the dynamics of growing wetting layers at surfaces [35] and the dynamics of capillary waves [36]. Furthermore, we note that in the static behaviour the Ising regime around $T_{\rm c}(L, h)$ is extremely small for large film thickness L. Generally, there is a crossover from Ising to mean field behaviour further away from the critical point. The extension of a reduced temperature interval around the critical point where Ising critical behaviour is observable can be quantified by the Ginzburg number, Gi. While in the bulk ordering with short-range interactions the Ginzburg number is of order unity [37], it vanishes exponentially with the film thickness L in the case of an interface localization–delocalization transition for three-dimensional films [24, 38] and two-dimensional films [39]. (In the latter case, there occurs a rounded transition [8] from the state with a delocalized interface to the state that contains domains with localized interfaces in this Ising critical region, and these domains are exponentially large in L in the direction along the boundaries.)

An additional motivation for the study of nonequilibrium relaxation at criticality is that for standard critical phenomena in the bulk such studies also allow accurate estimates of various static critical exponents [40–46]. For example, the static structure factor $S(k, t)$ of an Ising magnet is predicted to scale as [40]

$$S(k, t) = [\ell(t)]^{\gamma/\nu} \tilde{S}(k\ell(t)), \qquad \ell(t) \propto t^{1/z} \tag{1}$$

where γ, ν are the critical exponents of the susceptibility and $\ell(t)$ is a kind of dynamically growing correlation length, respectively. For standard systems in the bulk, relations such as equation (1) seem to hold at rather short times already [45]. Thus, it is interesting to test relations similar to equation (1) also for the interface localization–delocalization transition.

As a first step, we study a two-dimensional system and assume a single-spin-flip kinetic Ising model which does not conserve the order parameter. In $d = 2$ dimensions, one considers a strip of finite width L confined by straight line boundaries. In two-dimensional Ising films no truly long-range order develops for finite temperatures, because the system is infinitely

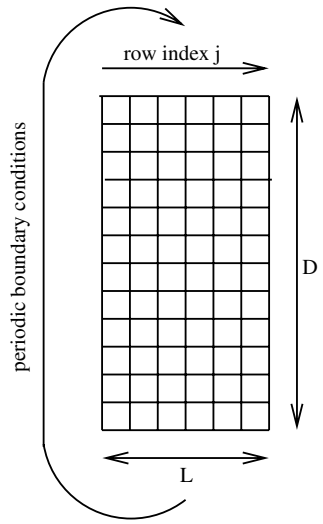

Figure 2. Illustration of the geometry of the simulated system.

extended in one spatial direction only (quasi-one-dimensional) [48]. For the one-dimensional Ising model the true transition occurs at $T = 0$, and the Glauber dynamics of the kinetic Ising model in one dimension is known exactly. At the critical temperature, $T_{cb}(d = 1) = 0$, one finds $\tau \propto \xi^2$, i.e., $z = 2$ [49].

In this work, however, we consider the ordering at the finite wetting transition temperature $T_w(h)$ of the two-dimensional Ising model, since $T_w(h)$ can be taken as an effective transition temperature of the rounded interface localization–delocalization transition of the thin film. Since the system is quasi-one-dimensional one expects that the interface localization–delocalization transition at $T_c(h, L)$ is rounded. For large L the rounding of this transition is so small that practically it can hardly be distinguished from a sharp phase transition at $T_w(h)$. The disadvantage of the rounding in a quasi-one-dimensional system is outweighed by the exact knowledge of the wetting transition temperature due to work by Abraham [47] and the ease of visualization of the system configurations.

The manuscript is organized as follows: after a short description of the theoretical background, we describe in section 3 the numerical procedure for the simulation of the Ising model in confined geometries. The results are presented and discussed in section 4, while the conclusions are summarized in section 5.

2. Theoretical background

We consider the time evolution of a d-dimensional thin Ising film of thickness L confined by competing walls (cf figure 2) after a quench from $T = \infty$ (where the spin configuration is completely disordered) to $T = T_c(h, L)$ ($=T_w(h)$ here). As explained for $d = 2$, the system is quasi-one-dimensional and the critical interface localization–delocalization transition rounded off. In a strict sense, in $d = 2$, there is no thermodynamic transition at the pseudo-critical temperature $T_c(h, L)$ and different quantities (e.g. specific heat or magnetic susceptibility) used to locate the effective transition temperature will yield different estimates. The difference between these estimates, the extent of the rounding in the temperature, and the difference between the pseudo-critical temperature $T_c(h, L)$ and the wetting critical temperature $T_w(h)$

is of the same order and vanishes fast with the film thickness L. Instead of locating an effective, pseudo-critical temperature $T_c(h, L)$, we define the pseudo-critical temperature as $T_c(h, L) \equiv T_w(h)$ using the exact analytical expression for the wetting transition of the two-dimensional Ising model [47]. L denotes the thickness of the film and D characterizes the extension in the remaining $d-1$ directions. The number of lattice sites is $N = LD^{d-1}$. In $d > 2$, of course, a well defined $T_c(h, L)$ distinct from $T_w(h)$ exists [6, 8, 38], but this case is not considered in the present simulational study.

