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Coarse-grained properties of three-dimensional Ising systems

S A Newlove and A D Bruce

Department of Physics, University of Edinburgh, UK

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Abstract. The universal coarse-grained properties of three-dimensional Ising systems are investigated with the aid of Wilson's recursion formula. The Helmholtz function is obtained in the critical regions both above and below the critical point; the coarse-grained free energy functional, believed to control spinodal decomposition, is also determined. The crossover from non-Gaussian (critical) to Gaussian (central limit) behaviour in the coarse-grained-coordinate distribution is investigated in both high- and low-temperature phases.

1. Introduction

It is now generally appreciated that the universal features of the behaviour displayed by a system near its critical point reflect a deeper universality in the spectrum of configurations formed by the system coordinates, coarse-grained to eliminate system-specific microscopic details. The seeds of this perception are to be found in the key papers developing the renormalisation group method (Kadanoff 1966, Wilson 1971); indeed, the idea is implicit, and apparent to varying degrees, in all the variants of this technique which have since been developed. In recent years the idea has found more explicit recognition in a number of studies focussing directly on the coarse-grained configuration spectrum. Particular attention has been given to two interrelated quantities: the *coarse-grained-coordinate probability density function* and the *coarse-grained Helmholtz functional.*

It is with these functions that we will be principally concerned in this paper. We shall restrict our attention to the Ising universality class in space dimension $d = 3$; the relevant ordering coordinates may thus be defined by a scalar field which we shall denote by $\{u(x)\}$. By 'coarse-grained coordinate' we shall mean the field $\{u_\Lambda(x)\}$ obtained by eliminating from $\{u(x)\}$ those Fourier components associated with wavevectors larger than a cut-off Λ. Physically the coordinate $u_\Lambda(x)$ represents the spatial average of the local field over a 'block' of linear dimension $\sim\Lambda^{-1}$ centred on the point x; we shall refer, loosely, to the set $\{u_\Lambda(x)\}$ as 'block' coordinates.

The block coordinate probability density function (PDF), $P_\Lambda(u_\Lambda(x))$, is of interest at formal, conceptual and practical levels. Its formal properties and significance have been explored by a number of authors (Cassandro and Jona-Lasinio 1978, and references therein). For block sizes Λ^{-1} *large* compared to ξ, the system correlation length, the PDF is Gaussian (Baker and Krinsky 1976) with a mean which is a measure of the equilibrium order parameter and a variance proportional to the associated susceptibility. For block sizes Λ^{-1} *small* compared to ξ the distribution is, in general, expected to be non-Gaussian (Gallavotti and Martin Löf, 1975). The existence of such non-Gaussian limiting forms is at the heart of an appealing probability-based view of the

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renormalisation group, advanced by Jona-Lasinio (1975). In a subsequent series of studies (Bruce *et al* 1979, Bruce 1981a) the universality of the block coordinate PDF was established (for Λ^{-1} and ξ large compared to microscopic lengths) and the form of the distribution determined exactly in $d = 1$ (for arbitrary $\Lambda\xi$), and approximately in dimensions $d = 2$ and 3 in the region $\Lambda^{-1} \ll \xi$, using the recursion-formula realisation of the renormalisation group due to Wilson (1971). These studies emphasise the conceptual value of the distributions which lie in their capacity to illuminate the nature of the configurational building blocks appropriate to a universality class. Finally, at a more immediately practical level Binder (1981; see also Binder and Landau 1984) has shown how the distributions and their moments may be analysed to yield critical indices and locate critical points and phase boundaries. Although this approach makes no explicit recourse to renormalisation group formalism it has much in common with the Monte Carlo renormalisation group methods pioneered by Swendsen (1982) and, like the latter, has clear cut advantages over the conventional analysis of Monte Carlo data, which may be traced to the use which it makes of the multiple-local-coordinate correlation functions implicit in the block coordinate distributions.

The coarse-grained Helmholtz functional (CGHF), $F_\Lambda(\{u_\Lambda(x)\})$, is intimately related to the coarse-grained coordinate PDF. Whereas the latter is the generating function for configurations of a single block coordinate $u_\Lambda(x)$, the former defines (is the configurational energy for) a coarse-grained representation of the partition function which is the generating function for the configurations of the entire block coordinate field $\{u_\Lambda(x)\}$. The CGHF assumes two particularly familiar limiting forms. In the regime $\Lambda^{-1} \gg \xi$ the function F_Λ effectively prescribes the true ('thermodynamic') Helmholtz function; on the other hand, in the regime $\Lambda^{-1} \ll \xi$ (but with Λ^{-1} still large compared to microscopic length scales) the CGHF is simply related to the fixed point 'Hamiltonian' of the (momentum-space) renormalisation group transformation (Wilson and Kogut 1974). There is, however, a further intermediate regime, which has attracted attention and which will be of particular interest here: the CGHF evaluated *below* the critical point for $\Lambda\xi$ equal to (or of the order of) unity is believed to define a configurational energy which controls the time-evolution of the large-scale structures involved in spinodal decomposition (Langer 1974). Indeed, the form of this function is an essential ingredient of the theory of this process developed by Langer *et al* (1975). In the latter studies the authors made the (then) reasonable assumption that the relevant CGHF might be represented by a Landau Ginzburg form; deficiencies of the theory which could be attributed to the inadequacy of this parameterisation were noted. Subsequently Kawasaki *et al* (1981) calculated the form of the CGHF (in $d = 3$) within a renormalisation group framework, utilising a perturbation expansion to first order in $\varepsilon = 4 - d$. Most recently Kaski *et al* (1984) have attempted to identify this function on the basis of Monte Carlo studies of the block coordinate configurations whose spectrum it controls.

