

## Growth of order in vector spin systems; scaling and universality

This article has been downloaded from IOPscience. Please scroll down to see the full text article.

1990 J. Phys. A: Math. Gen. 23 5897

(<http://iopscience.iop.org/0305-4470/23/24/028>)

View [the table of contents for this issue](#), or go to the [journal homepage](#) for more

Download details:

IP Address: 129.252.86.83

The article was downloaded on 01/06/2010 at 09:56

Please note that [terms and conditions apply](#).

# Growth of order in vector spin systems: scaling and universality

A J Bray and K Humayun

Department of Theoretical Physics, The University, Manchester M13 9PL, UK

Received 9 August 1990

**Abstract.** The growth of order in vector spin systems with non-conserved order parameter ('model A') is considered following an instantaneous quench from infinite to zero temperature. The results of numerical simulations in spatial dimension  $d = 2$  and spin dimension  $2 \leq n \leq 5$  are presented. For  $n \geq 4$ , a scaling regime (where a characteristic length scale  $\bar{L}(t)$  emerges) is entered for sufficiently long times, with  $L(t) \sim t^{1/2}$ . The autocorrelation function  $A(t)$  decays with time as  $A(t) \sim t^{-(d-\lambda)/2}$ , and the exponent  $\lambda(n)$  agrees well with the predictions of the  $1/n$ -expansion. The cases  $n = 2$  and  $3$  are more complicated, due to the non-trivial role played by topological singularities, i.e. vortices ( $n = 2$ ) and Polyakov solitons ( $n = 3$ ). For  $n \geq 4$ , universal amplitudes and scaling functions characterizing the energy relaxation and the equal-time correlation function are identified. It is argued that for  $d \geq 3$ , where an ordered phase exists at low temperature, such universal quantities characterize the entire ordered phase.

## 1. Introduction

Recent years have seen renewed interest in the ordering dynamics of a system quenched into the ordered phase from a high-temperature equilibrium state. For a conserved order parameter (model B in the classification of Hohenberg and Halperin [1]) this process is phase separation by 'spinodal decomposition', while for a non-conserved order parameter (model A of [1]) it corresponds to an order-disorder transition (see e.g. [2]). In both cases there is evidence for a scaling regime at late times, where physical quantities depend on time only through the length scale  $L(t)$  which, for a scalar order parameter, describes the typical scale of the domains of ordered phase which have formed at time  $t$ .

Much of the recent interest stems from the idea [3–5] that the ordering is driven by a ' $T = 0$  renormalisation group (RG) fixed point' of the dynamics, since this would provide a natural framework in which to understand the scaling phenomena observed. Such an approach has been used [4, 5] to determine the domain growth exponent  $\phi$  ( $L(t) \sim t^\phi$ ) for a conserved order parameter, and to investigate the role of long-range correlations in the initial conditions [6]. Within the RG approach  $\phi = 1/z$ , where  $z$  is the 'dynamical exponent at the  $T = 0$  fixed point'. For a conserved order parameter one obtains [4, 5]  $\phi = 1/3$  and  $1/4$  for scalar and vector order parameters respectively, the former in agreement with conventional Lifshitz–Slyosov scaling [7]. For a non-conserved order parameter, the RG provides no prediction: conventional arguments, however, give  $z = 2$  for a scalar order parameter [8]. The result for vector order

parameters is less clear-cut:  $z = 2$  follows (essentially from dimensional analysis) if one assumes that  $L(t)$  is the only important length scale at late times [5]. The role of possible topological singularities, however, which may provide additional length scales, has to be carefully considered.

In this paper we consider the ordering kinetics of  $n$ -dimensional spins ( $n \geq 2$ ), in spatial dimension  $d = 2$ , for a non-conserved order parameter. This work extends the recent studies of  $d = 1$  systems by Newman *et al* [9] which we will refer to as I. In addition we discuss the possibility, raised in I, that the amplitudes characterizing the decay of the excess energy at  $T = 0$  and the growth of the 'domain scale'  $L(t)$  are universal numbers. We present numerical evidence in favour of this hypothesis at  $T = 0$ . Finally we argue that, since a  $T = 0$  RG fixed point controls the entire low-temperature phase, temperature-independent universal amplitudes and scaling functions can be defined which describe ordering at all  $T < T_c$  whenever  $T_c > 0$ .

The conventional scaling forms for the order parameter correlation function and its Fourier transform are [2]

$$C(\mathbf{r}, t, t) = f_e(r/L(t)) \quad (1)$$

$$C_{\mathbf{k}}(t, t) = L(t)^d g_e(kL(t)) \quad (2)$$

where the subscript 'e' indicates an equal-time correlation function. Correlations of the order parameter at two different times are also of interest, since it has been shown [10] that these involve a new, non-trivial exponent. If  $\mathbf{S}(\mathbf{r}, t)$  is the order parameter field, we define  $C(\mathbf{r}, 0, t) = \langle \mathbf{S}(\mathbf{x}, 0) \cdot \mathbf{S}(\mathbf{x} + \mathbf{r}, t) \rangle$ , where the angle brackets indicate an average over both initial conditions and thermal noise (if present). General scaling considerations [11] suggest

$$C(\mathbf{r}, 0, t) = L(t)^{-\bar{\lambda}} f(r/L(t)) \quad (3)$$

$$C_{\mathbf{k}}(0, t) = L(t)^\lambda g(kL(t)) \quad (4)$$

where  $C_{\mathbf{k}}(0, t)$  is the Fourier transform of  $C(\mathbf{r}, 0, t)$  and

$$\bar{\lambda} = d - \lambda$$

follows from dimensional analysis. Scaling forms can also be written down for general times  $t, t'$ , but no new exponents are involved.

By expanding about the exactly soluble  $n = \infty$  limit, the forms (1)–(4) have been verified by explicit calculation to  $O(1/n)$  for a non-conserved order parameter (model A) quenched to zero temperature [10], with the results  $L(t) \sim t^{1/2}$  (i.e.  $z = 2$ ) and

$$\lambda = d/2 - (4/3)^{d/2} (2d(d+2)/9) B(d/2+1, d/2+1) (1/n) + O(1/n^2) \quad (5)$$

where  $B(x, y) = \Gamma(x)\Gamma(y)/\Gamma(x+y)$  is the beta function [12], and  $\Gamma(x)$  is the gamma function [12]. Note that  $\lambda$  is a non-trivial function of  $d$  and  $n$ . equation (5) shows that  $\lambda$  is a non-trivial exponent even for  $d = 1$ .

Numerical results for  $d = 1$  and  $2 \leq n \leq 5$  have been presented in I. There it was found that  $d = 1$  systems can be divided into two classes according to the value of  $n$ : for  $n \geq 3$  the behaviour is qualitatively the same as for  $n = \infty$  (e.g.  $\phi = 1/2$ ), whereas for  $n = 2$  different behaviour is obtained, with  $\phi = 1/4$ . For  $n \geq 4$  the results for

$\lambda$  are in good quantitative agreement with the  $1/n$ -expansion (5) truncated at lowest non-trivial order.