For the time evolution, we expect several distinct stages: in the first stage, small domains with magnetizations $\pm m_b$ (where m_b denotes the spontaneous magnetization of the Ising model in the bulk at the considered temperature $T_c(h, L) < T_{cb}$) are growing everywhere in the system, except in the layers directly adjacent to the walls, where rather a uniform layer with a magnetization that has the same sign as the surface field may grow. Note, however, that the growth of the layers is not related to the wetting layer growth considered by Lipowsky [35], since in the latter work one rather considers growth of wetting layers at the surface of a semi-infinite system which is in thermal equilibrium at the coexistence curve in the bulk, with uniform magnetization far away from the surface, and one assumes the temperature T to be larger than the wetting transition temperature, $T_w(h)$. Furthermore, the system in the bulk is highly nonuniform. The dynamics resembles somewhat the intensively studied problem of surface-directed spinodal decomposition [50–56]. However, in the latter problem the order parameter is conserved, while in the present problem it is not, and both for the problem of critical dynamics [34, 57] and the problem of the growth of domains in the bulk for $T < T_{cb}$ (also called 'phase ordering dynamics') [40, 57–59] it is known that the presence or absence of conservation laws has a major effect on the observed laws for relaxation and/or growth. In particular, for the case where no conservation law whatsoever applies, such as the single-spin-flip kinetic Ising model [25–33, 41, 49] or related field-theoretical 'model A' [34], there is consensus that linear dimensions $\ell(t)$ of domains in the bulk grow with the Lifshitz [60]–Cahn–Allen [61] law,

$$\ell(t) \propto t^x, \qquad x = 1/2 \tag{2}$$

and the equal-time structure factor $S(k, t)$,

$$S(\vec{k}, t) = \frac{1}{N}\left\langle \sum_{\mathbf{r},\mathbf{r}'} \exp[\mathrm{i}\vec{k}\cdot(\mathbf{r}-\mathbf{r}')]\sigma_{\mathbf{r}}(t)\sigma_{\mathbf{r}'}(t)\right\rangle, \tag{3}$$

where $\sigma_{\mathbf{r}}$ denotes the spin variable at site $\mathbf{r}$, grows as [57–59]

$$S(\vec{k}, t) = [\ell(t)]^d \tilde{S}(k\ell(t)). \tag{4}$$

$\tilde{S}(\zeta)$ is a scaling function with a maximum at $\zeta = 0$ (remember that $\ell(t)$ can be defined by $S(k = \ell^{-1}(t), t) = S(0, t)/2$, see for instance [40]). By the average in equation (3), we denote an average over many statistically independent realizations of the time evolution with different initial conditions that all correspond to temperature $T = \infty$. This average is necessary, since $S(\vec{k}, t)$ is not self-averaging [62]. Note that $S(\vec{k}, t)$ is normalized such that for an initial random starting configuration $S(\vec{k}, 0) = 1$, since only the terms $\mathbf{r} = \mathbf{r}'$ contribute, and $\sigma_{\mathbf{r}} = \pm 1$ with equal probability. We also recall that [40] $S(0, t) = N\langle[M(t)]^2\rangle$, where $M(t)$ denotes the time-dependent magnetization

$$M(t) = \frac{1}{N}\sum_{\mathbf{r}} \sigma_{\mathbf{r}}(t). \tag{5}$$

Therefore, one concludes that $N\langle[M(t)]^2\rangle = [\ell(t)]^d \tilde{S}(0)$, and since $\tilde{S}(0)$ is a constant of order unity which we may absorb in the scale of $\ell(t)$, one may alternatively define $\ell(t)$ as

follows [40]:

$$\ell(t) = (N\langle[M(t)]^2\rangle)^{1/d}. \tag{6}$$

Note that equation (3) does not subtract a term $\langle\sigma_{\mathbf{r}}(t)\rangle\langle\sigma_{\mathbf{r}'}(t)\rangle$, and hence $S(k, t)$ for $t \to \infty$ is not dominated by the standard structure factor in equilibrium, $S(k) = (1/N)\sum_{\mathbf{r},\mathbf{r}'} \exp[\mathrm{i}\vec{k} \cdot (\mathbf{r} - \mathbf{r}')][\langle\sigma_{\mathbf{r}}\sigma_{\mathbf{r}'}\rangle - \langle\sigma_{\mathbf{r}}\rangle\langle\sigma_{\mathbf{r}'}\rangle]$, which only would be a correction to equation (4), but rather by a δ-function at $k = 0$ representing long-ranged order. Equation (4) describes the rounding of this δ-function (i.e. Bragg peaks) by the finite domain size.

From equations (2) and (6) one predicts that in the very early stages of the quench to $T < T_{\mathrm{cb}}$, where $\ell(t) \ll L$ and no interface running parallel to the walls separating positive and negative magnetization has yet been established, one observes bulklike two-dimensional phase ordering dynamics for $T < T_{\mathrm{cb}}$ and a scaling with a trivial exponent

$$\langle[M(t)]^2\rangle \propto N^{-1}t^{d/2} = N^{-1}t \qquad (d = 2). \tag{7}$$

However, when $\ell(t)$ has grown to about the size $L/2$, an interface starts to develop, and domains start to grow that are very anisotropic in shape, with linear dimensions in the directions parallel to the wall much longer than perpendicular to it. Then the system approaches its equilibrium and the static critical behaviour is characterized by the $(d-1)$-dimensional Ising universality class. If $d > 2$ and hence a well defined non-zero critical temperature $T_{\mathrm{c}}(h, L)$ exists, one could speculate that in this regime equation (1) should hold, i.e.,

$$\langle[M(t)]^2\rangle \propto N^{-1}t^{\gamma/z\nu} = N^{-1}t^{(d''-2\beta/\nu)/z}, \tag{8}$$

where hyperscaling relations [63] have been used, $d'' = d - 1$ being the dimensionality of the system in the directions in which the system is still infinite, and also the critical exponents β, γ, ν, z should be that of a $(d-1)$-dimensional system. However, our system is quasi-one-dimensional, $d'' = 1$. The kinetics exponents for $d'' = 1$ are known exactly [49], but this ordering kinetics rather corresponds to a quench to $T = 0$ and not to $T_{\mathrm{w}}(h)$. As a consequence, it is still completely unknown what growth law one should expect to hold instead of equation (8) in our case ($d = 2$) where we quench to $T = T_{\mathrm{w}}(h)$, at times where $l(t)$ exceeds the size $L/2$ (in the direction parallel to the walls).

