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Non-equilibrium dynamics of the Ising model for $T \leqslant T_c$

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Abstract. The growth of order in Ising models with non-conserved order parameter is considered for quenches to final temperatures $T_f = 0$ and $T_f = T_c$. The results of numerical simulations in spatial dimension $d = 2$ are presented. In all cases a scaling regime is entered for sufficiently long times, where the characteristic length scale is the 'domain size', $L(t) \sim t^{1/2}$, for $T_f = 0$, and the 'non-equilibrium correlation length', $\xi(t) \sim t^{1/z}$, for $T_f = T_c$. The equal-time correlation function has the expected scaling forms $f(r/L(t))$ and $r^{-(d-2+\eta)} f_c(r/\xi(t))$ for $T_f = 0$ and T_c respectively. The scaling function $f_c(x)$ has interesting short-distance behaviour which is elucidated using scaling arguments and by ε- and $1/n$-expansions. The $T = 0$ scaling function $f(x)$ depends on whether the spin correlations present in the initial conditions are of long or short range, as does the exponent $\bar{\lambda}$ which describes the decay of the autocorrelation function, $A(t) = [\langle S_i(t) \rangle S_i(0)] \sim L(t)^{-\bar{\lambda}}$. Results for a quench from the equilibrium critical state to $T_f = 0$ are consistent with theoretical predictions.

1. Introduction

One of the difficult outstanding problems in phase transitions is that of the ordering dynamics of a system quenched into the ordered phase from a high temperature equilibrium state [1]. It has been shown that the ordering process depends crucially on whether the order parameter of the system (the magnetization in the case of a ferromagnet) is conserved or not. For a conserved order parameter (model B) this is the phenomenon of phase separation or 'spinodal decomposition'. Here we are interested in the dynamics of systems with a scalar, non-conserved order parameter (model A), which corresponds to an order-disorder transition.

For quenches into the ordered phase, the time-dependent structure factor $S_k(t) = [\langle \phi_k(t) \phi_{-k}(t) \rangle]$, (where ϕ_k is a Fourier component of the scalar order parameter field, while angle brackets and square brackets indicate averages over thermal noise, if present, and over initial conditions respectively) and its Fourier transform, the equal-time correlation function, are found to exhibit the following scaling forms [1]:

$$S_k(t) = L(t)^d g(kL(t)) \tag{1}$$

$$C(\boldsymbol{r}, t) = f(r/L(t)) \tag{2}$$

where $L(t)$ is the 'domain scale' and $L(t) \sim t^{1/2}$ for a non-conserved scalar order parameter [2].

For a quench to T_c, on the other hand, conventional critical scaling implies the scaling forms

$$S_k(t) = k^{-2+\eta} g_c(k\xi(t)) \tag{3}$$

$$C(\boldsymbol{r}, t) = r^{-(d-2+\eta)} f_c(r/\xi(t)) \tag{4}$$

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where $\eta=\frac{1}{4}$ for the 2D Ising model. The 'non-equilibrium correlation length' $\xi(t)$ [3] (our $\bar{\lambda}_c \equiv d-\lambda_c$ is called λ_c in [3]) is the length scale over which critical static correlations have been established at time t. Dynamical scaling gives $\xi(t)\sim t^{1/z}$ where z is the dynamical exponent.

Another important quantity, whose significance has only recently become apparent, is the response of the order parameter field to the initial condition, defined by $G_k(t)=[\partial\langle\phi_k(t)\rangle/\partial\phi_k(0)]$. For quenches into the ordered phase, and to the critical point respectively, it has the scaling forms

$$G_k(t)=L(t)^{\lambda}g_R(kL(t)) \qquad T<T_c \tag{5}$$

$$G_k(t)=\xi(t)^{\lambda_c}g_{R_c}(k\xi(t)) \qquad T=T_c \tag{6}$$

where the scaling functions $g(x)$ have $g(0)=\text{constant}$. It has been shown [4] that the exponent λ_c is a new critical exponent characterizing non-equilibrium critical dynamics, i.e. it is not related to z or the static exponents. Very recently, the analogous exponent λ for quenches into the ordered phase has been calculated in a $1/n$-expansion for an n-component vector order parameter [5]. Again, it is non-trivial, and unrelated to the exponent describing the growth of domains with time.

Renormalization group (RG) treatments of domain growth dynamics [6–8] have led to the idea that a $T=0$ RG fixed point controls the domain growth for all $T<T_c$, i.e. that thermal fluctuations are irrelevant to the asymptotic dynamics of the ordering system, their contribution being limited primarily to the renormalization of temperature-dependent amplitudes in (1), (2) and (5). Note that the domain scale also has a temperature-dependent amplitude, $L(t)\simeq A(T)t^{1/2}$ [8]. The new non-trivial exponent λ characterizes a critical behaviour which is 'self-organized' because it is obtained throughout the ordered phase as a consequence of the attractive (i.e. stable) nature of the $T=0$ fixed point. This is in contrast with the critical fixed point, which is repulsive (i.e. unstable) in character.

One of the most interesting questions in the field of ordering kinetics is to what extent the results are universal, i.e. independent of microscopic details associated with the Hamiltonian, equation of motion, or initial conditions. It has long been understood that the equation of motion is important, in that the results (the form of the domain growth law, the structure factor scaling function, etc) depend on whether the order parameter is conserved (model B) or non-conserved (model A) [1]. The class of models defined by the equation of motion $\partial\phi_k/\partial t=-\Gamma_k\delta H/\delta\phi_{-k}$, with $\Gamma_k\sim|k|^{\mu}$ for $k\to 0$, interpolate between model B ($\mu=2$) and model A ($\mu=0$), and corresponds to 'super-diffusive' transport of a conserved order parameter for $0<\mu<2$. An RG analysis [8] shows that the exponent ϕ characterizing the domain growth (via $L(t)\sim t^{\phi}$) is given by $\phi=1/(1+\mu)$ for $\mu>1$ and $\phi=\frac{1}{2}$ (the non-conserved result) for $\mu<1$.

A similar analysis can be carried out with respect to long-range forces in the Hamiltonian, if it contains a term of the form $H_{LR}=J_{LR}\sum_k|k|^{\rho}\phi_k\phi_{-k}$, with $\rho<2$. For $\mu>1$, general RG arguments [8] give $\phi=1/(d+\mu-y)$, where d and y are the spatial dimensionality and the 'scaling dimension of H at the $T=0$ fixed point' respectively. For a scalar order parameter with long-range forces, one finds [9] $y=d-1$ for $\rho>1$ and $y=d-\rho$ for $\rho<1$. Hence $\phi=1/(1+\mu)$ and $1/(\rho+\mu)$ for $\rho>1$ and $\rho<1$ respectively.