For  $d = 2$ , we find that only for  $n \geq 4$  is the behaviour qualitatively the same as for  $n = \infty$ . The values obtained for  $\lambda$  are again in reasonable quantitative agreement with (5). For  $n \leq 3$ , the  $T = 0$  relaxation is strongly affected by the existence of topological singularities, i.e. vortices for  $n = 2$  and Polyakov solitons [13] for  $n = 3$ .

The paper is organized as follows. Section 2 contains a short discussion of the dynamical model and the quantities calculated in the simulations. The results of are presented in section 3, along with a discussion of universality at  $T = 0$ . Universality at general  $T < T_c$  is discussed in section 4. It is emphasized that, for general  $T$ , the scaling forms (1) and (2) require the  $T$ -dependent prefactor  $M^2$ , where  $M$  is the equilibrium order parameter. This factor is important if systems at different temperatures are to be compared on the same scaling plot. The paper concludes with a summary and discussion of the results.

## 2. General considerations

Following section 1, we work with spins of fixed length ( $|\mathbf{S}_i| = 1$ ). The Hamiltonian is

$$H = - \sum_{(i,j)} \mathbf{S}_i \cdot \mathbf{S}_j \quad (6)$$

where the sum is over nearest-neighbour pairs and we have set the exchange interaction to unity. With model A dynamics the rate of change of a spin is proportional to the component of the local field (due to its neighbours) perpendicular to the spin. The equation of motion is therefore

$$d\mathbf{S}_i/dt = \mathbf{h}_i - (\mathbf{h}_i \cdot \mathbf{S}_i) \mathbf{S}_i \quad (7)$$

$$\mathbf{h}_i = \sum_j \mathbf{S}_j \quad (8)$$

where the sum in (8) is over the nearest neighbours of  $i$ .

In the continuum limit, which is useful for a discussion of scaling properties, equation (6) becomes

$$H = \frac{1}{2} \int d^d x (\nabla \mathbf{S})^2 \quad (9)$$

ignoring higher-order spatial derivatives and dropping a constant equal to the ground-state energy. For completeness, we also give the continuum limit of the equation of motion, derived in section 1:

$$\partial \mathbf{S} / \partial t = \nabla^2 \mathbf{S} + (\nabla \mathbf{S})^2 \mathbf{S} \quad (10)$$

In equation (10), we have taken the kinetic coefficient  $\Gamma$  to be unity. This corresponds to a particular choice for the units of time. More generally, there would be a factor  $\Gamma$  on the right-hand side of (10).

At  $T = 0$  equations (7) and (8), supplemented by an initial condition on the  $\{\mathbf{S}_i\}$ , completely specifies the dynamics. In the simulations we chose as an initial condition the state in which each spin is randomly oriented (over its hypersphere of possible directions) independently of the others, i.e. the equilibrium state at infinite temperature.

The central concept in the data analysis is the ‘domain’ scale  $L(t)$ , i.e. the length scale characterizing, via equation (1), the spatial extent of the spin correlations at time  $t$ . Provided a scaling regime described by (1) and (2) exists,  $L(t)$  can be extracted rather directly from the data by studying the decay of the excess energy  $\Delta E(t)$  with time. From the continuum Hamiltonian (10), the mean excess energy per unit volume (or per site in the lattice model) is

$$\begin{aligned} \Delta E(t) &= \frac{1}{2} \langle (\nabla \mathbf{S})^2 \rangle = \frac{1}{2N} \sum_{\mathbf{k}} k^2 \langle \mathbf{S}_{\mathbf{k}}(t) \cdot \mathbf{S}_{-\mathbf{k}}(t) \rangle \\ &\sim \int d^d k k^2 L(t)^d g_e(kL(t)) \sim L(t)^{-2}. \end{aligned} \quad (11)$$

This result requires that the sum over  $k$  be dominated by  $k$  of order  $L(t)^{-1}$ , i.e. that the integral converges at large  $k$ , such that the use of the scaling form (2) for the time-dependent structure factor is appropriate. It fails for a *scalar* order parameter, where the excess energy resides in domain walls of finite thickness  $w \ll L(t)$ . For this case the excess energy is of order  $1/w$  per unit area of wall, giving  $\Delta E(t) \sim 1/wL(t)$  for the excess energy density, since the wall area in a volume  $L(t)^d$  is of order  $L(t)^{d-1}$ .

From the  $d = 2$  simulations discussed below we find, for  $n \geq 4$ ,  $\Delta E(t) \sim 1/t$ , implying  $L(t) \sim t^{1/2}$  in agreement with the large- $n$  behaviour and with dimensional analysis based on  $L(t)$  being the only important scale [5]. With this choice of  $L(t)$ , furthermore, the equal-time correlation function  $C(r, t, t)$  is found to scale precisely as predicted by (1). No such simple scaling, however, is observed for  $n = 2$  or 3.

The third quantity that we compute in the simulations is the ‘autocorrelation function’  $A(t) = \langle N^{-1} \sum_i \mathbf{S}_i(t) \cdot \mathbf{S}_i(0) \rangle$ , where  $N$  is the number of spins, i.e.  $A(t) = C(0, 0, t)$ . From (3), we expect this to decay with time as  $A(t) \sim L(t)^{-\bar{\lambda}}$ , i.e.  $A(t) \sim t^{-\lambda/2}$  for  $n \geq 4$ , where  $\bar{\lambda} = 2 - \lambda$  for  $d = 2$ . The data fulfil these expectations, and allow a fairly precise determination of  $\lambda$  for  $n \geq 4$ .

### 3. Simulation results

#### 3.1. $n \geq 4$

Simulations were performed for  $d = 2$  systems of  $N = 200 \times 200$  sites, with periodic boundary conditions. At each site a spin of unit length is constrained to the surface of a hypersphere of dimension  $n$ . The system is set up with each spin having an independently random orientation, corresponding to an infinite-temperature equilibrium configuration. We now envisage an instantaneous quench to  $T = 0$  where the non-equilibrium dynamics of the system are governed by equations (7) and (8). Since the system is at  $T = 0$  there is no thermal noise. Results are averaged over an ensemble of 20 independently generated initial configurations.

Simulation of the ordering process corresponds to iterating the finite difference version of (7) with time step  $\Delta t$ . For the first 5000 iterations we set  $\Delta t = 0.01$

For subsequent iterations we set  $\Delta t = 0.05$  since by this time the spins will have a high degree of local correlation. We have checked that the results are insensitive to the choice of  $\Delta t$ . An important point to note is that converting (7) to a difference equation (i.e. finite  $\Delta t$ ) does not exactly preserve the length of a spin, although the error is only  $O(\Delta t)^2$ . Thus, after each iteration, every spin is rescaled to unit length.

During the simulation we compute the following quantities.