Alternatively, we consider the very late stage of approach to equilibrium, where the order parameter profile across the film develops towards its equilibrium shape. Assuming that the important fluctuations are those of the interface that runs between regions that already have the bulk average magnetization, we are tempted to extend the description of the transition in terms of the capillary wave Hamiltonian [24, 38, 8] to the dynamics. In fact, this yields a model of the type considered by Grant [36], in d dimensions,

$$\frac{\partial h(\vec{\rho}, t)}{\partial t} = -D^* \frac{\delta\mathcal{F}}{\partial h(\vec{\rho}, t)} + \eta(\vec{\rho}, t) \qquad \text{with } \mathcal{F}[h] = \frac{\Sigma}{2}\int \mathrm{d}^{d-1}\boldsymbol{\rho}\,(\nabla h)^2 \tag{9}$$

where $h(\boldsymbol{\rho}, t)$ is the local position of the interface, measured relative to its mid-point $z^* = L/2$, $\boldsymbol{\rho} = (x, y)$ is a coordinate in the directions parallel to the interface, and $1/D^*$ is a constant setting the timescale. Grant employed a capillary wave Hamiltonian $\mathcal{F}$, where Σ denotes the interfacial stiffness. η is a random force that satisfies the dissipation–fluctuation relation

$$\langle\eta(\vec{\rho}, t)\eta(\vec{\rho}\,', t')\rangle = 2k_{\mathrm{B}}T\,D^*\delta(\vec{\rho} - \vec{\rho}\,')\delta(t - t'). \tag{10}$$

While Grant [36] considered a freely fluctuating interface, we here have to include the effect of the wall potentials. Above the critical temperature of the interface localization–delocalization transition $T > T_{\mathrm{c}}(h, L)$, these wall potentials are responsible for making the correlation length $\xi_{\parallel}$ of interfacial fluctuations parallel to the wall finite [24, 38]. However, right at $T_{\mathrm{c}}(h, L)$ one recovers within the linear mean-field description of the interface localization–delocalization transition capillary waves on all length scales, such that the problem reduces

exactly to the same problem as studied by Grant [36], apart from the fact that he studied the growth of the width $W(t)$ of an initially flat interface with time, obtaining

$$W(t) \propto t^{(3-d)/4}. \tag{11}$$

In our case, this result could apply only as long as $W(t) < L$, since the interface is confined between the two parallel walls. Hence, one concludes that $W(t)$ for an initially flat interface grows at $T_c(h, L)$ until a time τ_R defined from $W(t = \tau_R) = L/2$, which yields

$$\tau_R \propto L^4. \tag{12}$$

It is tempting to assume that the same timescale τ_R also controls the dynamics to equilibrium here. Then, the dynamics of interface fluctuations also controls the relaxation time of the magnetization.

3. The confined Ising ferromagnet with competing fields and the Monte Carlo simulation method

The Hamiltonian H corresponding to the Ising model with competing surface fields in a confined geometry of size $L \times D$ ($L \ll D$) (cf figure 2) is given by

$$H = -J \sum_{\langle ij,mn \rangle}^{D,L} \sigma_{ij}\sigma_{mn} - h_1 \sum_{i=1}^{D} \sigma_{i1} - h_L \sum_{i=1}^{D} \sigma_{iL}, \tag{13}$$

where σ_{ij} are the Ising spin variables at the site of coordinates (i, j) and they may assume two different values, namely $\sigma_{ij} = \pm 1$. $J > 0$ is the coupling constant of the ferromagnet and the first sum of equation (13) runs over all the nearest-neighbour pairs of spins such that $1 \leqslant i \leqslant D$ and $1 \leqslant j \leqslant L$. The second (third) sum corresponds to the interaction of the spins placed at the surface layer $j = 1$ ($j = L$) of the film where a short-range surface magnetic field h_1 (h_L) acts. Open boundary conditions are assumed along the D-direction of the film where the fields act. In this manuscript, only the case of competing surface fields such that $h_1 = -h_L$, in the absence of any bulk magnetic field, is considered. So, hereafter $h = |h_1| = |h_L|$ will be used generically to specify the short-range surface magnetic field that is measured in units of the coupling constant J.

The evolution of the Ising film is simulated using the standard Metropolis algorithm. The time is measured in Monte Carlo steps (mcs), such that during one mcs we attempt to flip all $L \times D$ spins of the sample once on average. The Ising magnet in two dimensions and in the absence of any external magnetic field undergoes a second order order–disorder transition at the Onsager critical temperature $k_B T_{cb}/J = 2/\ln(1+\sqrt{2}) = 2.269\ldots$ [23]. In the following, temperatures are reported in units of T_{cb}.

Simulations are started using disordered configurations with zero initial magnetization ($m_0 \equiv 0$). Subsequently, the dynamic approach to the stationary regime is followed measuring relevant quantities (see below) and taking averages over many different initial configurations. For a suitable range of fields and temperatures, the formation of an interface between magnetic domains of opposite directions running along the film is observed. Such an interface undergoes a localization–delocalization transition (as the temperature is raised keeping h constant). This interface localization–delocalization transition is the signature of the wetting phase transition taking place in the limit $L \to \infty$. The wetting phase diagram has been calculated exactly by Abraham [47], yielding

$$\exp(2J/k_B T) \cdot [\cosh(2J/k_B T) - \cosh(2h_c/k_B T)] = \sinh(2J/k_B T), \tag{14}$$

where $h_c(T)$ is the critical surface field (the inverse function of the wetting temperature $T_w(h)$).