In this paper we extend this programme of studies in a number of directions. We present the results of a variety of calculations based on Wilson's (1971) recursion formula. The recursion formula has long been known to yield reasonable values for $d = 3$ critical indices. The remarkable agreement between the recursion-formula-based calculations of the block distribution function (in the $\Lambda^{-1} \ll \xi$ limit) reported by Bruce *et al* (1979) and the results of Monte Carlo simulation (Binder 1981) lead us to believe that the recursion formula also generates a perhaps surprisingly faithful representation of other universal characteristics of the coarse-grained configuration spectrum. In § 2 we recall the recursion formula explicitly, study its properties in the critical region

both above and below the critical point and explore its implications for critical point amplitude ratios. The latter calculations serve two useful functions. Firstly they offer a further check on the capacities of the recursion formula: we find, in particular, that it predicts the susceptibility amplitude ratio with modest success. Secondly they enable us to parameterise the theory so that it is consistent with the known value of the universal amplitude combination connecting thermodynamic properties with the correlation length (Stauffer *et al* 1972), which is not unambiguously prescribed within the recursion formula framework. In § 3 we proceed to determine the Helmholtz free energy in both high- and low-temperature phases: we find that the recursion formula yields the anticipated convex structure although the predicted 'finite-size' corrections to the limiting form (in the low-temperature phase) are, we shall see erroneous. We then establish the form of the CGHF for $\Lambda\xi = 1$, $T < T_c$, and compare the result with the simple form assumed by Langer *et al* (1975) and the form calculated by Kawasaki *et al* (1981): there are marked differences at both quantitative and qualitative levels. In § 4 we turn to the block PDF. We extend the analysis reported previously (Bruce 1981a) which was confined to the regime $\Lambda^{-1} \ll \xi$; we calculate the PDF for a range of $\Lambda\xi$ values both above and below the critical point, thus interpolating between the non-Gaussian form and the (two) Gaussian limits. In addition to their conceptual value, these results have potentially observable implications for scattering studies of critical point fluctuations; these we discuss briefly.

2. Recursion formula studies

2.1. The recursion formula

We begin by reviewing briefly the arguments leading to the approximate recursion formula, emphasising those aspects of its derivation which will prove important in our subsequent studies.

Consider the partition function of a $d = 3$ scalar model belonging to the Ising universality class. The partition function is defined by a functional integral over a Boltzmann weight prescribed by a configurational energy ('Hamiltonian') which we write in the form

$$\mathcal{H}_0 = \Omega^{-1} \int \mathrm{d}^d x \{\bar{q}^{-2}(\nabla u(x))^2 + V_0(u(x))\}. \tag{2.1}$$

This form is chosen for convenience; the parameters Ω and $\bar{q}$ will be defined below. Any scalar continuum model can be written in this form simply by a suitable choice of scales for the ordering and spatial coordinates. In the representation (2.1) the field $u(x)$ is presumed to have a Fourier decomposition which includes only modes of wavevectors $|q| < \Lambda$. The recursion formula describes a mode-decimation operation whereby Fourier components with wavevectors $|q| > \frac{1}{2}\Lambda$ are integrated from the partition function. Thus, writing $u(x) = u_>(x) + u_<(x)$, where $u_<$ contains fluctuations with wavevectors less than $\frac{1}{2}\Lambda$ and $u_>$ incorporates the remaining fluctuations with wavevectors intermediate between $\frac{1}{2}\Lambda$ and Λ we perform the functional integral on $u_>$ to obtain an effective Hamiltonian $\mathcal{H}'$ for $u_<$. If we neglect the term independent of $u_<$ in $\mathcal{H}'$ then

$$\mathcal{H}' \equiv \mathcal{H}'(\{u_<\}) = \Omega^{-1} \int \mathrm{d}^d x \{\bar{q}^{-2}(\nabla u_<^2\} + I_1 \tag{2.2}$$

where

$$I_1 \equiv I_1(\{u_<\}) = -\ln \frac{\int Du_> \exp[-\Omega^{-1} \int d^d x \{\bar{q}^{-2}(\nabla u_>)^2 + V_0(u_< + u_>)\}]}{\int Du_> \exp[-\Omega^{-1} \int d^d x \{\bar{q}^{-2}(\nabla u_>)^2 + V_0(u_>)\}]}. \tag{2.3}$$

In order to cast the function I_1 in a tractable form the recursion formula makes certain simplifying approximations. There are two equivalent approaches to understand these approximations—we can argue either in momentum space or in position space. The position space or 'phase cell' approach is due to Wilson (1971); a pedagogical derivation can be found in Ma (1976). The alternative approach is due to Polyakov (unpublished) and is presented by Wilson and Kogut (1974). We now briefly outline this approach. It is possible to set up a perturbative expansion of the right-hand side of equation (2.3). The denominator removes all the graphs without any external lines ('vacuum to vacuum' graphs) and the logarithm removes all the disconnected graphs.