(i) The excess energy per spin

$$\Delta E(t) = 2 - \left\langle N^{-1} \sum_{\langle i,j \rangle} \mathbf{S}_i(t) \cdot \mathbf{S}_j(t) \right\rangle.$$

(ii) The equal-time correlation function

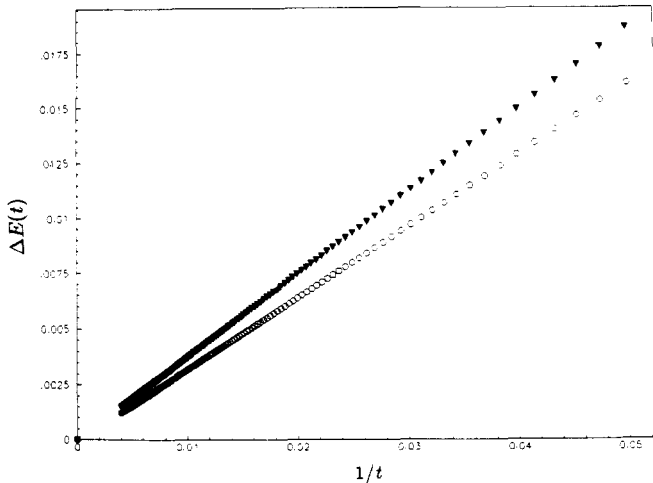
$$C(r, t, t) = \left\langle N^{-1} \sum_i \mathbf{S}_i(t) \cdot \mathbf{S}_{i+r}(t) \right\rangle$$

where here  $i + r$  indicates a site displaced by  $r$  lattice spacings, relative to site  $i$ , along a lattice axis. Displacements along both  $x$ - and  $y$ -axes are included in the average.

(iii) The autocorrelation function

$$A(t) = \left\langle N^{-1} \sum_i \mathbf{S}_i(t) \cdot \mathbf{S}_i(0) \right\rangle.$$

In all cases  $\langle \dots \rangle$  indicates the average over the ensemble of initial configurations.



**Figure 1.** Relaxation of the excess energy per spin for:  $\blacktriangledown$ ,  $n = 4$ ;  $\circ$ ,  $n = 5$ . A fit to  $\Delta E = a(n)/t$  gives the amplitudes  $a(n)$  listed in table 1.

For  $n = 4$  and  $5$  we find that the system enters a scaling regime, i.e. the equal-time correlation function scales as in (1), after  $\sim 10$  real time units. To determine the  $t$ -dependence of  $L(t)$  we plot  $\Delta E(t)$  against  $1/t$ . 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  $t \geq 20$  are shown), which extrapolate nicely through the origin, confirms the asymptotic time dependence  $\Delta E(t) \sim 1/t$  and implies, via (11), that  $L(t) \sim t^{1/2}$  for  $n \geq 4$ . Hence we can write, asymptotically

$$\Delta E(t) \sim a(n)/t \quad t \rightarrow \infty. \quad (12)$$

The coefficients  $a(n)$  for  $n = 4, 5$  are listed in table 1. These values are of interest because we conjecture that they are *universal*, i.e. independent of the initial conditions, provided that any correlations present at  $t = 0$  are short-ranged, and independent of the details of the Hamiltonian, provided the interactions remain short-ranged. Such universality can be explicitly demonstrated for  $n = \infty$ , with  $a(\infty) = d/8$ , as shown in I. Note that a necessary condition for universality is that the energy relaxes as  $1/t$ . This requirement follows upon demanding that  $\Delta E(t)$  be invariant under a simple rescaling of the Hamiltonian.

**Table 1.** Exponents and amplitudes extracted from the data for  $n \geq 4$ . The exponent  $\bar{\lambda}$  is deduced from the decay of the autocorrelation function,  $A(t) \sim t^{-\bar{\lambda}/2}$ , using the data in figure 5;  $\lambda \equiv 2 - \bar{\lambda}$  for  $d = 2$ ;  $\lambda_{1/n}$  is the theoretical prediction (5) including the  $O(1/n)$  term;  $a(n)$  is the amplitude in the energy relaxation,  $\Delta E \rightarrow a(n)/t$ , extracted from figure 1;  $b(n)$  is the parameter describing the best Gaussian fit to the equal-time correlation function,  $C(r, t, t) \simeq \exp\{-b(n)r^2/t\}$ . The final row gives the exact results for these quantities when  $n = \infty$ .

$n$	$\bar{\lambda}$	$\lambda$	$\lambda_{1/n}$	$a(n)$	$b(n)$
4	1.11(1)	0.89(1)	0.901	0.374(1)	0.171(2)
5	1.06(1)	0.94(1)	0.921	0.322(1)	0.148(2)
$\infty$	1	1	1	1/4	1/8

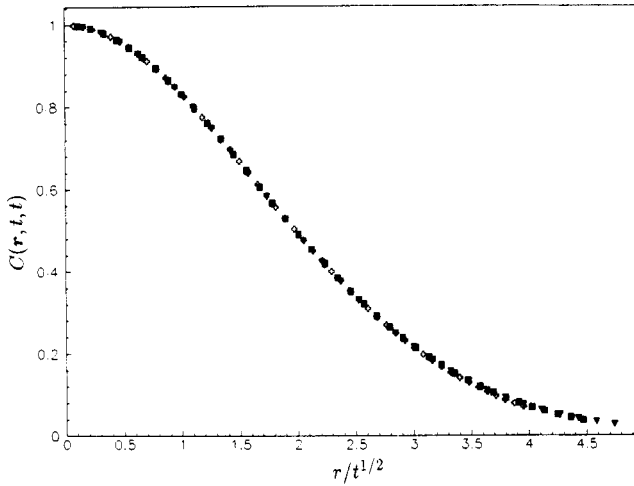
Data for the equal-time correlation function  $C(r, t, t)$  are presented in figures 2 and 3, where the abscissa is in each case the scaling variable  $r/t^{1/2}$ . The excellent collapse of the data on to universal scaling curves confirms both the scaling form (1) and the result  $L(t) \sim t^{1/2}$  deduced from the energy relaxation. The scaling functions are close to Gaussian, and fits to the form  $C(r, t, t) = \exp(-b(n)r^2/t)$  yield the parameters  $b(n)$  listed in table 1. Exact solution of the model for  $n = \infty$  yields a Gaussian scaling function, with  $b(\infty) = 1/8$  for all  $d$  [9]. The  $n = \infty$  results for  $d = 2$  are included in table 1 for comparison.