Very recently the role of initial conditions in determining universality classes has been discussed [10]. It has been shown that new universality classes are obtained when there are long-range, power-law correlations of the form $[\phi(r)\phi(0)]\sim r^{-(d-\sigma)}$ in the initial conditions. Such correlations do not affect the growth exponent ϕ, but do change scaling functions and the value of the exponent λ which characterizes the correlation with the initial conditions in the non-conserved case. For initial conditions with sufficiently short-range correlations, $\sigma < \sigma_c = d - 2\lambda_{SR}$, the exponent λ retains its short-range value λ_{SR} [10]; λ_{SR} has been calculated to $O(1/n)$ for an n-component non-conserved order parameter [5]. For long-range correlations, $\sigma > \sigma_c$, however, λ acquires a σ-dependence, of the predicted form $\lambda_{LR} = (d - \sigma)/2$ [10].

The exponent λ is most simply measured through the time dependence of the correlation with the initial condition, or 'autocorrelation function',

$$\begin{aligned} A(t) &= [\langle\phi(\boldsymbol{x}, t)\rangle\phi(\boldsymbol{x}, 0)] \\ &= \sum_{\boldsymbol{k}} [\langle\phi_{\boldsymbol{k}}(t)\rangle\phi_{-\boldsymbol{k}}(0)]. \end{aligned} \tag{7}$$

For initial conditions which are Gaussian random variables with correlator

$$[\phi_{\boldsymbol{k}}(0)\phi_{-\boldsymbol{k}'}(0)] = \Delta_{\boldsymbol{k}}\delta_{\boldsymbol{k},\boldsymbol{k}'} \tag{8}$$

it is easy to show that

$$[\langle\phi_{\boldsymbol{k}}(t)\rangle\phi_{-\boldsymbol{k}}(0)] = \Delta_{\boldsymbol{k}} G_{\boldsymbol{k}}(t). \tag{9}$$

The proof proceeds by integrating the left-hand side by parts. For a non-Gaussian distribution of initial conditions, we expect the same result to hold as far as the scaling limit is concerned (although a proper RG treatment would be needed to justify this). The numerical results presented below confirm these expectations. Equations (5), (7) and (9) yield

$$A(t) \sim t^{-(d-\lambda_{SR})/2} \equiv t^{-\bar{\lambda}_{SR}/2} \qquad T < T_c,\ \sigma < \sigma_c \tag{10}$$

$$A(t) \sim t^{-(d-\sigma-\lambda_{LR})/2} \equiv t^{-\bar{\lambda}_{LR}/2} \qquad T < T_c,\ \sigma > \sigma_c \tag{11}$$

these equations defining the exponents $\bar{\lambda}$.

Similarly, for power-law correlations of the form (8), with $\Delta_{\boldsymbol{k}} \sim |\boldsymbol{k}|^{-\sigma}$ for $\boldsymbol{k} \to 0$, the structure factor was shown in [10] to contain a 'long-range' contribution of the form $S_{\boldsymbol{k}}^{LR}(t) = k^{-\sigma} t^{\lambda} s(k^2 t)$, with $s(0) = \text{constant}$. In comparison with the general scaling form (1), $S_{\boldsymbol{k}}^{LR}(t)$ makes a negligible contribution to the full $S_{\boldsymbol{k}}(t)$ for $\sigma < \sigma_c$. For $\sigma > \sigma_c$, $S_{\boldsymbol{k}}^{LR}(t)$ is part of the scaling function, which becomes long-ranged in space, i.e. $g(x) \sim x^{-\sigma}$ for $x \to 0$ in (1). In real space, this means that for $\sigma > \sigma_c$ the equal time correlation function decays as

$$C(\boldsymbol{r}, t, t) \sim (L(t)/r)^{d-\sigma} \qquad \text{for } r \gg L(t) \text{ and } T < T_c. \tag{12}$$

A case of special experimental interest is when the initial condition is the equilibrium critical state, i.e. when $\sigma = 2 - \eta$. For the 2D Ising spin system, we would then expect $A(t) \sim t^{-1/16}$, and $C(\boldsymbol{r}, t, t) \sim (\sqrt{t}/r)^{1/4}$ for $r \gg \sqrt{t}$, when the system is quenched to zero temperature from the equilibrium state at T_c. Our simulation results confirm the above predictions.

In this paper three different quenches are studied: (i) from $T = \infty$ to $T = 0$; (ii) from $T = T_c$ to $T = 0$; and (iii) from $T = \infty$ to $T = T_c$. These are discussed in sections 2, 3 and 4 respectively. For quench (i), Fisher and Huse† [11] and Furukawa [12] have previously measured λ_{SR} for the $d = 2$ Ising model, but their results differ. We find $\lambda_{SR} \simeq 1.24$, in reasonable agreement with [11]. We also show that the scaling

† Our $\bar{\lambda} \equiv d - \lambda$ is called λ by these authors.

hypothesis (2) is obeyed, and that the scaling function $f(x)$ is isotropic. For the quench to $T=0$ from the equilibrium critical state (quench (ii)), problems associated with 'critical slowing down' are avoided by using an accelerated convergence algorithm due to Wolff [13] to equilibrate the system at T_c. The simulation results confirm (11) and (12) for the $2-d$ Ising model. For the quench to T_c (quench (iii)), we obtain $d-\lambda_c \equiv \bar{\lambda}_c = 1.59 \pm 0.02$, in excellent agreement with Huse [3]. The scaling function $f_c(x)$ (4) for this quench shows interesting behaviour for $r/\xi(t) \ll 1$, which is accounted for by scaling arguments and analytic computation of the short-distance expansion for the structure factor.

2. Equilibration at $T=0$ following a quench from $T=\infty$

The Hamiltonian of our system is the conventional Ising Hamiltonian

$$H = -\sum_{\langle i,j\rangle} S_i S_j \tag{13}$$

where the sum is over nearest-neighbour pairs and the exchange interaction has been set to unity. Monte Carlo simulations were performed for lattice sizes of up to $N = 1000 \times 1000$ spins, with periodic boundary conditions. Data for smaller sizes show that the results presented here for $N = 1000^2$ are not significantly finite-size affected. The system is initially given a random configuration and then quenched to zero temperature, where it evolves using conventional 'heat-bath' dynamics, adapted to $T=0$† and vectorized by sequential updating of each sublattice in turn. The results are averaged over an ensemble of 160 independently generated initial configurations, with the final time measurement being at 800 MCS. (1 MCS means one update of both sublattices). These systems are larger than those studied in references [11] ($N = 400^2$) and [12] ($N = 500^2$), the run times are longer and twice as many initial states are included.