To evaluate the remaining graphs we have to make some simplifications. Of these we need recall here only the key rule defining the approximation within which integrals over 'internal' momenta (necessarily in the range between $\frac{1}{2}\Lambda$ and Λ) are evaluated. According to this rule all factors of momentum-squared appearing in such integrals are replaced by an 'average', $\bar{q}^2$. The remaining trivial integral $(2\pi)^{-d} \int_{\Lambda/2<|q|<\Lambda} d^d q$ then defines a constant which we denote by Ω^{-1}. These statements are to be regarded as the definitions of the parameters Ω and $\bar{q}^2$ (which appear in (2.1)). Specifically we note that

$$\Omega = \frac{d(2\pi)^d 2^d \Lambda^{-d}}{S_d(2^d - 1)} \tag{2.4a}$$

which for $d = 3$ reduces to

$$\Omega = \tfrac{48}{7}\pi^2 \Lambda^{-3}. \tag{2.4b}$$

The parameter $\bar{q}^2$ is less unambiguously defined. One might take as the defining relation either

$$(2\pi)^{-d} \int_{\Lambda/2<|q|<\Lambda} d^d q \, q^2 = \Omega^{-1} \bar{q}^2 \tag{2.5a}$$

or

$$(2\pi)^{-d} \int_{\Lambda/2<|q|<\Lambda} d^d q \, q^{-2} = \Omega^{-1} \bar{q}^{-2}. \tag{2.5b}$$

This is an ambiguity to which we shall return. For the moment we note simply that, given these approximations, the perturbative expansion may be resummed to give

$$I_1(\{u_<\}) = -\Omega^{-1} \int d^d x \ln \frac{\int dy \exp(-y^2 - \frac{1}{2}V_0(y + u_<) - \frac{1}{2}V_0(y - u_<))}{\int dy \exp(-y^2 - V_0(y))}. \tag{2.6}$$

Substituting this result into equation (2.2) we have that

$$\mathcal{H}'(\{u_<\}) = \Omega^{-1} \int d^d x \{q^{-2}(\nabla u_<)^2 + V'(u_<)\} \tag{2.7a}$$

where

$$V'(u) = -\ln\{I(u)/I(0)\} \tag{2.7b}$$

and

$$I(u) = \int_{-\infty}^{\infty} \mathrm{d}y \exp[-y^2 - \tfrac{1}{2}V_0(y+u) - \tfrac{1}{2}V_0(y-u)]. \tag{2.7c}$$

To complete the renormalisation group transformation it is convenient to rescale $u_<$ and x (in $\mathscr{H}'$) in such a way that the configurational energy expressed in terms of the rescaled coordinates, $\mathscr{H}_1$, has the same form as the initial Hamiltonian $\mathscr{H}_0$ (2.1). Explicitly we define

$$x' \equiv x/b; \qquad b \equiv 2 \tag{2.8a}$$

$$u' \equiv \alpha^{-1} u_<; \qquad \alpha \equiv b^{1-d/2}. \tag{2.8b}$$

Then, dropping the redundant primes, the coarse-grained configurational energy can be written as

$$\mathscr{H}_1 = \Omega^{-1} \int \mathrm{d}^d x \{\bar{q}^{-2}(\nabla u(x))^2 + V_1(u(x))\} \tag{2.9}$$

where

$$V_1(u) = -2^d \ln(I(\alpha u)/I(0)). \tag{2.10}$$

Equations (2.7) through (2.10) define the recursion formula; iterating the procedure defined by these equations generates a sequence of potentials $V_l (l = 1, 2 \ldots)$ defining configurational energies $\mathscr{H}_l$ containing fluctuations of maximum wavevector $\Lambda/2^l$.

2.2. Evolution of the potentials V

We have seen that, under the action of the recursion formula, the interaction (gradient term) in the effective Hamiltonian is invariant, while the potential evolves according to (2.10). In order to investigate the implications of the formula we have to specify the initial potential V_0. According to the conventional doctrine of universality the essential characteristics of the critical point behaviour should be independent of the specific parameterisation we choose. There is substantial supporting evidence for this viewpoint (see for example Nickel 1982) although the issue has not been conclusively settled (see for example Freedman and Baker 1982). Here we shall presuppose the conventional view and choose the specific (convenient) parameterisation

$$V_0(u) = r_0 u^2 + g_0 u^4; \qquad g_0 = \tfrac{1}{2} \tag{2.11}$$

where r_0 is a parameter which is taken to be an analytic function of temperature.