Results for the autocorrelation function,  $A(t)$ , are given in figure 4 for  $n = 4, 5$ . The linear behaviour of the  $-\ln A(t)$  against  $\ln t$  plots confirms the anticipated result, namely

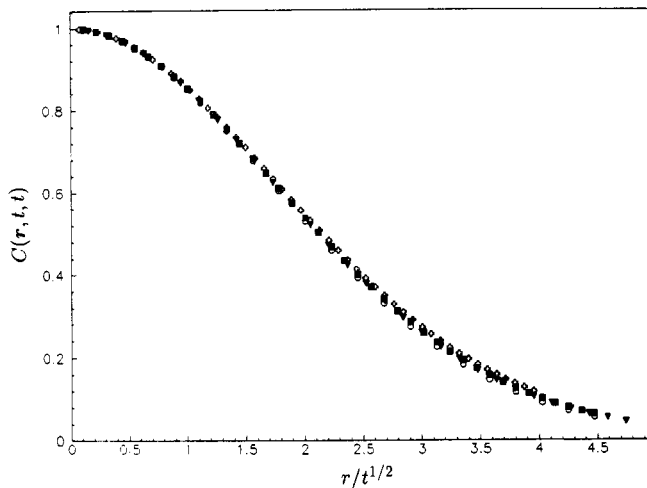
$$A(t) \sim t^{-\bar{\lambda}/2} \quad (13)$$

with  $\bar{\lambda} = \bar{\lambda}(n)$ . The results for  $\bar{\lambda}$  and  $\lambda \equiv d - \bar{\lambda}$  are given in table 1, and compared with the prediction, equation (5) with  $d = 2$ , of the  $1/n$ -expansion. The agreement is surprisingly good.

The errors quoted in table 1 are purely statistical, and take no account of any systematic errors associated with a failure to reach the asymptotic regime. The straightness of the lines in figures 1 and 4, however, and the excellent collapse of the data in the scaling plots of figures 2 and 3, suggest that the asymptotic regime is reached rather quickly for  $n \geq 4$ , since the data scales well for  $t \geq 10$ . The systematic errors



**Figure 2.** The equal-time correlation function  $C(r, t, t)$ , plotted against the scaling variable  $r/t^{1/2}$ , for  $n = 4$ :  $\circ$ ,  $t = 20$ ;  $\nabla$ ,  $t = 40$ ;  $\blacksquare$ ,  $t = 80$ ;  $+$ ,  $t = 160$ .



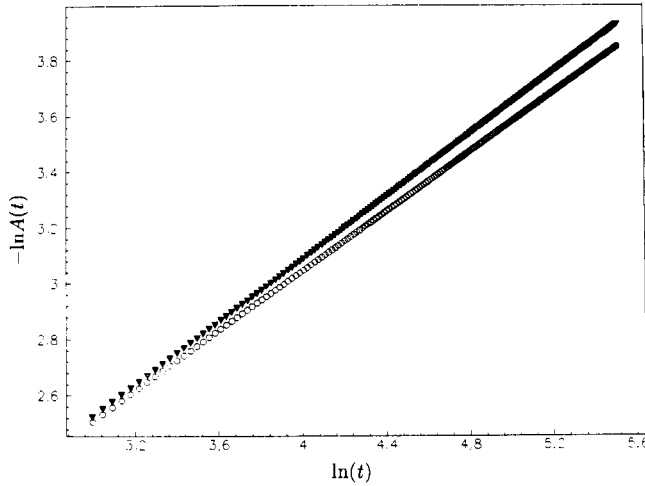
**Figure 3.** Scaling plot of the equal-time correlation function for  $n = 5$ . Symbols as for figure 2.

associated with the finite temporal extent of the simulations can be estimated from the exact solution, on the lattice, of equation (7) for  $n = \infty$  (see I). The result suggests that these systematic errors should be smaller than the statistical errors quoted in table 1.

### 3.2. $n = 2$

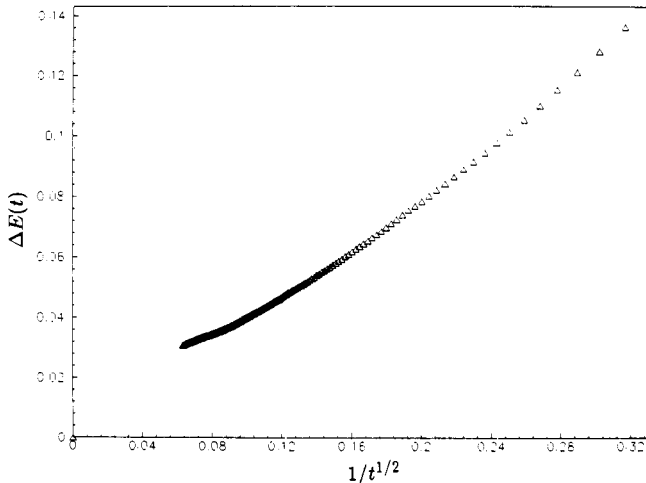
The energy relaxation data for  $n = 2$  is shown in figure 5. In contrast to  $n \geq 4$  (and also  $n = 3$ , see below) the excess energy does not seem to relax to zero at infinite time, but rather to saturate at a non-zero limiting value. We ascribe this phenomenon to the presence of a finite density of vortices and anti-vortices, which are not relaxed





**Figure 4.** Time dependence of the autocorrelation function  $A(t)$ , plotted as  $-\ln A(t)$  against  $\ln t$ , for:  $\blacktriangledown$ ,  $n = 4$ ;  $\circ$ ,  $n = 5$ . The values of the exponents  $\lambda$  ( $A(t) \sim t^{-\lambda/2}$ ), deduced from the slopes, are listed in table 1.

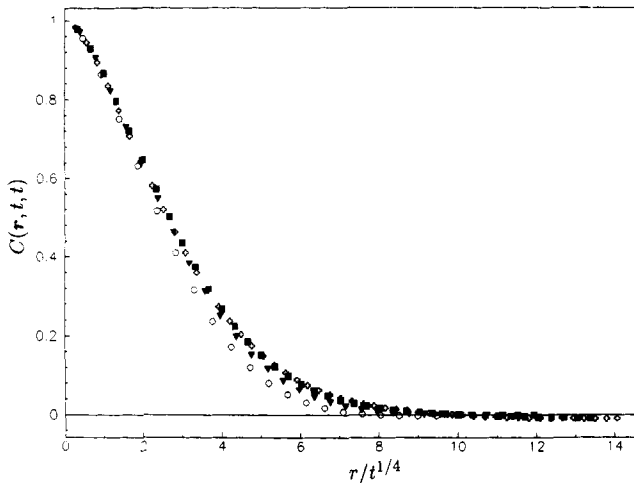
out by the dynamics of equation (7): each spin is parallel to its local field and the vortex/anti-vortex state is a local (metastable) minimum of the Hamiltonian (6). We have verified, by explicit inspection of the spin configurations, the presence of vortices and anti-vortices, with a typical separation of about 13 lattice spacings. The vortex positions are stable under the dynamics.



**Figure 5.** Relaxation of the excess energy per spin for  $n = 2$ . The choice for  $1/t^{1/2}$  as abscissa is motivated by the results obtained for  $d = 1$  in [9]. Note that  $\Delta E(t)$  does not seem to be approaching zero as  $t \rightarrow \infty$ .