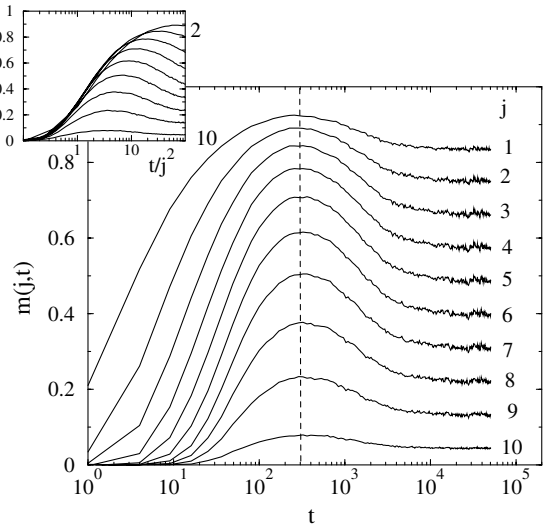

Figure 3. Linear–logarithmic plot of the row magnetization $m(j,t)$ versus time (measured in mcs). Note that each row is identified on the right-hand side of the figure. Results obtained for $h_w = 0.7229$ and $T_w = 0.700$, that corresponds to a critical point of the wetting phase diagram according to Abraham [47]. The lattice size is $L = 20$, $D = 1024$, and results are averaged over 1000 different initial conditions. The dashed curve shows the location of the maxima of the row magnetization and has been drawn to guide the eyes. In the inset the data are plotted versus t/j^2 (j being the row index).

The magnetization in layers parallel to the walls (rows) measured along the L-direction and averaged over the D-direction is given by

$$m(j,t) = \left\langle \frac{1}{D} \sum_{i=1}^{D} \sigma_{ij}(t) \right\rangle \tag{15}$$

where $\langle\rangle$ corresponds to averages taken over different realizations of the quench. The row magnetizations describe the magnetization profiles $m(j)$, $1 \leqslant j \leqslant L$, for any desired time t.

Also, the kth moment of the magnetization of the film is measured as

$$m^k(t) = \left\langle \left[\frac{1}{LD} \sum_{i=1}^{D} \sum_{j=1}^{L} \sigma_{ij}(t) \right]^k \right\rangle. \tag{16}$$

4. Results and discussion

Figure 3 shows linear–logarithmic plots of the row magnetization $m(j,t)$ versus time, obtained by starting from disordered configurations. The dynamical evolution has been followed at the critical point ($T_w = 0.7$, $h_w = 0.7229$) of the wetting phase diagram given by equation (14). This choice of temperature ($T_w = 0.7$) is arbitrary; in principle the behaviour is the same in the whole regime $0 < T < T_{cb}$. However, we want to avoid temperatures close to T_{cb} (then the bulk correlation length would be large) and we also want to avoid low temperatures where the interface would become non-rough over rather large scales. It is observed that within a short-time regime the absolute value of the row magnetization $m(j,t)$ increases monotonically, and reaches maximal values at a certain time τ_{max}, that is almost independent of the row j. This is a

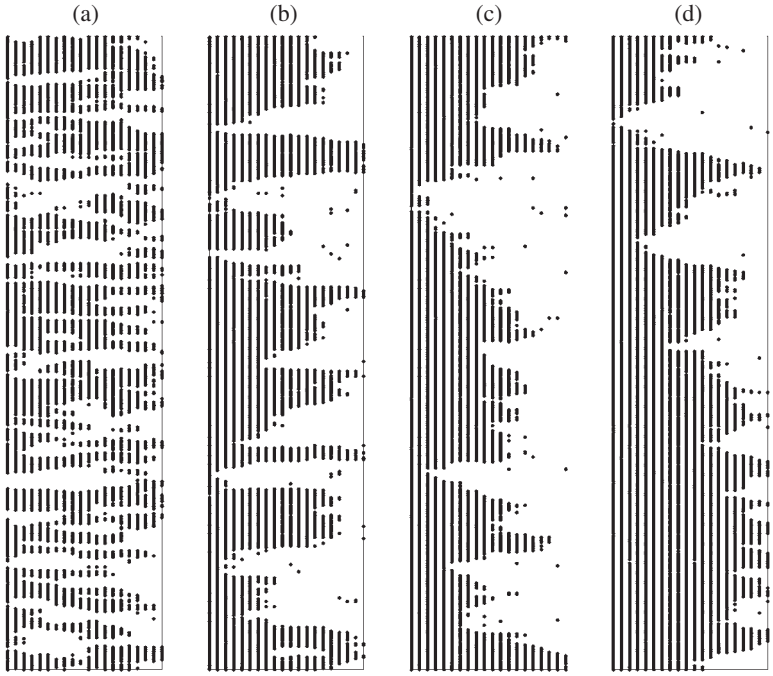

Figure 4. Typical snapshot configurations obtained during the dynamic evolution of the film towards the stationary state. The lattice size is $L = 20$, $D = 512$ and the snapshots were obtained for $h_w = 0.7229$ and $T_w = 0.700$. (a) $t = 10$ mcs, (b) $t = 80$ mcs, (c) $t = 300$ mcs and (d) $t = 20\,000$ mcs. Note that the scale of the coordinate along the films is chosen as a factor of 6.4 smaller than the scale perpendicular to the film.

surprising, unexpected result. Subsequently, $|m(j, t)|$ decreases, reaching a plateau during the long-time regime, that corresponds to the (averaged) stationary values of film magnetization.

Qualitatively, the behaviour of the row magnetization can be understood with the aid of snapshots of configurations shown in figure 4. At very early times ($t = 10$ mcs in figure 4(a)), a sequence of magnetic domains with up and down orientations, running along the L-direction, are observed. During this initial regime the time evolution of the absolute value of the row magnetization depends on the scaling variable t/j^2 as shown in the inset of figure 3. In the bulk, one has a situation similar to that observed in the absence of fields close to bulk criticality [2, 3]. However, at this stage the surface fields cause the onset of spins nucleating (parallel to each field) in the ultimate vicinity of the surfaces, while these fields are still not relevant at the centre of the film. The overall effect is a minor increase of the magnetization close to the surface of the films while the magnetization of the bulk remains negligible (see figure 3). For $t = 80$ mcs (figure 4(b)) a rough interface between domains of spins up and down has emerged. The nucleation of spins close to the surface still continues and the surface fields start to play a role in the centre. Due to these effects the absolute value of the magnetization of all rows increases (see figure 3). Even at this stage, domains attached to the surfaces and having opposite orientations develop almost independently from each other. At $t = 300$ mcs (figure 4(c)) the row magnetizations reach maxima for all rows, indicating the onset of interference between the domains growing attached to opposite surfaces. Then, an interface that runs parallel to the surfaces has formed. It is smoother than in equilibrium, yet the excursions are of the order of the film width, L. After this stage and for the stationary state, $t = 20\,000$ mcs in figure 4(d),