We proceed now to discuss the evolution of the potentials V_l for different values of the temperature (i.e. r_0). By symmetry we need only keep track of $V_l(u)$ for $u > 0$. The iterates become sufficiently complicated after one iteration to prevent an analytic study of the recursion formula. Instead we have to use appropriate numerical techniques. It will, however, prove helpful to record, first, one specific analytic implication of (2.10). Suppose, in particular that V_l has a 'sharp' minimum at u_l so that near u_l

$$V_l(u) \approx V_l(u_l) + m_l^2 (u - u_l)^2 \tag{2.12}$$

with m_l^2 large. Then for $\alpha u \sim u_l$ a steepest descent analysis of equation (2.10) yields (Golner 1973a)

$$V_{l+1}(u) = 2^d V_l(u_l) + 4m_l^2 (u - \alpha^{-1} u_l)^2 + C \tag{2.13}$$

where

$$C = -2^d \ln\left(\int dy\, e^{-m_l^2 y^2} \Big/ I(0) \right). \tag{2.14}$$

To summarise equation (2.13) we note that if a deep minimum exits in V_l then a deep minimum is always present in later iterations of the potential and the position of the minimum moves out by a factor $\alpha^{-1} = 2^{1/2}$ each successive iteration. We also note that the corresponding mass term at a deep minimum of the potential is increased by a factor of 4 on each successive iteration (i.e. $m_{l+1}^2 = 4m_l^2$).

The (critical) fixed point of the recursion formula is obtained by locating the critical value, r_{0c}, of the parameter r_0 such that, after a few iterations, the sequence of the potentials V_l settles to a 'stable' (l-independent) form V^*; the closer r_0 is to the 'true' value of r_{0c} the larger is the number of iterations over which the potential is stable and the closer is the observed potential (in this regime) to the 'true' fixed point potential. With the specific numerical techniques we have adopted we find $r_{0c} = r_{0c}(g_0 = \frac{1}{2}) = -1.666\,8606\ldots$; the associated fixed point potential is displayed in figure 1, reproducing Wilson's (1971) original result.

Now consider the situation where r_0 is close to but actually larger than r_{0c}. Initially V_l converges to V^*. For large enough l values, however, V_l evolves away from V^* (figure 2) into a 'Gaussian' regime where the origin is the sole minimum, and is 'sharp' (in the sense of (2.12)). Then, in these conditions ($r_0 > r_{0c}$, $l \to \infty$), we may write

$$V_l(u) \approx 4^l m^2 u^2 \tag{2.15}$$

for the (small) range of u-values which contribute significantly to ensemble averages calculated with $\mathcal{H}_l$. This limiting behaviour (and, in particular, the value of the parameter m^2 which it defines) will be exploited in the following subsection.

Now suppose that the chosen value of r_0 is slightly less than r_{0c}. Then, beyond the regime where $V_l \sim V^*$, instead of crossing over into the regime where the origin is the only minimum, the iterates always have other deeper minima. Initially the origin is a maximum and there are only two minima at $\pm u_l$. The value of u_l and the depth of the

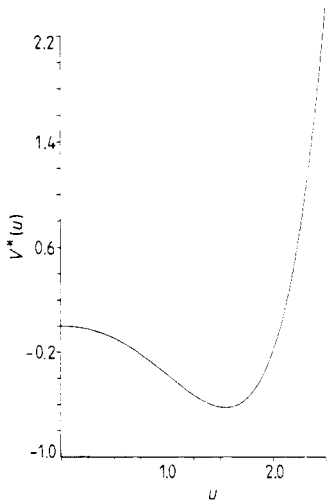

Figure 1. The fixed point potential.

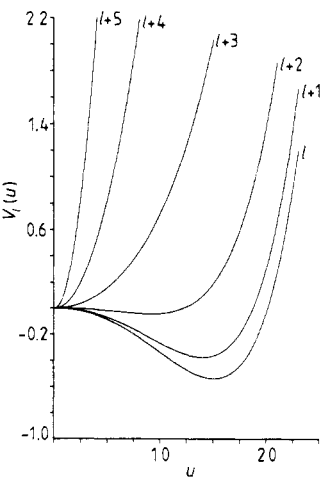

Figure 2. The large l behaviour of $V_l(u)$ for $T > T_c$.

minima below the origin slowly increase until we arrive at the situation depicted in figure 3(*a*). In this figure V_l has a sufficiently deep minimum that it forces the origin of the next iterate to be a local minimum also. Subsequently the iterates become very peaked as originally noted by Wilson (1971). Figure 3(*b*) illustrates the result obtained by carrying out the next iteration. Once the iterates have crossed over into the many minima regime then with each successive iteration all the minima move outwards by a factor α^{-1} and the minima become sharper. It also transpires that the number of minima increases: if V_l has $n(>2)$ minima then V_{l+1} has $(2n-1)$ minima. We also note that, with each iteration, the depth of the lowest minimum below the origin increases and between the origin and the lowest minimum the maximum height attained by V_l increases. It is only possible to carry out a small number of further iterations, once the multiple peaks have appeared, before the computational time required to obtain the next iterate becomes quite substantial.