In the absence of a well defined scaling regime for the energy relaxation at  $T = 0$ , one does not expect the correlation function to scale well. The data are presented

in figure 6, plotted against  $r/t^{1/4}$ . Somewhat surprisingly, the collapse of the data is quite good apart from the earliest time,  $t = 20$  (and, to a lesser extent,  $t = 40$ ). The choice of  $r/t^{1/4}$  as scaling variable is motivated by the results obtained in  $d = 1$  (see I), where  $r/t^{1/4}$  scaling was obtained analytically by linearizing the equation of motion in angular variables. This is valid when neighbouring spins are almost parallel, which is the case for  $d = 1$  at late times. The same calculation can be extended to  $d = 2$  if one ignores vortices, and  $r/t^{1/4}$  scaling is again obtained [9]. It is not immediately clear how this result would be affected by the ‘frozen’ vortices present in the simulations. Furthermore, if vortices and antivortices are allowed to annihilate, either by introducing temperature or by using a ‘soft-spin’ Hamiltonian, quite different results might be obtained.



**Figure 6.** Scaling plot for the equal-time correlation function for  $n = 2$ , using  $r/t^{1/4}$  as scaling variable.  $n = 4$ :  $\circ$ ,  $t = 20$ ;  $\blacktriangledown$ ,  $t = 40$ ;  $\blacksquare$ ,  $t = 80$ ;  $+$ ,  $t = 160$ .

### 3.3. $n = 3$

The case  $n = 3$  is also difficult to interpret. A preliminary log-log plot of excess energy against time suggests a  $t^{-2/3}$  decay law. Therefore we plot (figure 7) the excess energy directly against  $1/t^{2/3}$ . This plot yields, for  $t > 30$ , a good straight line that extrapolates through the origin, suggesting that there is no residual energy in this case and, from (11), that the characteristic scale grows as  $L(t) \sim t^{1/3}$ . However, an attempted collapse of the data for the equal-time correlation function using  $r/t^{1/3}$  as scaling variable is not convincing: the data are ‘undercollapsed’, suggesting that a scaling variable  $r/t^\phi$  with  $\phi > 1/3$  is required. No value of  $\phi$ , however, produces a good collapse over the whole range of the scaling variable.

While we have been unable to account explicitly for the form of the data, it is possible that  $n = 3$  is a special case, distinct from  $n \geq 4$ , for the following reason. The continuum equation of motion (10) possesses stationary solutions (in which the right-hand side vanishes) other than the ground state. These are the soliton (or instanton) solutions identified by Polyakov [13]. While these seem to be weakly unstable on the lattice, the initial configuration may inject a number of such objects into the system.

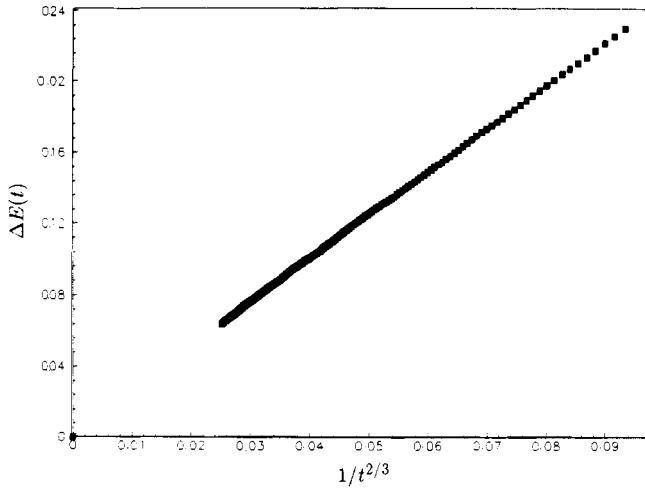


Figure 7. Relaxation of the excess energy per spin for  $n = 3$ , plotted against  $1/t^{2/3}$ .

The presence of these topological structures influences the dynamics in a way which we do not yet understand. As for the case  $n = 2$ , more work is required to clarify the situation.

After this work was completed, we received a preprint from Mondello and Goldenfeld in which the case  $n = 2$ ,  $d = 2$  was studied using a ‘cell dynamics simulation’, equivalent to using a Langevin equation with a ‘soft-spin’ Hamiltonian, at  $T = 0$  [14]. This dynamics allows vortex-antivortex annihilation. The authors find a pre-asymptotic behaviour  $L(t) \sim t^{3/8}$ , crossing over to  $L(t) \sim t^{1/2}$  at later times. This suggests that asymptotically  $n = 2$  belongs to the same class of systems as  $n \geq 4$ . It would be interesting to apply a similar approach to  $n = 3$ . Our work strongly suggests that fixed-length spin models yield the correct asymptotic behaviour for  $n \geq 4$ .

#### 4. Universality

For a scalar order parameter, it has been observed empirically that the scaling function for the equal-time correlation function  $C(r, t, t)$  is universal if  $r$  is scaled by a suitably defined domain scale  $L(t)$ , extracted from the data itself (see e.g. [15] for recent studies of systems with a conserved scalar order parameter). Here we interpret this universality in terms of the  $T = 0$  fixed point controlling the asymptotic dynamics, and suggest explicit forms for  $L(t)$  in terms of independently measurable equilibrium properties of the system. We also note that equations (1) and (2) require a prefactor  $M^2$  for general  $T$ .

In the context of a non-conserved vector order parameter, the question of universality in ordering kinetics was raised in I, where it was suggested that, in addition to  $C(r, t, t)$ , the amplitude  $a(n)$  in the energy relaxation,  $\Delta E \rightarrow a(n)/t$ , might be universal at  $T = 0$ . In subsection 4.1 we present numerical evidence for universality at  $T = 0$ . For this purpose we revert to the  $d = 1$  systems studied in I, and specialize to  $n = 3$ . The results should be qualitatively similar for all  $n \geq 3$  in  $d = 1$  and for all  $n \geq 4$  in  $d = 2$ . In subsection 4.2 we suggest that an extended form of universality holds for  $T < T_c$  when  $T_c > 0$ .

#### 4.1. Universality at $T = 0$

The simulation details of these  $d = 1$  systems were described in I. The basic idea underlying universality is that, on large length and time scales, the system can be described by the continuum Hamiltonian (9) and corresponding equation of motion (10), independent of the microscopic details of the model, with the proviso that the Hamiltonian contains only short-range interactions and the initial conditions only short-range correlations. These latter restrictions specify a universality class for the model.

To test this idea we consider systems with both nearest-neighbour interactions  $J_1$  and next-nearest-neighbour interactions  $J_2$ . Then the continuum Hamiltonian becomes  $H = (\rho_s/2) \int d^d x (\nabla \mathbf{S})^2$  instead of (9), where the spin-wave stiffness  $\rho_s$  is defined by  $\Delta E(\theta) = (\rho_s/2)(\theta/L)^2$ , this being the energy cost per spin of imposing a twist of  $\theta$  in the spin direction over a length  $L$ . Since  $\theta/L$  is the twist across each bond, we have

$$\rho_s = J_1 + 4J_2. \quad (14)$$

The corresponding equation of motion acquires a factor  $\rho_s$  on the right-hand side of (10).