During the simulation we compute the following quantities:

(1) The excess energy per spin,

$$\Delta E(t) = 2 - \left[N^{-1} \sum_{\langle i,j\rangle} S_i(t) S_j(t) \right].$$

(2) The equal-time correlation function,

$$C(r,t) = \left[N^{-1} \sum_i S_i(t) S_{i+r}(t) \right]$$

where here $i+r$ indicates a site displaced by r lattice spacings, relative to site i. Displacements along lattice axes and lattice diagonals are included.

(3) The autocorrelation function,

$$A(t) = \left[N^{-1} \sum_i S_i(t) S_i(0) \right].$$

† At $T=0$ moves which decrease, leave unchanged or increase the energy are accepted with probability 1, $\frac{1}{2}$ or 0 respectively.

In all cases [...] indicates the average over the ensemble of initial configurations.

Since the excess energy resides in domain walls, and the area of wall in a volume $L(t)^d$ is of order $L(t)^{d-1}$, the excess energy per spin should scale as

$$\Delta E(t) \sim L(t)^{-1}. \tag{14}$$

To determine the t-dependence of $L(t)$ we plot $\Delta E(t)$ against $1/t^{1/2}$. The data are presented in figure 1 where, as elsewhere in this paper, the errors are smaller than the symbols. The excellent linearity of the data (times $\geqslant 100$ are shown), which extrapolate nicely through the origin, confirms the asymptotic time dependence $\Delta E(t) \sim 1/t^{1/2}$ and implies, via (14), that $L(t) \sim t^{1/2}$ as expected [1, 2].

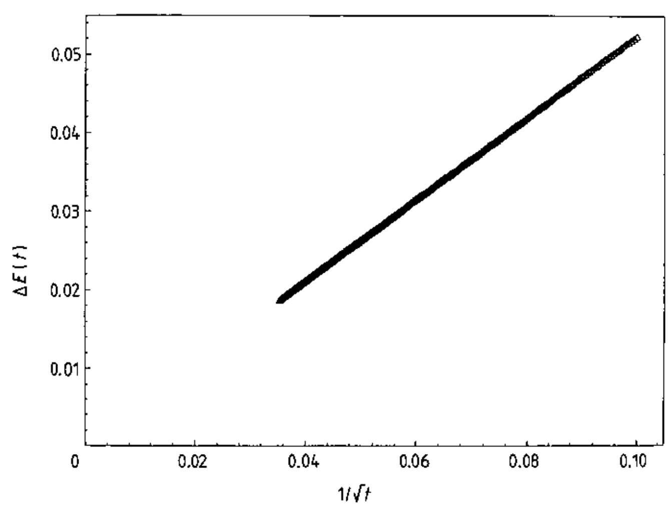

Figure 1. Relaxation of the excess energy for the 2D Ising model following a quench from $T=\infty$ to $T=0$. The data, which represent an average of 160 histories of a 1000^2 system, confirm the expected relation $\Delta E(t) \propto t^{-1/2}$, with proportionality constant $\simeq 0.521$. Times between 100 MCS and 800 MCS are plotted: there are small departures from linearity for $t < 100$ MCS, where the data are not yet fully in the scaling regime.

Data for the equal-time correlation function $C(r, t)$ is presented in figure 2, where the abscissa is the scaling variable $r/t^{1/2}$. $C(r, t)$ is calculated for sites separated by r lattice spacings along the lattice axes and in the direction of the lattice diagonals. The excellent collapse of the data onto a universal curve confirms both the scaling form (1) and the result $L(t) \sim t^{1/2}$ deduced from the energy relaxation. We can also conclude that the system is isotropic as $C(r, t)$ scales perfectly in the direction of the lattice axes and along the lattice diagonals, with the same scaling function $f(x)$. This function is linear at small x, in agreement with Porod's law [14]. The scaling function is in good agreement with that proposed by Mazenko [15] (which would be obscured by the data points if included in figure 2), after a suitable rescaling of the abscissa.

Results for the autocorrelation function $A(t)$ are presented in figure 3. The linear behaviour of $-\ln A(t)$ against $\ln t$ confirms the anticipated result $A(t) \sim t^{-\bar{\lambda}_{SR}/2}$, with $\bar{\lambda}_{SR} \simeq 1.2$. There is, however, a slight but discernible curvature in the data, such that the slope increases slowly with time. Therefore, the data were analysed using the procedure introduced for studies of spinodal decomposition [16], and also used in

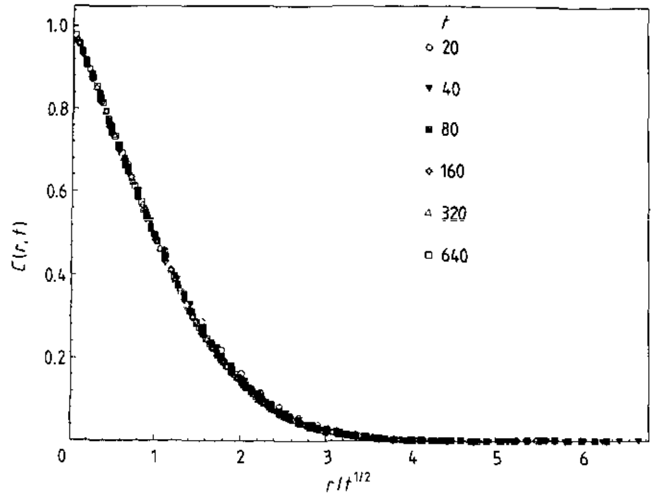

Figure 2. Scaling plot for the equal-time correlation function of the 2D Ising model following a quench from $T=\infty$ to $T=0$. Displacements along lattice diagonals as well as lattice axes are included: there is no evidence for any anisotropy in the scaling function. The data represent an average of 160 histories of a 1000^2 system, for times up to 640 MCS. Small departures from scaling are just observable at the earliest times, $t=20$ and 40.