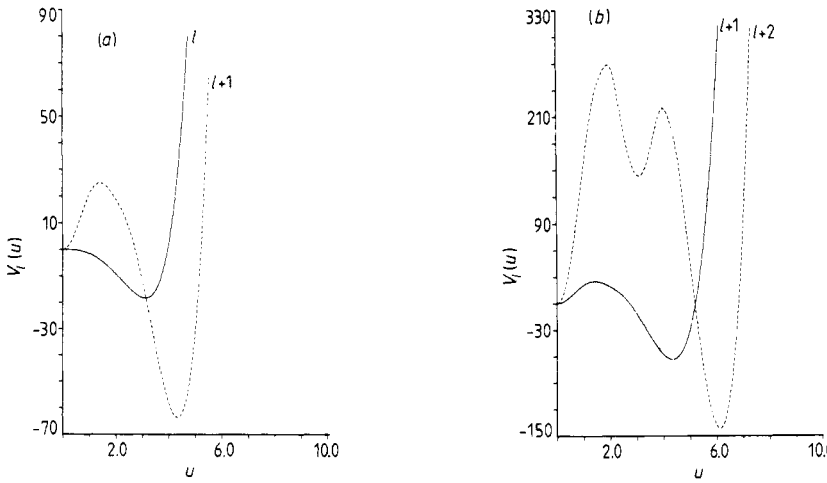

Figure 3. The large l behaviour of $V_l(u)$ for $T < T_c$. (*a*) Stage 1, (*b*) stage 2.

The essential features of the behaviour noted above and displayed in figures 3(*a*, *b*) can readily be understood analytically. Consider, in particular, the character of the deepest minimum, u_l, in V_l. Exploiting (2.13) and assuming that the integral $I(0)$ in (2.14) will be dominated by the symmetry related minima at $\pm u_l$ we find that near the deepest minimum u_{l+1} of the potential V_{l+1},

$$V_{l+1}(u) \approx -4u_{l+1}^2 + 4m_l^2(u-u_{l+1})^2. \tag{2.16}$$

Recalling that $u_{l+1} = 2^{1/2}u_l$ we see that this result implies that (in the $l \to \infty$ limit, for $r_0 < r_{0c}$) the behaviour of the renormalised potential may be written as

$$V_l(u) = -2^{l+2}M_s^2 + 4^l m^2(u - 2^{l/2}M_s)^2 \tag{2.17}$$

for u-values which are sufficiently close to the minimum of V_l to contribute significantly to averages evaluated in the ensemble prescribed by $\mathscr{H}_l$. The thermodynamic significance of the parameters M_s and m^2 defined by (2.17) will be developed in the next section. We defer to § 3.1 a discussion of the physically pathological proliferation of

minima in the potential iterates, for large l: this behaviour manifests itself in incorrect predictions for finite size corrections to the Helmholtz function in the ordered phase.

2.3. Universal amplitude ratios

The results summarised in the preceding section have immediate implications for three key observables: the order parameter (spontaneous magnetisation) M, the associated susceptibility χ and the correlation length ξ.

Consider first the order parameter

$$M = \lim_{h \to 0^+} \lim_{V \to \infty} V^{-1} \int d^d x \langle u(x) \rangle \tag{2.18}$$

when $V \equiv \int d^d x$ is the system volume and h is the field conjugate to the order parameter. Recalling the scale transformations introduced in (2.8) we see that

$$M = 2^{-l/2} M_l \tag{2.19}$$

where M_l is the order parameter for the system defined by the renormalised Hamiltonian $\mathcal{H}_l$. For $T > T_c$ ($r_0 > r_{0c}$) of course M_l vanishes identically (c.f. the behaviour of V_l depicted in figure 2). For $T < T_c$ ($r_0 < r_{0c}$), however, it is clear physically that M_l will coincide with the deepest minimum $u = +u_l$ of the potential V_l, the positive minimum being singled out by the (renormalised) field h_l inherent in the strategy by which the order parameter is defined. Recalling the behaviour (2.17) we conclude that, in zero field

$$M = M_s. \tag{2.20}$$

To determine the susceptibility and correlation length we consider the propagator

$$g(q) = \int d^d x \{\langle u(0)u(x) \rangle - \langle u(0) \rangle \langle u(x) \rangle\} \exp(i q \cdot x) \tag{2.21}$$

in terms of which we may make the identifications

$$\chi \equiv g(q = 0) \tag{2.22a}$$

$$\xi^2 = -(d/dq^2) \ln g(q)|_{q=0} \tag{2.22b}$$

the latter relationship defining the *second moment* correlation length (see e.g. Tarko and Fisher 1975). Recalling, once again, the transformations (2.8) we see that, provided $q < \Lambda/2^l$,

$$g(q) = 2^{2l} g_l(2^l q). \tag{2.23}$$

To determine g_l we may formally envisage setting up a loop expansion about the deepest minimum in V_l. For large l we may neglect corrections to the leading (Gaussian) behaviour finding simply that