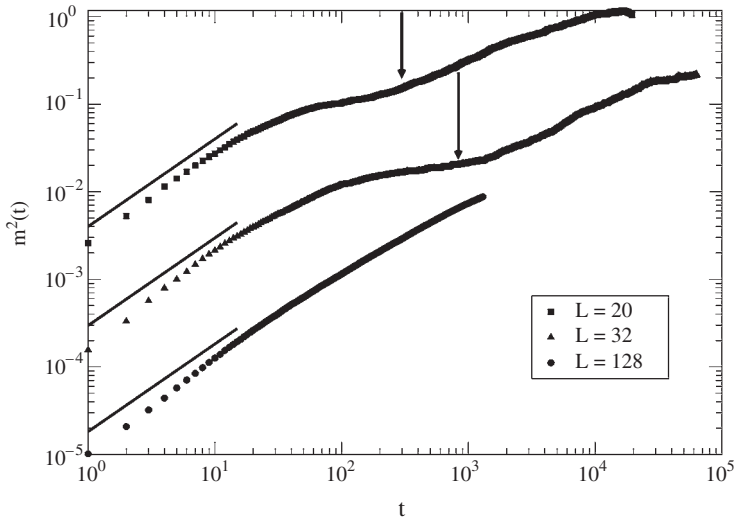

Figure 5. Log–log plots of the second moment of the magnetization $m^2(t)$ versus time (measured in mcs). Results obtained for $h_w = 0.7229$ and $T_w = 0.700$ and using lattices of different width L, as shown in the figure. The full lines show the behaviour according to equation (7). The arrows show the location of the maxima of the row magnetization and have been drawn to guide the eyes. The data are shifted along the vertical axis for the sake of clarity.

excursions of the interface up to the boundaries of the film are built up and cause a small decrease of the row magnetization (see figure 3). The occurrence of the maxima in the row magnetizations corresponds to the presence of a plateau in the log–log plot of $m^2(t)$ versus t (cf figure 5), while for much shorter times the relation (cf equation (7)) $m^2(t) \propto t$ is verified in figure 5.

Assuming a diffusive-like behaviour in the development of correlations within domains attached to the surfaces, as discussed previously along the description of the results shown in figure 4 and also suggested by the scaling observed in the inset of figure 3, it may be expected that the time at the occurrence of the maxima should be linked to the lattice width according to the following relationship:

$$\tau_{max} \propto L^2. \tag{17}$$

Figure 6 shows that a plot of $\tau_{max}^{1/2}$ versus L gives a straight line, confirming the proposal of equation (17). Note that we observe at short times a two-dimensional growth characteristic for bulk ordering at $T < T_{cb}$. As the strength of the surface interactions corresponds exactly to a second-order wetting transition, they are not strong enough to nucleate a single-domain layer of spins with sign that corresponds to the wall interaction, which then grows and extends further into the film. Only for stronger surface fields or higher temperature, $T \gg T_w(h)$, could one expect a diffusive growth of a laterally homogeneous layer of spins at the walls, which would then lead to $\tau_{max} \propto \Delta j^2$, where Δj denotes the distance from the surface.

At the wetting temperature $T_w(h)$ and within the stationary regime, the magnetization profile is simply linear [64] and it is given by

$$m(j) = m_b(-1 + 2j/L), \tag{18}$$

except in the immediate vicinity of the boundaries. In equation (18), m_b is the bulk magnetization of the Ising model at $T = T_w(h)$. Defining the width W of the interfacial profile as the second moment of the profile [65], it follows that $W \propto L$ [66].

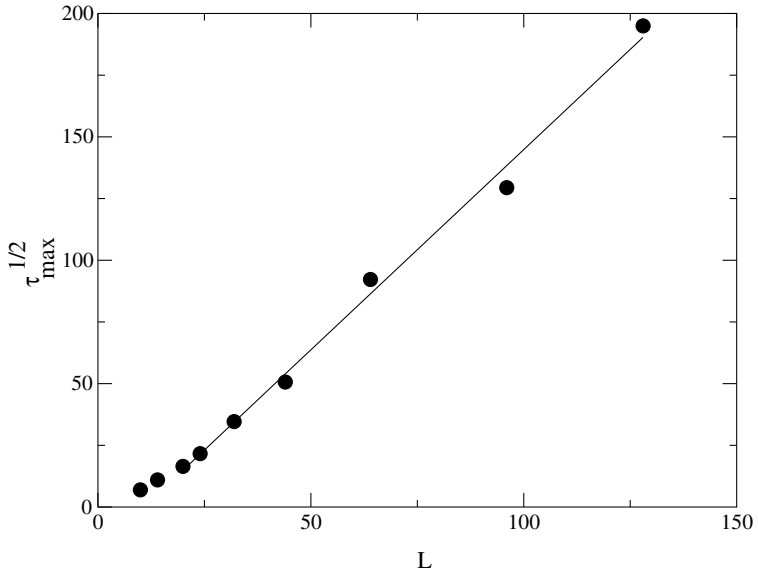

Figure 6. Plot of $\tau_{max}^{1/2}$ versus L. Data obtained for $h_w = 0.7229$ and $T_w = 0.700$.

Figure 7(a) shows that the magnetization profiles obtained numerically are, in fact, linear in agreement with the theoretical calculations [64]. Of course, for very small L such as $L = 10$ and 14 corrections to scaling occur, as expected. However, during the dynamic evolution towards the stationary state and particularly when the row magnetization exhibits a maximum, the magnetization profiles adopt a sigmoidal shape, as shown in figure 7(b). This quantifies the observation that the interface in this intermediate regime is smoother than in equilibrium (cf figure 2(c)). These profiles are fitted quite accurately by means of error functions and the interface width resulting from the fits depends linearly on L (see the inset of figure 7(b)). In this transient regime far from equilibrium a simple scaling behaviour of the profile does not seem to hold.