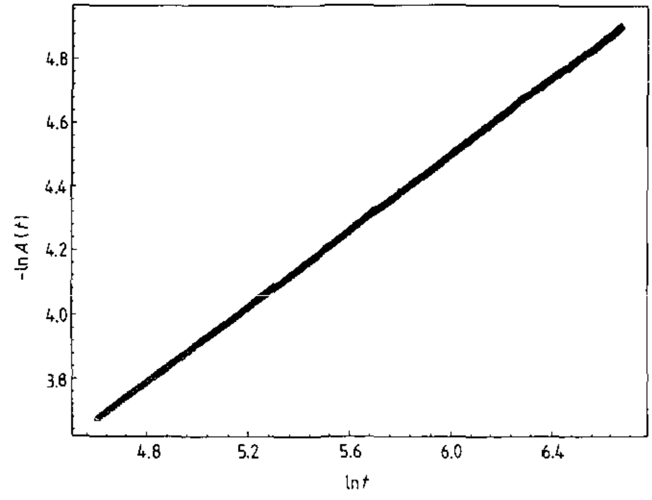

Figure 3. Time dependence of the autocorrelation function $A(t)$ for the 2D Ising model following a quench from $T=\infty$ to $T=0$. The slope, $\bar{\lambda}/2 \simeq 0.60$, increases slowly with time in a manner analysed in detail in figure 4.

[11], where an effective exponent is defined via

$$\bar{\lambda}_{\rm eff}(t) = -\log_{10}[A(t)/A(10t)]/\log_{10}[\Delta E(t)/\Delta E(10t)].$$

This effective exponent is shown against $\Delta E(t)$ in figure 4. It is natural to guess that the deviation of $\bar{\lambda}_{\rm eff}(t)$ from the asymptotic $\bar{\lambda}_{\rm SR}$ is due to effects that vanish as the length-to-area ratio of the domains [11]. Therefore one expects that the deviations may vanish as $\bar{\lambda}_{\rm eff}(t) - \bar{\lambda}_{\rm SR} \sim \Delta E(t)$. If we ignore the short 'plateau' in the data for the

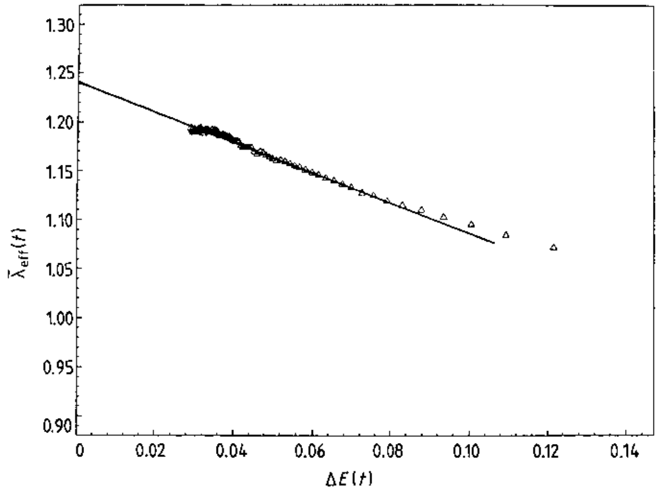

Figure 4. Effective exponent $\bar{\lambda}_{eff}$, defined in the text, as a function of the excess energy. Extrapolating to $\Delta E = 0$ gives $\bar{\lambda} \simeq 1.24$.

latest times, which is probably due to increasing statistical noise at late times, the data in figure 4 extrapolate to a value $\bar{\lambda}_{SR} \simeq 1.24$, to be compared to the value 1.25 obtained by Fisher and Huse [11] and conjectured to be exact. The trend is such that an asymptotic exponent $\bar{\lambda}_{SR} = 1.25$ certainly cannot be excluded. The value $\bar{\lambda}_{SR} \simeq 1.30$ obtained by Furukawa [12], however, does seem to be outside any reasonable extrapolation of the data.

3. Equilibration at $T = 0$ following a quench from T_c

The main motive behind this study is to test the prediction of new universal behaviour when the initial conditions exhibit long-range power-law correlations [10]. Preliminary results have been presented in [10]. The case of greatest experimental relevance is when the system is quenched from the equilibrium state at T_c. The correlations are then long-range, with $\sigma = 2 - \eta = 1.75$ for the 2D Ising model. To observe this new universal behaviour the system must be in the long-range universality class, $\sigma > \sigma_c = d - 2\lambda_{SR}$ [10]. But $\lambda_{SR} \equiv d - \bar{\lambda}_{SR} \simeq 0.76$ for the 2D Ising model, so the condition $\sigma > \sigma_c$ is well satisfied for the equilibrium critical state.

Equilibration at T_c suffers from critical slowing down. Although the equilibration time, τ, is finite for a finite system, it can be very large at the critical point. This puts severe restrictions on simulating large lattices which are needed to reduce finite-size effects and to obtain better statistics. At criticality, τ grows as $\tau \sim L^z$, where L is the linear size of the system, and z is the dynamic critical exponent. Since $z \sim 2.15$ for the 2D Ising model [17], and the simulation time must be much longer than τ for equilibrium to be established, this presents a major limitation if one is using standard Monte Carlo techniques for equilibrating the system. The above problem was overcome by preparing equilibrium states at $T = T_c = 2/\ln(1+\sqrt{2})$ using the accelerated convergence algorithm of Wolff [13], which involves flipping a large, stochastically generated, cluster of spins in one Monte Carlo 'move'. The state thus generated was then quenched to $T = 0$ and evolved using conventional 'heat bath' dynamics. We simulated systems of $N = 250^2$

spins, with periodic boundary conditions, and the results were averaged over 100 independent initial configurations.

For an infinite lattice, the equilibrium state at T_c has the following form for the equal-time correlation function [18]: $C_\infty(r)=K/r^{1/4}$, where K is a constant. For a finite lattice of linear dimension L, however, the equilibrium correlation function $C_L(r)$ should exhibit (for r and L both large compared to the lattice spacing) the finite-size scaling form $C_L(r)=r^{-1/4}c(r/L)$. With periodic boundary conditions, one expects $c(x)\geqslant K$, i.e. $C_L(r)\geqslant C_\infty(r)$, and this is indeed found. We define the 'equilibration time' τ for the Wolff algorithm to be, for given L, the time beyond which $r^{1/4}C_L(r)$ is essentially time-independent. From figure 5, where we plot $r^{1/4}C_L(r,t)$ against $r(r\leqslant 50)$ for $L=250$ and various times t, we conclude that $\tau\leqslant 160$ ws, where a 'Wolff step' ws corresponds to 'marking' N sites [13]. The open squares in figure 5 were obtained by averaging over times between 200 and 3200 ws. It is clear that there is no significant evolution of $C_L(r)$ after 160 ws.