$$g_l(q) = \Omega/2(\bar{q}^{-2} q^2 + 4^l m^2) \tag{2.24}$$

from which, invoking (2.22), (2.23) we find immediately

$$\chi = \Omega/2m^2, \qquad \xi = (\bar{q}m)^{-1}. \tag{2.25a, b}$$

By determining the values of m and M_s corresponding to various values of $\delta r \equiv r_0 - r_{0c}$ we can, then, with the aid of these results, determine the indices and amplitudes characterising the power law behaviour of χ, ξ and M as functions of the 'reduced

temperature' δr. In practice we used r_0 values such that $|\delta r| \leqslant 5 \times 10^{-5}$. The key results are

$$2\beta = \tfrac{1}{2}\gamma = \nu = 0.609 \pm 0.001 \tag{2.26a}$$

and

$$(f_+/f_-)^2 = C_+/C_- = 5.3 \pm 0.1. \tag{2.26b}$$

The relationships amongst the indices in (2.26*a*), and the link (2.26*b*) between the amplitude ratio for the correlation length (f_+/f_-) and that associated with the susceptibility (C_+/C_-) are corollaries of the '$\eta = 0$' approximation inherent in the recursion formula (in the form used here; cf Golner 1973b). The result for the index ν merely reproduces that reported by Wilson (1971). The result for the ratio C_+/C_- is, to our knowledge, new. The reliability of the two predictions is comparable: the best estimates currently available give $\nu = 0.629$ (see e.g. Pawley *et al* 1984) and $C_+/C_- = 5.06$ (Tarko and Fisher 1975).

There is one further critical amplitude combination which is, in principle, prescribed by our results. This is the combination which relates the scales of the thermodynamic variables (χ and M) to that of the correlation length (Stauffer *et al* 1972, Bervillier 1976). It may be defined by

$$S = f_+^d B^2 / C_+ \tag{2.27}$$

where B is the amplitude associated with the order parameter power law. In contrast to the susceptibility amplitude ratio this combination involves the parameters Ω and $\bar{q}$. Specifically we find from the numerical studies

$$S = 11.55(\Omega \bar{q}^3)^{-1}. \tag{2.28}$$

The parameter Ω is prescribed by (2.4*b*). However, as noted in § 2.1 the parameter $\bar{q}$ is less clearly defined: (2.5*a*), gives $\bar{q} = 0.815\Lambda$ while (2.5*b*) gives $\bar{q} = 0.764\Lambda$. In the light of this ambiguity we choose to adopt a different strategy. We forego the attempt to determine the universal quantity S; instead we exploit (2.28) together with the best available independent estimate of S to assign a value to the parameter $\bar{q}$. In tuning the link between thermodynamic and correlation length scales in this fashion we hope to enhance the reliability of our calculation of the CGHF (§ 3.2), in which this link plays a crucial role. Specifically, then, utilising the series-based result (Tarko and Fisher 1975), $S = 0.254$ we find

$$\bar{q} = 0.875\Lambda \tag{2.29}$$

which may be compared, without too much embarrassment, with the possible *a priori* assignments indicated above.

3. Mesoscopic and macroscopic free energies

The 'mesoscopic' or 'coarse-grained' Helmholtz free energy functional is defined by

$$F_{\Lambda_1} \equiv F_{\Lambda_1}(\{u_{\Lambda_1}(\boldsymbol{x})\}) = -\ln \int_> Du \exp\{-\mathscr{H}_0\} \tag{3.1a}$$

where the functional integral extends over the Fourier components of the field with wavevectors in the range $\Lambda_1 < |q| < \Lambda$. The coarse-grained coordinates $u_{\Lambda_1}(\boldsymbol{x})$ thus

contain only Fourier components with wavevectors $|q| < \Lambda_1$. Explicitly

$$u_{\Lambda_1}(x) = \int_{|q|<\Lambda_1} \frac{d^d q}{(2\pi)^d} \exp(-iq \cdot x) u(q) \tag{3.1b}$$

where the set $\{u(q); |q| < \Lambda\}$ defines a complete Fourier representation of the ordering field $u(x)$.

The recursion formula enables us to study these functions for values of Λ_1 of the form $\Lambda_1 = \Lambda/2^l$; accordingly, to simplify the notation, we shall represent $F_{\Lambda/2^l}(\{u_{\Lambda/2^l}(x)\})$ simply by $F_l(u)$. To within configuration-independent (constant) terms which we shall not explore, the functionals F_l are simply related to the sequence of effective Hamiltonians $\mathcal{H}_l$. Specifically, recalling the scale transformations (2.8) we find

$$F_l = \int d^d x \{\Omega^{-1} \bar{q}^{-2} (\nabla u)^2 + f_l(u)\} \tag{3.2a}$$

where

$$f_l(u) = \Omega^{-1} 2^{-dl} V_l(\alpha^{-l} u). \tag{3.2b}$$

The ('thermodynamic') Helmholtz function is then prescribed by the limiting form of f_l

$$f(M) = \lim_{l\to\infty} \lim_{V\to\infty} V^{-1} F_l(u = M) = \lim_{l\to\infty} f_l(M). \tag{3.3}$$