As observed in figure 3, for $t > \tau_{max}$ the row magnetization exhibits a decay until the stationary regime is established. It has been found that, in all cases, such a decay can be well fitted by an exponential relaxation of the form

$$m(t) = \Delta m \exp(-(t - \tau_{max})/\tau_R) + m_s, \tag{19}$$

while a power-law decay can safely be ruled out. In equation (19) m_s is the row magnetization in the stationary regime, τ_R is the relaxation time and $\Delta m = m_{max} - m_s$, where m_{max} is the maximum value of the row magnetization (i.e. measured at $t = \tau_{max}$). So, fitting the data using equation (19), as shown in figure 8, the relaxation time can be obtained.

The relaxation of the magnetization to its equilibrium value goes along with the equilibration of the smooth interface position around τ_{max} to the strongly fluctuating one at longer times. Hence, the dynamics of interface fluctuations described by equation (12) sets the timescale and we expect that τ_R may depend on the lattice size according to $\tau_R \propto L^n$ with $n = 4$. As shown in figure 9, $n = 4$ yields a good fit. The exponential decay of the row magnetization is also observed above the wetting critical curve, i.e. for $h_w = 0.7229$ and $T > T_w = 0.700$, and the dependence of the relaxation time on the lattice size is also compatible with equation (12), as shown in figure 9.

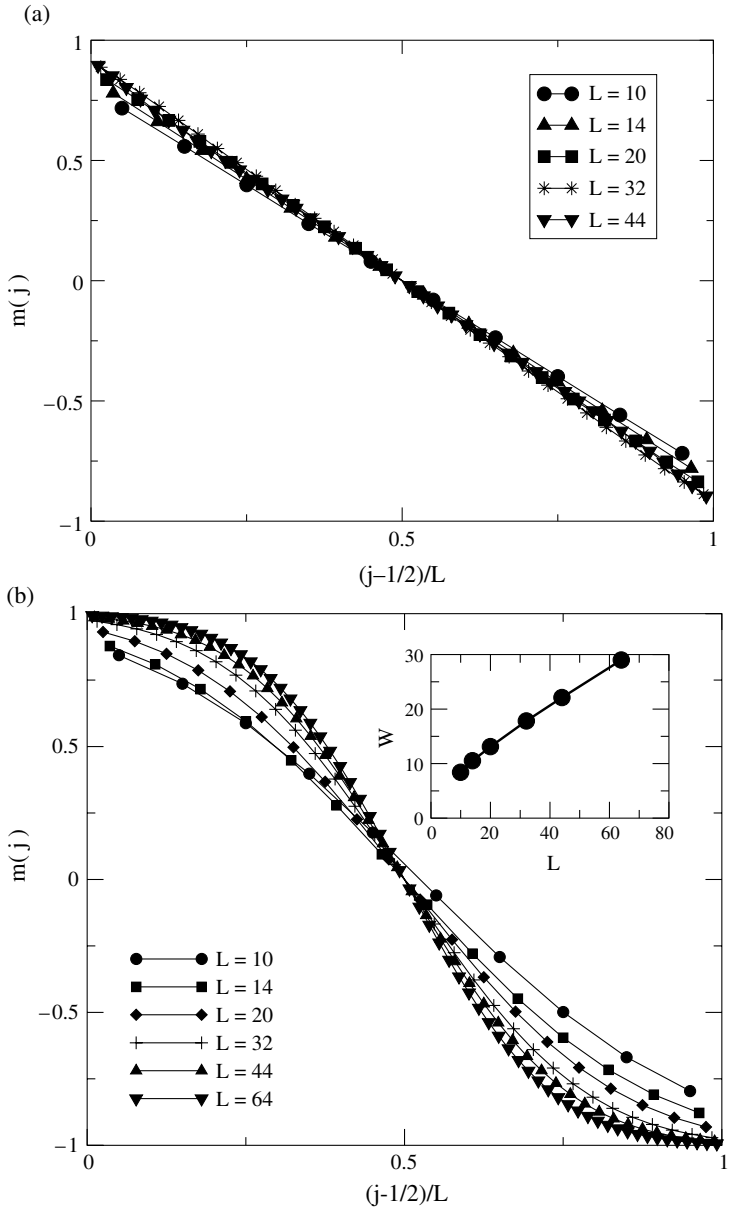

Figure 7. Plots of the magnetization profiles $m(j)$ versus j for lattices of different width. (a) Data obtained during the stationary regime for $h_w = 0.7229$ and $T_w = 0.700$. (b) As in case (a) but measured at τ_{max} when the row magnetizations exhibit a maximum. The inset shows the dependence of the interface width (W) on L. Note that the lattice rows were labelled from 1 to L and, hence, the film centre is at $L/2 + 1/2$. Therefore, $1/2$ needs to be subtracted from the row index j in the scaling representation.

5. Conclusions and outlook

A numerical study of the dynamical approach to the stationary regime at $T_w(h)$ for confined Ising films with antisymmetric surface fields reveals that the row magnetizations exhibit a