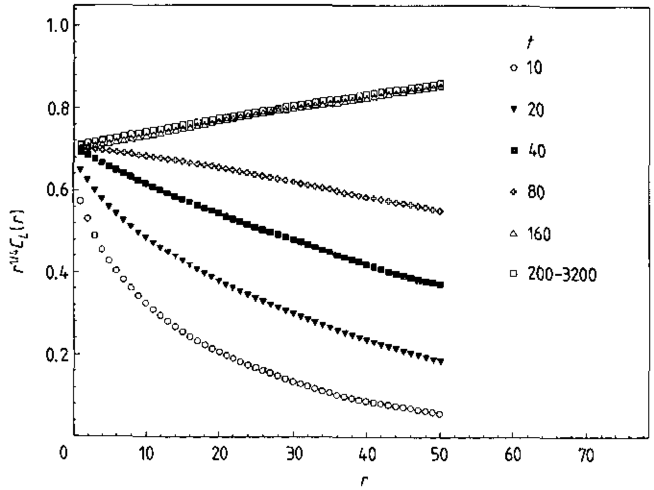

Figure 5. Spin–spin correlation function, multiplied by $r^{1/4}$, for the 2D Ising model at T_c, obtained using the Wolff algorithm, after various elapsed times from a random initial state. *No further evolution is observed after 160 ws.* The data represent an average of 100 histories of a 250^2 system. The open squares were obtained by averaging over 100 times between 200 and 3200 ws for a single history.

We found that the equilibrated system at T_c had a short 'decorrelation time' ρ (defined as the time for essentially complete decorrelation of the magnetization—see figure 6—rather than a $1/e$-time) of around 15 ws. This implies that once we have generated an equilibrium state at T_c from a given random initial configuration (corresponding to a particular state at infinite temperature) it becomes a completely new equilibrium critical state after ρ ws, where $\rho\ll\tau$. Therefore to create an ensemble of equilibrium states at T_c, we only needed to generate one equilibrium critical state from a random initial configuration. Subsequent new equilibrium states were generated by applying the Wolff algorithm to the previous critical equilibrium state for a further ρ ws, instead of starting from a new random initial configuration, hence saving a considerable amount of CPU time. The value of ρ was estimated from the magnetization correlation function in equilibrium. Figure 6 shows a plot of $\langle M(t_0)M(t_0+t)\rangle/\langle M(t_0)^2\rangle$

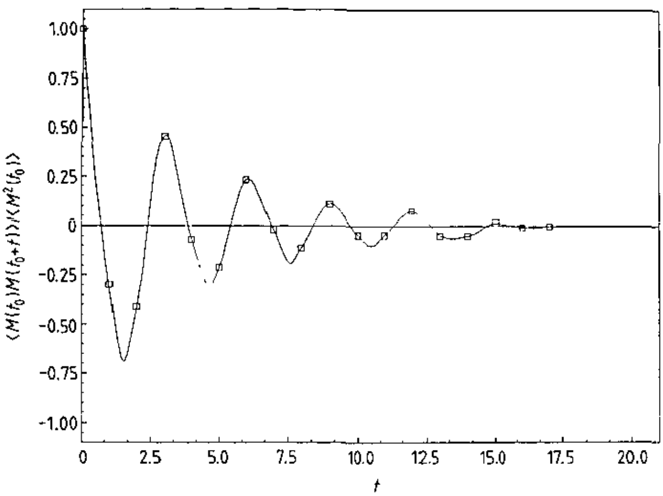

Figure 6. Magnetization–magnetization correlation function in equilibrium for a 250^2 2D Ising system updated according to the Wolff algorithm. The continuous curve is included as a guide to the eye. Decorrelation is essentially complete after 15 ws.

against t, where $\langle\ldots\rangle$ indicates an average over different values of time t_0, and the magnetization $M(t)$ of the sample is defined as $M(t) = (1/N)\sum_i S_i(t)$. The magnetization correlation function becomes essentially zero for $t > \rho \sim 15$. To allow a safety margin we equilibrated the initial random state for 200 ws, and took states at subsequent intervals of 30 ws as independent equilibrium states. It is noteworthy that the 'decorrelation time' ρ for the Wolff algorithm is much shorter than the 'equilibration time' τ. This is not surprising, given the nature of the algorithm: the size of the typical clusters generated increases as the system approaches equilibrium.

The equal-time correlation function $C(r, t)$ following the quench to $T = 0$ is presented in scaling form in figure 7. We actually plot $\tilde{C}(r, t) = C_L(r, t)[C_\infty(r)/C_L(r)]$, where C_∞ and C_L were defined above. This correction is designed to remove, as far as possible, finite-size (boundary) effects in the spatial correlations at $t = 0$, this being the dominant finite-size effect present. These arise due to the long-range initial correlations built in the system due to the system being in an equilibrium state at T_c. A further refinement was to select only initial equilibrium states with magnetization per spin $|M| < 0.01$. If all equilibrium states are included, the data fall on the same scaling curve at short times, but break away at later times. This is because $|M|$ is typically quite large at T_c for the $N = 250^2$ systems studied here: finite-size scaling yields $|M| \sim L^{-\beta/\nu} = L^{-1/8}$, so we expect $|M| \sim 0.6$ for $L = 250$, a result confirmed by the simulations. As a result, the system usually reaches a single domain quite quickly, taking the system out of the scaling regime. (The large typical values of $|M|$ in equilibrium at T_c is presumably responsible for the oscillations in figure 6.) Selecting initial states with small $|M|$ enables us to artificially expand the scaling regime. Since the probability distribution for M has the scaling form $P(M) = L^{\beta/\nu} f(ML^{\beta/\nu})$, our procedure corresponds to selecting states from a narrow band in the centre of the distribution. In practice this was achieved by selecting the first state generated with $|M| < 0.01$ after at least 30 ws had elapsed from the previously selected state.

To test the prediction (12) for the asymptotic behaviour of the scaling function, i.e. $\tilde{C}(r, t) \sim (\sqrt{t}/r)^{1/4}$ in this case, we plotted the product $(r/\sqrt{t})^{1/4}\tilde{C}(r, t)$ against $r/\sqrt{t}$.