Consider first the high-temperature phase, for which we will record simply the predictions for the Helmholtz function itself. Our recursion formula studies indicate that the limit prescribed in (3.3) is well defined, and that $f(M)$ is a convex function with a single minimum at the origin; the form of $f(M)$ for two different ξ values is shown in figure 4(a). More explicitly we find by combining (2.15), (3.2b) and (3.3) that, for small M,

$$f(M) = m^2 \Omega^{-1} M^2 + O(M^4) \tag{3.4a}$$

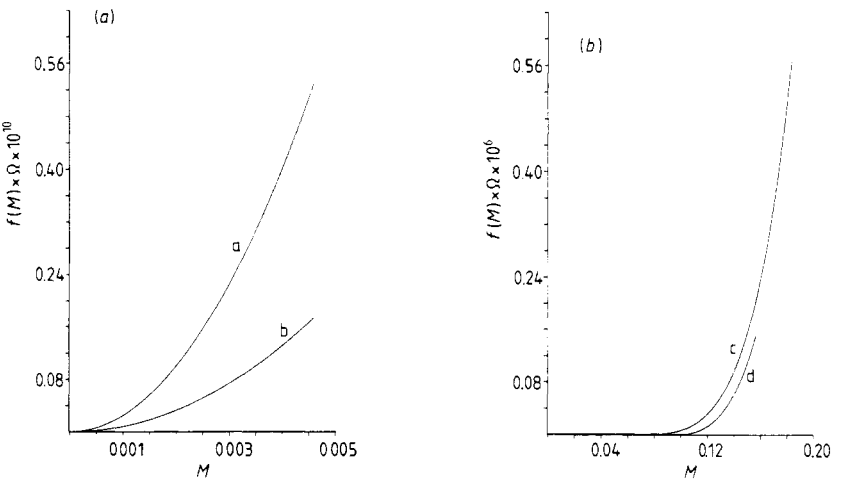

Figure 4. Helmholtz free energy $f(m)$ (a) for $T > T_c$; a, $\Lambda\xi = 7.22 \times 10^2$; b, $\Lambda\xi = 1.26 \times 10^3$, ($b$) for $T < T_c$: c, $\Lambda\xi = 5.46 \times 10^2$; d, $\Lambda\xi = 3.12 \times 10^2$.

implying

$$\chi^{-1} \equiv \partial^2 f(M)/\partial M^2 = 2m^2\Omega^{-1} \tag{3.4b}$$

in accord with (2.25*a*).

Now let us turn to the low-temperature phase. Here we shall be concerned not only with the thermodynamic limit (3.3), but also with the form of f_l for finite l. It will prove helpful to preface the presentation of our results for this regime with a brief discussion of the behaviour one might anticipate.

We begin by noting that (to within configuration-independent terms) the function $f_l(u)$ may be regarded as the free energy density of a 'block' of side $L \sim 2^l/\Lambda$. (Recall that the argument of the function f_l contains only Fourier components with wavevectors in the range $q < \Lambda/2^l$.) Given this identification the structure of $f_l(u)$ may be anticipated on the basis of rather general if heuristic arguments (Binder 1981, 1982, Kaski *et al* 1984). Specifically for l sufficiently large that the 'block size' L is large compared to ξ one may expect that the function $f_l(u)$ will have a double minimum structure expressing the dominance of single phase configurations. The principle characteristics of this structure are the *position*, the *depth* and the *width* (or *sharpness*) of the minimum.

It is clear that the *position* of the minimum will approach the equilibrium zero field order parameter M_s in the $l \to \infty$ limit. One might expect that this approach will be made monotonically from above: the location of the minimum in the function $f_l(u)$ identifies the order parameter of a system in which a class of fluctuations (namely those with wavevectors of $q < \Lambda/2^l$) have not been taken into account; rather generally fluctuations act to reduce the order parameter; the above conclusion follows.

The *depth* of the free energy minimum may be estimated on the basis of the observation (Binder 1981, 1982) that an ensemble in which a block has an order parameter xM_s $(-1 < x < 1)$ will be dominated by heterophase configurations in which fractions $\frac{1}{2}(1 \pm x)$ of the block have order parameters $\pm M_s$. The difference between the free energy of such an ensemble and that of the single phase ensemble (realised in the limit of an infinitesimal ordering field) resides in the free energy of the interface separating the two single phase regions. The specific form of this interface will reflect the block boundary conditions. However, for values of $|x|$ not too close to unity, its area must be of order L^{d-1}. The depth of the minimum in the coarse grained free energy *density* will thus be of order

$$\Delta f_l \sim L^{-d} \cdot L^{d-1}\sigma \sim \sigma\Lambda/2^l \tag{3.5}$$

where $\sigma \sim \xi^{-(d-1)}$ is the surface tension (free energy per unit interfacial area).