In the simulations we used  $J_1 = 1$  and  $J_2 = 0, 1/4, 3/4,$  and  $7/4$ , corresponding to  $\rho_s = 1, 2, 4$  and  $8$  respectively. If we assume that there is a single characteristic length scale  $L(t)$  at late times, we can estimate its time dependence from dimensional analysis of (10) (with a factor  $\rho_s$  on the right-hand side), namely  $1/t \simeq \rho_s/L(t)^2$ , to obtain  $L(t) \simeq (\rho_s t)^{1/2}$ . Similarly, equation (9) (with a factor  $\rho_s$  on the right) gives, for the excess energy density,  $\Delta E \simeq \rho_s/L(t)^2 \simeq 1/t$ , independent of  $\rho_s$ . Thus we expect to find, in the scaling regime

$$\Delta E(t) = a/t \quad (15)$$

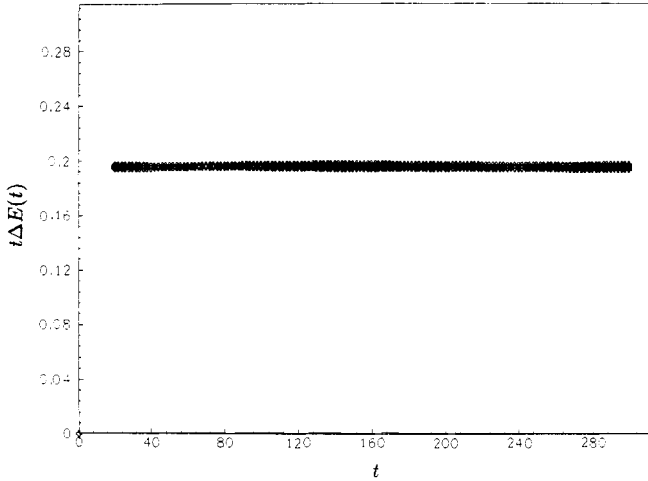
$$C(r, t, t) = f_e[r/(\rho_s t)^{1/2}] \quad (16)$$

with both  $a$  and  $f_e(x)$  universal.

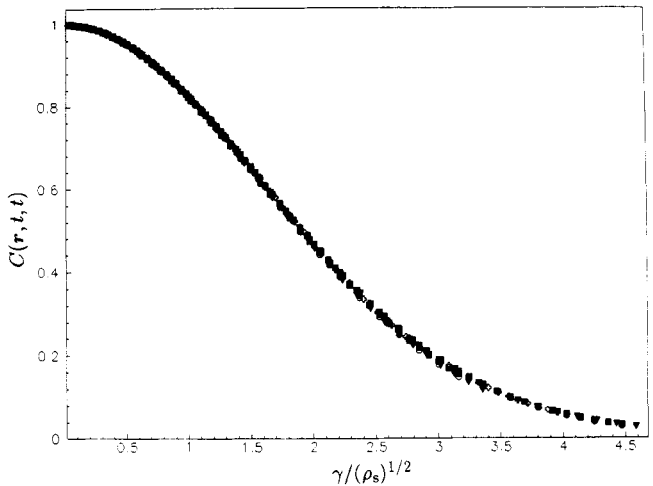
The data for  $\Delta E$  and  $C(r, t, t)$  are shown in figures 8 and 9, with the data obtained with different values of  $\rho_s$  superimposed. The results convincingly verify the forms (15) and (16). We conclude that the microscopic details of the model are indeed irrelevant in the scaling regime.

The above results also imply that the asymptotic behaviour of the system is independent of short-range correlations in the initial conditions. The arguments leading to (15) and (16) are equivalent to extracting the dependence on  $\rho_s$  by rescaling lengths through the change of variable  $\mathbf{x} = \rho_s^{1/2} \mathbf{x}'$ . Then  $\rho_s$  drops out of the equation of motion in the continuum limit. However,  $\rho_s$  reappears in the initial condition, since the length scale characterizing the range of the correlations is reduced by a factor  $\rho_s^{1/2}$  in the new variables. We conclude that the data collapse of figures 8 and 9 demonstrate independence of the initial conditions at late times as well as of the microscopic details of the model, subject to the caveat that any correlations in the initial conditions remain short-ranged. Initial conditions with long-range correlations can, however, be a relevant perturbation to the asymptotic dynamics [6].

As a link to the following section we should emphasize that the forms (15) and (16) are predicated on particular values for the 'kinetic coefficient',  $\Gamma = 1$ , and the spin



**Figure 8.** Relaxation of the excess energy per spin for  $d = 1$ ,  $n = 3$ , plotted as  $t\Delta E(t)$  against  $t$ . The data from systems with  $\rho_s = 1, 2, 4, 8$  are superimposed, as described in the text. The limit as  $t \rightarrow \infty$  gives, via equation (15), the universal energy amplitude  $a$  for these systems, and is consistent with the value  $a = 0.193(1)$  obtained in [9]. The ‘flatness’ of the data is an indication of how early the scaling regime sets in.



**Figure 9.** Universal scaling function  $f_e(x)$  (equation (16)) for  $d = 1$ ,  $n = 3$ . The data for  $\rho_s = 1, 2, 4, 8$  are superimposed.

length,  $|\mathbf{S}| = 1$  (or equivalently the equilibrium order parameter,  $M = 1$ ). In section 4.2 below we will include the effects of thermal fluctuations on these quantities to obtain generalized scaling forms for all  $T < T_c$ . To conclude this section we discuss what (15) and (16) become at  $T = 0$  for general kinetic coefficient  $\Gamma$  and spin length  $|\mathbf{S}| = M$ .

In the most general case the continuum Hamiltonian and equation of motion be-

come, instead of (9) and (10),

$$H = \frac{\rho_s}{2M^2} \int d^d x (\nabla \mathbf{S})^2 \tag{17}$$

$$\partial \mathbf{S} / \partial t = (\Gamma \rho_s / M^2) \{ \nabla^2 \mathbf{S} + M^{-2} (\nabla \mathbf{S})^2 \mathbf{S} \}. \tag{18}$$

Repeating, in this more general context, the dimensional analysis that previously led to  $L(t) \simeq (\rho_s t)^{1/2}$  now gives

$$L(t) \simeq \left( \frac{\Gamma \rho_s t}{M^2} \right)^{1/2}. \tag{19}$$

Similarly, dimensional analysis of (17) yields now

$$\Delta E(t) \simeq \frac{\rho_s}{L(t)^2} \simeq \frac{M^2}{\Gamma t}. \tag{20}$$

Then the general statement of universality at  $T = 0$  is

$$\Delta E(t) = a \frac{M^2}{\Gamma t} \tag{21}$$

$$C(r, t, t) = M^2 f_e \left[ r \left( \frac{M^2}{\Gamma \rho_s t} \right)^{1/2} \right] \tag{22}$$

with  $a$  and  $f_e(x)$  universal for a given  $n$  and  $d$ . We stress again that  $\Gamma$ ,  $\rho_s$  and  $M$  are simply constants in (21) and (22). In the following subsection they will become functions of temperature.