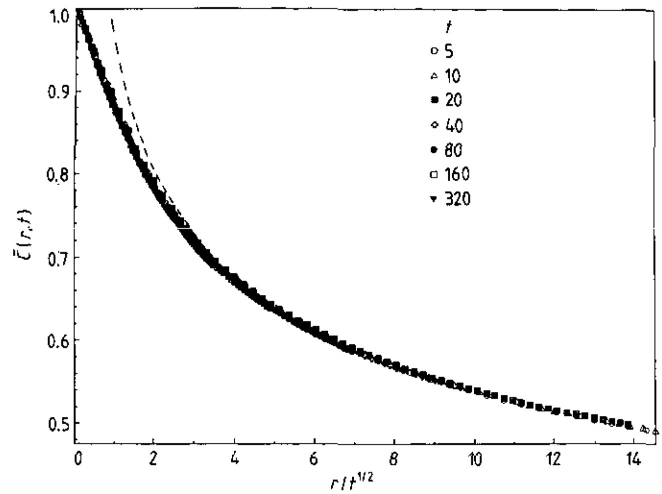

Figure 7. Scaling plot for the equal-time correlation function of the 2D Ising model, following a quench from $T=T_c$ to $T=0$. The data, which represent an average of 100 histories of a 250^2 system, have been adjusted for finite-size effects as described in the text. The broken curve shows the asymptotic behaviour $C(r,t) \simeq 0.96(\sqrt{t}/r)^{1/4}$.

In this form, the data saturates at $\simeq 0.96$ for $r/\sqrt{t} > 4$, implying $C(r,t) \simeq 0.96(\sqrt{t}/r)^{1/4}$ for large $r/\sqrt{t}$. The broken curve in figure 7 shows this asymptotic behaviour. This scaling function is quite different from that associated with the conventional quench from the high-temperature phase, shown in figure 2. The short-distance behaviour, however, is still linear, in accordance with Porod's law [14], which is simply a consequence of the sharp domain walls in a system with a scalar order parameter.

The results for the autocorrelation function are also consistent with the prediction $A(t) \sim t^{-1/16}$. In this case we were unable to correct simply for the finite-size effects

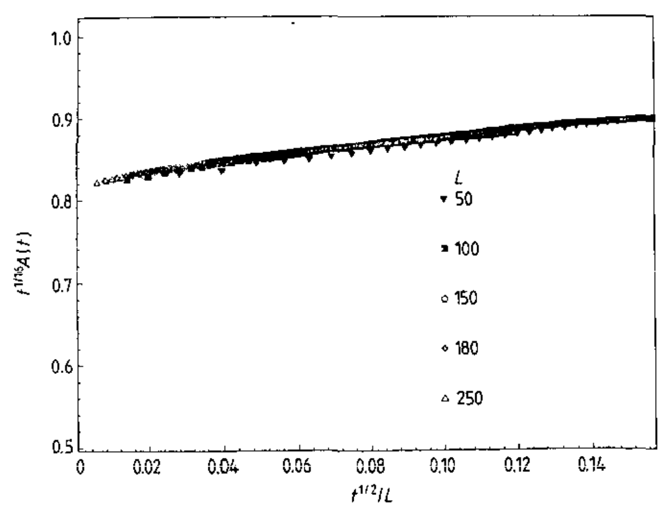

Figure 8. Finite-size scaling analysis of the autocorrelation function $A(t)$ for the 2D Ising model quenched from $T=T_c$ to $T=0$. The data are averaged over 200 histories for each system size. The excellent collapse of the data, except for the smallest system, verify the predicted form $A(t) \sim t^{-1/16}$.

on the initial condition which, as is clear from figure 5, yield a $C_L(r, 0)$ decreasing more slowly with r than $1/r^{1/4}$. As a result, we must employ finite-size scaling methods. Anticipating the finite-size scaling form $A(t) = t^{-1/16}a(\sqrt{t}/L)$, the argument of the scaling function a being the ratio of the domain scale to the system size, we plot (figure 8) $t^{1/16}A(t)$ against $\sqrt{t}/L$, for values of L in the range $50 \leq L \leq 250$. Except for the smallest system size, the data collapse is excellent, confirming the prediction made in [10]. The deviation from the scaling curve of the $L = 50$ data can be attributed to the relatively small values of t involved: $\sqrt{t}/L = 0.08$, for example, corresponds (for $L = 50$) to $t = 16$, which is not in the scaling regime.

4. Equilibration at T_c following a quench from $T = \infty$

For this quench we simulated lattice sizes up to 400×400 spins, with periodic boundary conditions. Data for smaller sizes show that the results presented here for $N = 400^2$ are not finite-size affected. Averages were taken over 1500 independent random initial conditions run for 400 MCS using a standard heat bath algorithm. Our main goals are to determine the exponent λ_c of (6), and the form of the scaling function $f_c(x)$ in (4). Rather than compute λ_c directly, we compute instead the equivalent exponent $\bar{\lambda}_c \equiv d - \lambda_c$, through a study of the autocorrelation function $A(t)$. Arguments identical to those leading to (10) give, for a quench to T_c,

$$A(t) \sim \xi(t)^{-\bar{\lambda}_c} \sim t^{-\bar{\lambda}_c/z} \tag{15}$$

for initial conditions with short-range correlations. This exponent has been measured previously by Huse [3], using a larger number of smaller systems, and our results are in good agreement with his. Our study of the scaling function $f_c(x)$ is, as far as we know, new and reveals interesting short-distance behaviour which we can understand from general scaling arguments.