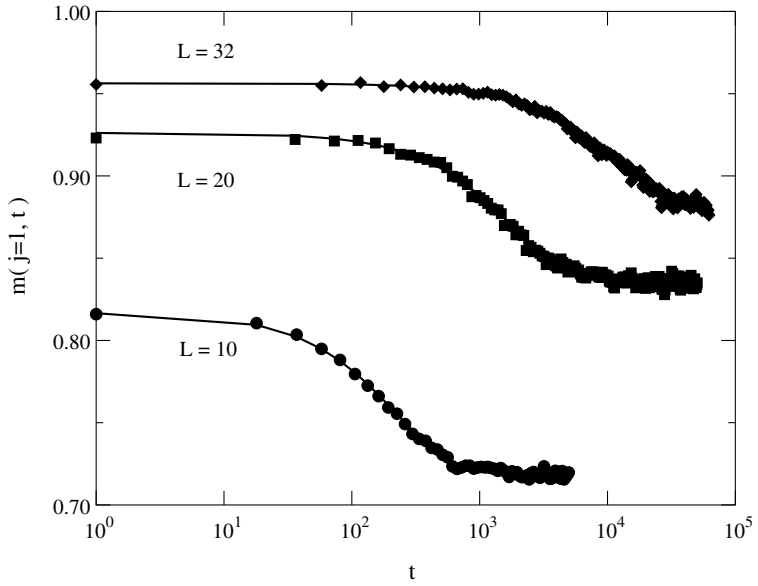

Figure 8. Plots of the decay of the magnetization of the first row (i.e. for $j = 1$) $m(t)$, measured for $t > \tau_{\max}$, versus t obtained for lattices of different width as indicated in the figure. The solid curves correspond to the best fits of the data using equation (19).

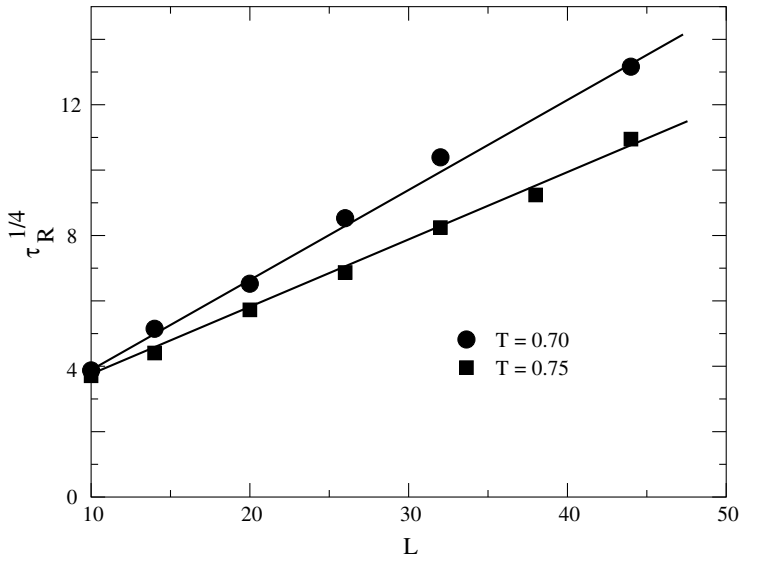

Figure 9. Plots of $\tau_R^{1/4}$ versus L as obtained by fitting the magnetization decay of the first row (see also figure 8). Data obtained keeping $h_w = 0.7229$ constant and two different temperatures $T_w = 0.700$ and $T = 0.75$, respectively. The solid lines have been draw to guide the eyes.

peak at a time $\tau_{\max} \propto L^2$. The kinetics in the initial stage corresponds to a diffusive growth of domains, which resembles the bulk ($d = 2$) kinetics at $T < T_{cb}$. This result suggests a diffusive-like propagation of the influence of the magnetic fields acting along the walls towards the bulk of the film, where the interface between domains of spins with opposite directions starts

to emerge. At the stage where the row magnetizations adopt their maxima, the configurations consist of two domains of opposite magnetization at the respective walls, which are separated by an interface. This interface runs parallel to the walls and exhibits smaller fluctuations of the interface position than in equilibrium. After the maxima, the row magnetizations relax exponentially with a characteristic time $\tau_R \propto L^4$ as suggested by theoretical arguments. In the stationary state at $T_w(h)$, the excursions of the interface are on the order of the film thickness itself.

We have restricted ourselves to two-dimensional films. In three dimensions the behaviour might be even richer. According to the short-time dynamic scaling Ansatz [45, 46] for quenches to the critical temperature $T_c(h, L)$, the second moment of the magnetization should behave as

$$m^2(t) = t^{c_2} \qquad \text{with } c_2 = (d - 1 - 2\beta/\nu)/z, \tag{20}$$

during some intermediate period. The interface localization–delocalization transition in $d = 3$ dimensions corresponds to the two-dimensional Ising universality class. Hence, one has $\beta = 1/8$ for the critical exponent of the order parameter and $\nu = 1$ for the correlation length exponent in the direction parallel to the interface, while the dynamic exponent of the Ising model is given by $z \simeq 2.169$ [31]. So, using these estimates in equation (20) one would obtain $c_2 \simeq 0.808$. Equation (20) implies that the idea that the interface localization–delocalization transition of an Ising film in d dimensions belongs to the universality class of the $(d - 1)$-dimensional Ising model can be carried over to the dynamics. We plan to study this problem in future work.

The dynamical behaviour of the confined Ising magnet with competing fields exhibits a rich ordering behaviour. Within this context, an extensive numerical study of the short- and long-time dynamics, aiming at an independent estimation of the critical exponents, is in progress.

Acknowledgments

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References

[1] Fisher M E and Nakanishi H 1981 *J. Chem. Phys.* **75** 5857
[2] Albano E V, Binder K, Heermann D W and Paul W 1989 *Surf. Sci.* **223** 151
[3] Albano E V, Binder K, Heermann D W and Paul W 1989 *Z. Phys.* B **77** 445
[4] Albano E V, Binder K, Heermann D W and Paul W 1990 *J. Stat. Phys.* **61** 161
[5] Brochard-Wyart F and deGennes P G 1983 *C. R. Acad. Sci. Paris* **279** 223
[6] Parry A O and Evans R 1990 *Phys. Rev. Lett.* **64** 439
[7] Swift M R, Owczarek A L and Indekeu J O 1991 *Europhys. Lett.* **14** 465
[8] Parry A O and Evans R 1992 *Physica* A **181** 250
[9] Binder K, Landau D P and Ferrenberg A M 1995 *Phys. Rev. Lett.* **74** 298
Binder K, Landau D P and Ferrenberg A M 1995 *Phys. Rev.* E **51** 2823
[10] Maciolek A and Stecki J 1996 *Phys. Rev.* B **54** 1128
[11] Müller M, Albano E V and Binder K 2000 *Phys. Rev.* E **62** 5281
[12] Fisher M E and Au-Yang H 1980 *Physica* A **101** 255
[13] Au-Yang H and Fisher M E 1980 *Phys. Rev.* B **21** 3956
[14] de Gennes P G 1985 *Rev. Mod. Phys.* **57** 827