#### 4.2. Universality for $T < T_c$

Given that the ordering kinetics is governed by a  $T = 0$  RG fixed point, it seems reasonable to assume that any universal quantities in the theory are properties of the fixed point itself. Furthermore, since the fixed point is attractive, these same universal quantities should characterize the entire ordered phase. Our viewpoint in this subsection is that this is indeed the case, and that the role of thermal fluctuations is limited to renormalizing the kinetic coefficient  $\Gamma$ , spin wave stiffness  $\rho_s$  and equilibrium order parameter  $M$ , so that these become functions of temperature given by their equilibrium values.

The validity of this result rests on there being no non-trivial renormalization of  $\Gamma$  at the  $T = 0$  fixed point [5]. For a vector order parameter, this assumption leads immediately to  $z = 2$  (i.e.  $L(t) \sim t^{1/2}$ ), and is equivalent to the assumption that the dimensional analysis which we performed above gives correct results [5]. This means that the discussion is limited to  $n$ -values for which  $L(t) \sim t^{1/2}$  and  $\Delta E(t) \sim 1/t$ , i.e. to the 'large- $n$ ' classes  $n \geq 3$  for  $d = 1$  and  $n \geq 4$  for  $d = 2$ , and possibly also to  $n = 2$  for  $d = 2$  [14].

One minor modification for  $T > 0$  is that the excess energy has to be replaced by the excess free energy in (21). Thus we conjecture that, throughout the ordered phase, the asymptotic time-dependence of the excess free energy is given by

$$\Delta F(t) = a M^2 / \Gamma t \tag{23}$$

and that of the equal-time correlation function is given by (22), where now  $M = M(T)$ ,  $\Gamma = \Gamma(T)$  and  $\rho_s = \rho_s(T)$  are the equilibrium values of these quantities in the ordered phase, and may be obtained from macroscopic measurements. For example,  $\rho_s(T)$  and  $\Gamma(T)$  can be deduced from the dependence on wavevector  $k$  and frequency  $\omega$  of the equilibrium transverse susceptibility  $\chi_T(k, \omega)$  in the limit  $k \rightarrow 0$ ,  $\omega \rightarrow 0$ , namely  $\chi_T(k, 0) \rightarrow M^2/\rho_s k^2$ , and  $\chi_T(0, \omega) \rightarrow \Gamma/(-i\omega)$ . The key point is that  $a$  and  $f_e(x)$  should be universal and independent of  $T$ .

For general  $T$ , equations (22) and (23) hold only when  $L(t)$  and  $r$  are both large compared to the thermal correlation length  $\xi$ . In the limit  $T \rightarrow T_c$  from below, one can insert the scaling behaviour  $M^2 \sim \xi^{-(d-2+\eta)}$ ,  $\rho_s \sim \xi^{-(d-2)}$  and  $\Gamma \sim \xi^{2-\eta-z}$ , where  $z$  is here the dynamic critical exponent, to obtain  $\Delta F(t) \sim \xi^{-d}(\xi^z/t)$ , consistent with static and dynamic critical scaling, and  $C(r, t, t) = \xi^{-(d-2+\eta)} f[(r/\xi)(\xi^z/t)^{1/2}]$ , again consistent with critical scaling.

The extension of these arguments to a conserved vector order parameter, and to conserved and non-conserved scalar order parameters, is discussed below.

## 5. Discussion and summary

The  $T = 0$  ordering kinetics of vector spin systems with non-conserved order parameter have been discussed. Numerical simulations in  $d = 2$  for  $2 \leq n \leq 5$  indicate the existence of an asymptotic scaling regime, with characteristic length scale  $L(t) \sim t^{1/2}$ , for  $n \geq 4$ . The scaling regime is associated with a  $1/t$  behaviour of the excess energy, and with the scaling form (1) for the equal-time correlation function. The correlation with the initial condition is described by the power-law form (13), and the exponent  $\bar{\lambda}$  is in reasonable agreement with the prediction of the  $1/n$ -expansion [10].

For  $n = 2$  the  $T = 0$ , fixed-length spin, Langevin dynamics employed seem to lead to metastable states, with non-zero vortex density at infinite time. Thus we do not believe that the asymptotic scaling regime is accessible by these methods, although the equal-time correlation function scales reasonably well against  $r/t^{1/4}$  for the times studied. It is interesting that  $L(t) \sim t^{1/4}$  is the result expected in the absence of vortices, and is in fact realized for  $d = 1$ . The  $r/t^{1/4}$  scaling obtained for  $d = 2$  will presumably break down when  $L(t)$  becomes comparable with the typical spacing of the frozen vortices. Recent studies using a 'cell dynamics simulation' (CDS), equivalent to a 'soft-spin' Hamiltonian, are consistent with  $L(t) \sim t^{1/2}$  at late times [14].

Similarly, for  $n = 3$  the data fail to scale well, even at short times, due presumably to the presence in the system of 'Polyakov solitons' [13]. It will be interesting to apply the CDS approach to this case.

For vector systems with  $\phi = 1/2$ , we have argued that the scaling function for the equal-time correlation function should be universal, i.e. independent of  $T$  as well as of microscopic details of the model, for all  $T < T_c$ , provided the scale length  $L(t)$  is expressed in terms of the appropriate macroscopic quantities  $M$ ,  $\Gamma$  and  $\rho_s$  as in (22). Similarly, we argue that the excess free energy should be associated with a universal amplitude, as in (23). This universal behaviour should, we believe, emerge as a property of the  $T = 0$  fixed point controlling the scaling regime. Universality with respect to the Hamiltonian has been demonstrated explicitly at  $T = 0$  for  $d = 1$ ,  $n = 3$ .

We conclude by discussing how such universality might emerge for a scalar order parameter (i.e.  $n = 1$ ). For a non-conserved scalar order parameter, the analogue of

(19) is [5]

$$L(t) \simeq \left( \frac{\Gamma \Sigma w t}{M^2} \right)^{1/2} \quad (24)$$

where  $\Sigma$  and  $w$  are the surface tension and domain wall thickness respectively. The explicit appearance of the latter is a consequence of the non-trivial renormalization of the kinetic coefficient at the  $T = 0$  fixed point for this case [5]. Also, the excess free energy density has the form  $\Delta F(t) \simeq \Sigma/L(t)$  for a scalar order parameter, so the analogues of (23) and (22) are given naively by

$$\Delta F(t) = a M \left( \frac{\Sigma}{\Gamma w t} \right)^{1/2} \quad (25)$$

$$C(r, t, t) = M^2 f_e \left[ r \left( \frac{M^2}{\Gamma w \Sigma t} \right)^{1/2} \right]. \quad (26)$$

It is tempting to conjecture that  $a$  and  $f_e(x)$  are here universal, as was suggested for the non-conserved vector case. This, however, requires us to provide a precise definition of the ‘interface thickness’  $w$ . In addition, it is not immediately clear what is meant by  $\Sigma$ , in (25) and (26), for lattice models where the surface tension can be anisotropic. By contrast, for lattice vector models the isotropy of the spin-wave stiffness  $\rho_s$  follows from the existence of the isotropic continuum limit (17). Setting these caveats aside, it will be interesting to carry out simulations of scalar systems for a range of temperatures below  $T_c$  to test whether, for example, the equal-time correlation function can be fitted to the form  $C(r, t, t) = M^2 f_e(r/Bt^{1/2})$ , where all the  $T$ -dependence is contained in  $M$  and  $B$ , as suggested by (26).