Data for the equal-time scaling function $f_c(x) = r^{1/4}C(r, t)$ is presented in figure 9, where the abscissa is the scaling variable $x = r/t^{1/z}$, with $z = 2.15$ [17]. The data collapse

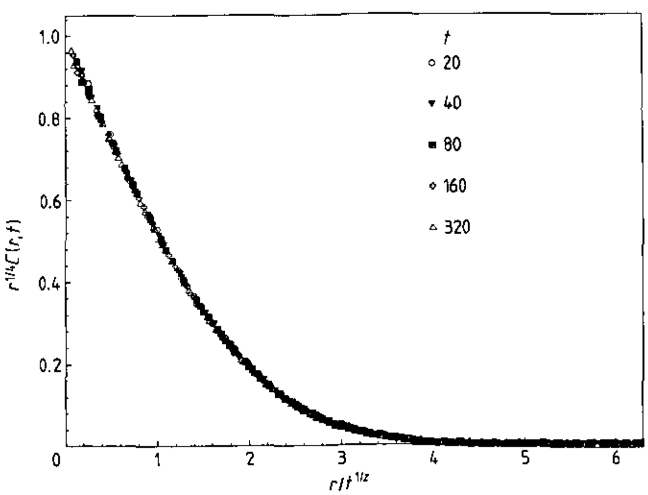

Figure 9. Scaling plot, with $z = 2.15$, for the equal-time correlation function of the 2D Ising model quenched from $T = \infty$ to $T = T_c$. The data are averaged over 1500 histories of a 400^2 system.

is excellent, confirming both the scaling form (4) and the value of z. Note that for small scaling variable the scaling function is almost linear. While this behaviour is superficially reminiscent of Porod's law for the scaling function at $T=0$ (section 2), its origin is quite different, and will be discussed in detail below.

The results for $A(t)$ and $\langle M^2(t)\rangle/N$ are presented in figure 10, where $M(t)$ is now the total magnetization of the sample. Well established power-law behaviour is seen for times 10–400 MCSs. The fit to $A(t)$ gives $\bar{\lambda}_c/z=0.74\pm0.01$, or $\bar{\lambda}_c=1.59\pm0.02$ when we use $z=2.15$. This result agrees with that of Huse [3]. The scaling expectation is that $\langle M^2(t)\rangle\sim t^{(2-\eta)/z}$ [3]; the slope in figure 10 is consistent with this, within the errors.

We consider now the scaling form (4) for $C(r, t)$, and determine the form of the scaling function for $r/t^{1/z}\ll 1$, i.e. the 'short-distance' expansion.

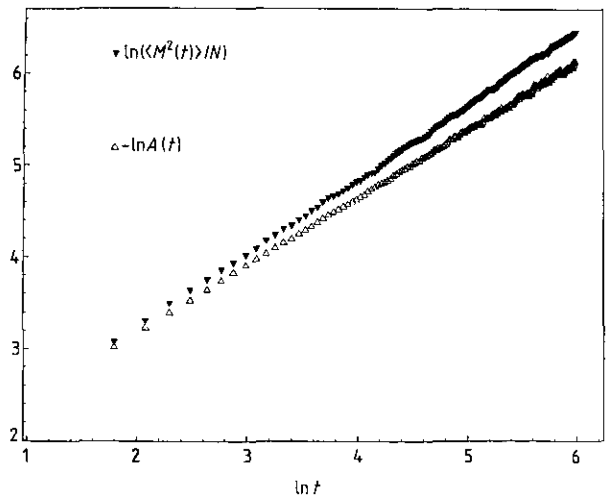

Figure 10. Time-dependence of the autocorrelation function $A(t)$ and the 'non-equilibrium susceptibility' $\langle M^2(t)\rangle/N$, for the 2D Ising model quenched from $T=\infty$ to $T=T_c$. The data are an average of 1500 histories of a system of $N=400^2$ spins.

4.1. Short-distance expansion: scaling arguments

Consider first the equilibrium correlation function just above T_c. It has the short-distance expansion [19]

$$\langle\phi(0)\phi(r)\rangle=\frac{\tilde{C}}{r^{d-2+\eta}}\left(1+\tilde{A}\left(\frac{r}{\xi}\right)^{(1-\alpha)/\nu}+\tilde{B}\left(\frac{r}{\xi}\right)^{1/\nu}+\ldots\right) \tag{16}$$

where ξ is the equilibrium correlation length, $\tilde{A}$, $\tilde{B}$, $\tilde{C}$ are constants and α, η, ν are the usual static critical exponents. In the non-equilibrium situation following a quench to T_c, the equal-time correlation function should have the same short-distance expansion (16), but with coefficients that now depend on the scaling variable t/ξ^z or, equivalently, on $\xi(t)/\xi$ where $\xi(t)\sim t^{1/z}$ is the 'non-equilibrium correlation length' of (4). Thus scaling implies that $C(r, t)$ has the short-distance expansion (16) but with $\tilde{A}$, $\tilde{B}$ and $\tilde{C}$ becoming functions of $\xi(t)/\xi$. These scaling functions should be such that the equilibrium result (16) is recovered in the limit $\xi(t)\gg\xi$. In this paper, we are interested in the non-equilibrium relaxation at T_c, which corresponds to the opposite limit $\xi(t) \ll \xi \to \infty$. In this limit, ξ should drop out of the expression for $C(r, t)$: effectively we replace ξ by $\xi(t)$ in (16), to obtain the desired short-distance expansion

$$C(r, t) = \frac{C'}{r^{d-2+\eta}} \left(1 + A'\left(\frac{r}{t^{1/z}}\right)^{(1-\alpha)/\nu} + B'\left(\frac{r}{t^{1/z}}\right)^{1/\nu} + \ldots\right) \tag{17}$$

where A', B', C' are new constants (in fact, $\tilde{C}$ and C' are equal since both are the equilibrium critical amplitude). For the 2D Ising model, $\alpha = 0$ and $\nu = 1$, so both terms in the bracket become linear in $r/t^{1/z}$ in agreement with the data in figure 9. (Actually, $\alpha = 0$ should probably be interpreted as a logarithm, implying a term in $(r/t^{1/z}) \ln(r/t^{1/z})$. This is also consistent with the data.)

Equation (17) has been derived from scaling considerations. In the following two subsections we calculate $C(r, t)$ explicitly to first order in $\varepsilon = 4 - d$, and leading order in $1/n$ for an n-component order parameter, and verify that the results are consistent with (17).

4.2. *The ε-expansion*

We can derive the small-r behaviour of $C(r, t)$ from the short-distance expansion for its Fourier transform $S_k(t)$. The calculation is a relatively straightforward extension of the work of Janssen *et al* [4].

The analysis starts from the continuum Langevin equation

$$\partial\phi_k^i/\partial t = -\Gamma_k \left\{(r + k^2)\phi_k^i + (u/L^d) \sum_{j,p,q} \phi_p^j \phi_q^j \phi_{k-p-q}^i\right\} + \xi_k^i(t) \tag{18}$$

where L^d is the volume of the system, i, j label Cartesian components in order parameter space, and $\xi_k(t)$ is a Gaussian white noise with correlator

$$\langle \xi_k^i(t) \xi_{-k'}^j(t')\rangle = 2\Gamma_k \delta_{i,j} \delta_{k,k'} \delta(t - t').$$

With an appropriate choice of units of time, we may take $\Gamma_k = 1$ for model A dynamics. We also take the distribution of initial conditions to be Gaussian with mean zero and correlator defined by a natural extension of (8): $[\phi_k^i(0)\phi_{-k'}^j(0)] = \Delta\delta_{i,j}\delta_{k,k'}$.