[15] Dietrich S 1988 *Phase Transitions and Critical Phenomena* vol 12, ed C Domb and J L Lebowitz (London: Academic) p 1
[16] Forgacs G, Lipowsky R and Nieuwenhuizen Th M 1991 *Phase Transitions and Critical Phenomena* vol 14, ed C Domb and J L Lebowitz (London: Academic)
[17] Parry A O 1996 *J. Phys.: Condens. Matter* **8** 10761
[18] Sullivan D E and Telo da Gama M M 1986 *Fluid and Interfacial Phenomena* ed C A Croxton (New York: Wiley)
[19] Iglói F and Indekeu I O 1990 *Phys. Rev.* B **41** 6836
[20] Ebner C, Hayot F and Cai J 1990 *Phys. Rev.* B **42** 8187
[21] Le Bouar Y, Loiseau A, Finel A and Ducastelle F 2000 *Phys. Rev.* B **61** 3317
[22] Ising E 1925 *Z. Phys.* **31** 253
[23] McCoy B M and Wu T T 1973 *The Two Dimensional Ising Model* (Cambridge, MA: Harvard University Press)
[24] Binder K, Evans R J, Landau D P and Ferrenberg A M 1996 *Phys. Rev.* E **53** 5023
[25] Yahata H and Suzuki M 1969 *J. Phys. Soc. Japan* **27** 1421
[26] Stoll E, Binder K and Schneider T 1973 *Phys. Rev.* B **8** 3266
[27] Tang S and Landau D P 1987 *Phys. Rev.* B **36** 567
[28] Wansleben S and Landau D P 1991 *Phys. Rev.* B **43** 6006
[29] Ito N 1993 *Physica* A **196** 591
[30] Stauffer D 1997 *Physica* A **244** 344
[31] Wang J S and Can C K 1998 *Phys. Rev.* E **57** 6548
[32] Wang J S 1999 *Computer Simulation Studies in Condensed Matter* vol 11, ed D P Landau and H B Schütter (Berlin: Springer) p 125
[33] See Landau D P and Binder K 2000 *A Guide to Monte Carlo Simulations in Statistical Physics* (Cambridge: Cambridge University Press) figure 4.14
[34] Hohenberg P C and Halperin B I 1977 *Rev. Mod. Phys.* **49** 435
[35] Lipowsky R 1985 *J. Phys. A: Math. Gen.* **18** L585
[36] Grant M 1988 *Phys. Rev.* **37** 5705
[37] Anisimov M A, Povodyrev A A, Kulikov V D and Sengers J V 1995 *Phys. Rev. Lett.* **75** 3146
[38] Binder K, Landau D P and Müller M 2003 *J. Stat. Phys.* **110** 1411
[39] Müller M and Binder K 2001 *Phys. Rev.* E **63** 021602
[40] Sadiq A and Binder K 1984 *J. Stat. Phys.* **35** 517
[41] Müller M and Paul W 1993 *J. Stat. Phys.* **75** 209
[42] Janssen H K, Schaub B and Schmittmann B 1989 *Z. Phys.* B **73** 539
[43] Lu Z B, Retschel U and Zheng B 1994 *J. Phys. A: Math. Gen.* **27** L837
[44] Schülke L and Zheng B 1995 *Phys. Lett.* A **204** 295
[45] Zheng B 1998 *Int. J. Mod. Phys.* B **12** 1419
[46] Zheng B 1999 *Comput. Phys. Commun.* **121/122** 338
[47] Abraham D B 1980 *Phys. Rev. Lett.* **44** 1165
[48] Fisher M E 1969 *J. Phys. Soc. Japan* **S26** 87
[49] Glauber R J 1963 *J. Math. Phys.* **4** 294
[50] Jones R A L, Norton L J, Kramer E J, Bates F S and Wilkins P 1991 *Phys. Rev. Lett.* **66** 1326
[51] Puri S and Binder K 1992 *Phys. Rev.* A **46** R 4487
[52] Puri S and Binder K 1994 *Phys. Rev.* E **49** 5359
[53] Krausch G 1995 *Mater. Sci. Eng.* R **14** 1
[54] Puri S and Frisch H L 1997 *J. Phys.: Condens. Matter* **9** 2109
[55] Binder K 1998 *J. Non-Equilib. Thermodyn.* **23** 1
[56] Puri S and Binder K 2002 *Phys. Rev.* E **66** 061602
[57] Onuki A 2002 *Phase Transition Dynamics* (Cambridge: Cambrdige University Press)
[58] Binder K 1991 *Materials Science and Technology* vol 5 *Transformations in Materials* ed R W Cahn, P Haasen and E J Kramer (Weinheim: VCH) p 405
[59] Bray A J 1994 *Adv. Phys.* **43** 357
[60] Lifshitz I M 1962 *Zh. Eksp. Teor. Fiz.* **42** 1354
Lifshitz I M 1962 *Sov. Phys.—JETP* **15** 939 (Engl. Transl.)
[61] Allen S M and Cahn J W 1979 *Acta Metall.* **27** 1085
[62] Milchev A, Binder K and Heermann D W 1986 *Z. Phys.* B **63** 527
[63] Fisher M E 1974 *Rev. Mod. Phys.* **46** 587
[64] Parry A O, Evans R and Nicolaides D B 1991 *Phys. Rev. Lett.* **67** 2987
[65] Jasnow D 1984 *Rep. Prog. Phys.* **47** 1059
[66] Albano E V, Binder K and Paul W 2000 *J. Phys.: Condens. Matter* **12** 2701