In a similar spirit, one can consider a conserved scalar order parameter. For this case, one expects [4, 5, 16]

$$L(t) \simeq \left( \frac{\lambda \Sigma t}{M^2} \right)^{1/3} \quad (27)$$

where  $\lambda$  is the ‘transport coefficient’ or ‘spin conductivity’ [4, 5, 16]. This gives, instead of (25) and (26),

$$\Delta F(t) = a \left( \frac{\Sigma^2 M^2}{\lambda t} \right)^{1/3} \quad (28)$$

$$C(r, t, t) = M^2 f_e \left[ r \left( \frac{M^2}{\lambda \Sigma t} \right)^{1/3} \right]. \quad (29)$$

Finally, for a conserved vector order parameter, one expects [4, 5]

$$L(t) \simeq \left( \frac{\lambda \rho_s t}{M^2} \right)^{1/4} \quad (30)$$

giving

$$\Delta F(t) = a \left( \frac{\rho_s M^2}{\lambda t} \right)^{1/2} \quad (31)$$

$$C(r, t, t) = M^2 f_e \left[ r \left( \frac{M^2}{\lambda \rho_s t} \right)^{1/4} \right]. \quad (32)$$



An additional caveat in this case is that, for a conserved vector order parameter with  $n = \infty$ , the scaling form (1) is known to fail due to the appearance of two marginally different length scales diverging as  $t^{1/4}$  and  $(t/\ln t)^{1/4}$ , leading to 'multiscaling' instead of simple scaling [17]. It is not known at present whether this phenomenon persists to finite  $n$ . Multiscaling has also been suggested in the context of a non-conserved scalar order parameter [18], although there is no evidence in this case for the failure of the scaling from (1) for the equal-time correlation function. The excellent scaling of the data presented in figures 2 and 3 also strongly suggests the validity of (1) for a non-conserved vector order parameter, at least for  $n \geq 4$ .

The prefactor  $M^2$  in (22), (26), (29) and (32) is important, and seems to have been overlooked in some previous analyses. Rogers *et al* [15], for example, study the Langevin equation for a conserved scalar 'soft-spin' model in  $d = 2$  with dimensionless thermal noise  $\epsilon = 0, 0.05, 0.2$  and  $0.5$ . The data for  $\epsilon = 0.5$  do not fall on the same scaling curve as the other data, which they attribute to the  $\epsilon = 0.5$  data not being in the scaling regime. A visual inspection of the data, however, reveals that the  $\epsilon = 0.5$  data is essentially just reduced by an overall factor of about 0.75 compared to the scaling curve. We interpret this, via equation (29), as corresponding to an equilibrium magnetization  $M$  of about 0.87 for this noise strength. In the study by Gunton *et al* [15], data from the  $d = 2$  kinetic Ising model at  $T = 0.6T_c$  collapse well onto data obtained from Langevin and CDS studies at  $T = 0$ . For  $T = 0.6T_c$ , however, the equilibrium magnetization is extremely close to unity, so the omission of the factor  $M^2$  in (29) would not be noticed.

The origin of the factor  $M^2$  is clear when one recalls that the scaling regime is defined by  $r$  and  $L(t)$  both being large compared with the thermal correlation length  $\xi$ , but  $r/L(t)$  arbitrary. For  $\xi \ll r \ll L(t)$  one has immediately  $C(r, t, t) = M^2$ , which also shows that  $f_e(0) = 1$ .

## Acknowledgments

AB thanks M A Moore and T J Newman for useful discussions. KH thanks Alex Szymanski (Manchester Computing Center) for technical assistance and the SERC for a Research Studentship.

## References

- [1] Hohenberg P C and Halperin B I 1977 *Rev. Mod. Phys.* **49** 435
- [2] Gunton J D, San Miguel M and Sahní P S 1983 *Phase Transitions and Critical Phenomena* vol 8, eds C Domb and J L Lebowitz (New York: Academic) p 267  
Furukawa H 1985 *Adv. Phys.* **34** 703  
Binder K 1987 *Rep. Prog. Phys.* **50** 783
- [3] Mazenko G F, Valls O T and Zhang F 1985 *Phys. Rev. B* **31** 4453  
Lai Z W, Mazenko G F and Valls P T 1988 *Phys. Rev. B* **37** 9481  
Vinals J, Grant M, San Miguel M, Gunton J D and Gawłinski E T 1985 *Phys. Rev. Lett.* **54** 1264  
Kumar S, Vinals J and Gunton J D 1986 *Phys. Rev. B* **34** 1908  
Roland C and Grant M 1988 *Phys. Rev. Lett.* **60** 2657  
Roland C and Grant M 1989 *Phys. Rev. B* **39** 11971
- [4] Bray A J 1989 *Phys. Rev. Lett.* **62** 2841
- [5] Bray A J 1990 *Phys. Rev. B* **41** 6724
- [6] Bray A J, Humayun K and Newman T J 1990 *Phys. Rev. B* to appear

- [7] Lifshitz I M and Slyosov V V 1961 *J. Chem. Phys. Solids* **19** 35
- [8] Lifshitz I M 1962 *Zh. Eksp. Teor. Fiz.* **42** 1354 (*Engl. transl. 1962 Sov. Phys.-JETP* **15** 939)  
Allen S M and Cahn J W 1979 *Acta Metall.* **27** 1085
- [9] Newman T J, Bray A J and Moore M A 1990 *Phys. Rev. B* **42** 4514
- [10] Newman T J and Bray A J 1990 *J. Phys. A: Math. Gen.* **23** L279  
Newman T J and Bray A J 1990 *J. Phys. A: Math. Gen.* **23** 4491
- [11] Furukawa H 1989 *J. Phys. Soc. Japan* **58** 216  
Furukawa H 1989 *Phys. Rev. B* **40** 2341
- [12] Abramowitz M and Stegun I A (eds) 1965 *Handbook of Mathematical Functions* (New York: Dover)
- [13] Rajaraman R 1982 *Solitons and Instantons* (North Holland: Amsterdam)
- [14] Mondello M and Goldenfeld N 1990 *preprint*
- [15] Rogers T M, Elder K R and Desai R C 1988 *Phys. Rev. B* **37** 9638  
Gunton J D, Gawlinski E T, Chakrabarti A and Kaski L 1988 *J. Appl. Cryst.* **21** 811
- [16] Huse D A 1986 *Phys. Rev. B* **34** 7845
- [17] Coniglio A and Zannetti M 1989 *Europhys. Lett.* **10** 575  
Congiglio A and Zannetti M 1989 *Preprint*
- [18] Roland C and Grant M 1989 *Phys. Rev. Lett.* **63** 551