The central quantity to compute is $G_k(t, t') = \langle \partial\phi_k^i(t)/\partial\xi_k^i(t')\rangle$, which is the response of the field at time t to thermal noise acting at time t'. Janssen *et al* [4] showed that Δ is an irrelevant variable and can be set to zero in all loop corrections. Therefore one only needs to average over thermal noise. To $O(\varepsilon)$ the result is [4]

$$G_k(t, t') = (t/t')^{\lambda_c/z} \exp\{-k^2(t - t')\} \qquad t > t' \tag{19}$$

with $\lambda_c/z = \varepsilon(n+2)/4(n+8)$.

The structure factor $O(\varepsilon)$ is simply

$$S_k(t) = 2\int_0^t \mathrm{d}t'\, G_k^2(t, t'). \tag{20}$$

Using (19), the integral can be evaluated asymptotically for large $k^2 t$ to give

$$S_k(t) = \frac{1}{k^2}\left[1 + \frac{(n+2)}{4(n+8)}\frac{\varepsilon}{k^2 t} + O\left(\frac{1}{k^4 t^2}\right)\right]. \tag{21}$$

To compare this result with the general form (17), we first Fourier transform the latter to obtain

$$S_k(t) = Ck^{-(2-\eta)}[1 + A(kt^{1/z})^{-(1-\alpha)/\nu} + B(kt^{1/z})^{-1/\nu} + \ldots] \tag{22}$$

where A, B, C are simply related to A', B', C'. Substituting the values of the exponents α, η, ν and z to $O(\varepsilon)$ [20], we get

$$S_k(t) = Ck^{-2}[1 + (A/k^2t)(1 + 3\varepsilon \ln(k^2t)/(n+8)) \\ + (B/k^2t)(1 + \varepsilon \ln(k^2t)\{(n+2)/2(n+8)\}) + O(\varepsilon^2)]. \tag{23}$$

Comparison with (22) gives $A = (n+2)^2\varepsilon/\{4(n-4)(n+8)\}$, $B = -6(n+2)\varepsilon/\{(n-4)(n+8)\}$ and $C = 1$.

4.3. *The large-n limit*

We can also compute the structure factor in the limit $n \to \infty$. Again, our result is a straightforward extension of reference [4]. For $n = \infty$, the response function is given exactly by (19), with $\lambda_c/z = (4-d)/4$, and the structure factor is given exactly by (20). Hence the asymptotic expansion for large k^2t is the same as (21), but with $(4-d)/4$ replacing $\varepsilon(n+2)/\{4(n+8)\}$:

$$S_k(t) = k^{-2}[1 + (4-d)/4k^2t + O(1/k^4t^2)]. \tag{24}$$

Substituting into (22) the values of the exponents α, η, ν and z for $n = \infty$ [20], and ignoring the higher-order terms gives

$$S_k(t) = Ck^{-2}[1 + A/k^2t + B/(kt^{1/2})^{d-2}].$$

Comparing with (24) gives $A = (4-d)/4$, $B = 0$ and $C = 1$ in the large-n limit. Naturally, these results agree with the large-n limit of the $O(\varepsilon)$ results.

5. Discussion and summary

The growth of order in Ising spin systems, following a quench to either $T = T_c$ or $T = 0$, has been studied by Monte Carlo simulations in two dimensions. For a quench to $T = 0$, the developing order corresponds to the growth of domains of the two pure phases. The form of the equal-time correlation function depends on whether the system is quenched from the high-temperature phase, when the system immediately after the quench possesses only short-range spin correlations, or from equilibrium at T_c, when long-range spin correlations are present. In the latter case, the large-argument form of the scaling function, and the exponent describing the decay of the autocorrelation function, are in agreement with theoretical predictions [10].

Since a $T = 0$ RG fixed point should describe domain growth throughout the ordered phase, the exponents and scaling functions obtained here for quenches to $T = 0$ should also describe domain growth for general temperatures $T < T_c$. Similarly, a quench from any initial temperature in the high temperature phase should give the same asymptotic results as a quench from $T = \infty$: any short-range correlations present in the initial condition become irrelevant when the domain scale $L(t)$ exceeds the correlation length of the initial condition.

For a quench from high temperatures to T_c, the developing order corresponds to the establishment of critical correlations over a length scale $\xi(t) \sim t^{1/z}$, a sort of 'non-equilibrium correlation length' analogous to the domain scale $L(t)$ for quenches to $T=0$. The exponent $\bar{\lambda}_c$ describing the decay of the autocorrelation function has been determined, and is in good agreement with the result of Huse [3]. We have also determined the scaling function $f_c(x)$ for the equal-time correlation function (equation (4)), and have shown that the small x behaviour is consistent with the short-distance expansion derived from scaling arguments and from ε- and $1/n$-expansions.

In the course of this work it was necessary, in order to investigate the role of initial conditions on the growth kinetics at $T=0$, to generate equilibrium states at T_c. Problems associated with critical slowing down were eliminated by employing the Wolff algorithm [13]. It was found that the system can be equilibrated in a reasonable time ($\sim$160 ws), but that this time is much longer than the correlation time for the magnetization in equilibrium, a result which is quite reasonable given the nature of the algorithm. The finite-size scaling function for the equilibrium spin–spin correlation function was also computed (the upper data set in figure 5), i.e. the function $c(x)$ in $C_L(r)=r^{-1/4}c(r/L)$. The dependence on x for $x \ll 1$ is almost linear (see figure 5), a fact which can be understood from a short-distance expansion for $c(x)$ analogous to that derived in section 4 for the equal-time correlation function at T_c. Essentially one just replaces the non-equilibrium correlation length $\xi(t)$ by the lattice size L in (17), to obtain $C_L(r)=(C/r^{1/4})[1+A(r/L)^{(1-\alpha)/\nu}+B(r/L)^{1/\nu}+\ldots]$, where A, B are new constants. For the 2D Ising model, $\alpha=0$ and $\nu=1$ imply a linear correction to the infinite lattice result, up to a possible logarithm.

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