The *width* of the minimum may be roughly characterised by identifying the value of u_l for which $f_l(u) \sim -\frac{1}{2}\Delta f_l$. Invoking the expectation that the second derivative of $f_l(u)$ at its minimum will, for large l, approach the inverse susceptibility χ^{-1}, we find that the value of u_l thus prescribed differs from that locating the minimum by

$$\Delta u_l \sim (\sigma\Lambda\chi/2^l)^{1/2}. \tag{3.6}$$

Finally we remark that these observations serve to illuminate the structure anticipated for the Helmholtz free energy itself (Griffiths 1967): specifically, the vanishing (in the $l \to \infty$ limit) of the free energy density cost of the interfaces associated with heterophase configurations (3.5) implies a Helmholtz function which is flat in the regime $-M_s < M < M_s$.

With these remarks in mind we now return to discuss the results yielded by the recursion formula in the ordered phase. We consider first the Helmholtz free energy.

Our recursion formula studies indicate that the limit (3.3) does exist, and that, moreover, it has the anticipated convex structure: the behaviour of $f(M)$ for two different ξ values is shown in figure 4(b). That the recursion formula does yield the correct (convex) structure in the $l \to \infty$ limit is a reflection of the fact that (in contrast to the majority of approximation schemes) it does, to a degree at least, incorporate the effects of heterophase configurations. It does not, however, treat these configurations faithfully: its failure in this regard shows up in the manner in which the function f_l approaches its $l \to \infty$ limit. Specifically, combining (2.17) and (3.2b) we see that the depth of the (deepest) minimum in f_l is of the form

$$\Delta f_l \sim 4M_s^2 \Omega^{-1}/2^{2l}. \tag{3.7}$$

Thus, although the well depth vanishes in the $l \to \infty$ limit it does so more rapidly than our general arguments would suggest (cf (3.5)). This failure can be traced to the nature of the approximation within which the gradient (interaction) term in the Hamiltonian (2.1) is treated in the recursion formula framework. This approximation is formally expressed on the substitution of the mean-square momentum $\bar{q}^2$ in the internal lines associated with the various graphical contributions to the expansion of the functional integral (2.3); physically, it presupposes that the predominant spatial structure within a block (described by the coordinate $u_>$) will be smooth and, in particular, will not occur on length scales small compared to the block size. In fact, this presupposition is clearly wrong in the limit of sufficiently large block size since the scale upon which the ultimately dominant intra-block structure will occur (the interfacial thickness) will actually be small on the scale of the block size. This same failure shows up in a more immediately obvious way in the fact that, for large l, the function $f_l(u)$, as calculated with the recursion formula, does not have a simple double-minimum form. The growing multiplicity of subsidiary (shallower) minima (shown in the large l behaviour of the potential V_l: cf figure 3) expresses the incapacity of the recursion formula to reflect faithfully the continuous spectrum of possible heterophase configurations.

Notwithstanding these clear deficiencies the recursion formula results are certainly sensible in a number of respects. Firstly we find that the position of the dominant (deepest) minimum of f_l does approach its large l limit from above. This behaviour has also been observed in recent Monte Carlo studies reported by Kaski *et al* (1984). Secondly the quantitatively resonable value which the recursion formula yields for the susceptibility amplitude ratio indicates that the curvature of the deepest minimum reflects reasonably well the curvature of the 'true' minimum: this correspondence suggests that, in fact, the renormalisation of the stucture of the deepest minimum by the heterophase fluctuations (erroneously characteristed by the recursion formula) is actually very small as, indeed, one would expect in view of the depth of the dominant minimum relative to the others. Finally, we note that the erroneous multiple-minimum structure begins to set in at values of $l > l_u$ where $2^{l_u} > 2\xi$. It is thus not excessively optimistic to hope that the structure of $f_l(u)$ for l values less than l_u will be both qualitatively and quantitatively reasonable. It is specifically to this regime that we now turn.

As noted in the introduction the CGHF for coarse graining lengths of the order of the correlation length has attracted particular attention in view of its potential relevance to the problem of spinodal decomposition. Specifically, within the framework developed by Langer *et al* (1975) and recently reviewed by Gunton *et al* (1983) the time evolution of the wavevector-dependent 'structure factor' (which appears to be the most experimentally accessible probe of the coarse-grained configurations) is

described by a set of dynamical equations for which the principal input is this CGHF. The specific form of the CGHF is thus of some interest. To facilitate comparison with earlier studies we follow Langer *et al* (1975), writing the CGHF in the form

$$f_l(u) = a^{-3} c\phi(u/M_s, 2^l/\Lambda\xi). \tag{3.8}$$

This scaling form should be appropriate in a region close enough to the critical point (ξ large compared to microscopic lengths) and for large enough coarse graining lengths ($l > l_0$ where l_0 is the first value of l for V^* is a good approximation to V_l). The parameter a gives a measure of the coarse-graining length and is chosen to be (Langer *et al* 1975)

$$a = (6\pi^2)^{1/3} 2^l/\Lambda. \tag{3.9}$$

The function ϕ is chosen to satisfy the normalisation conditions

$$\phi(0, 2^l/\Lambda\xi) = 0: \qquad \phi''(0, 2^l/\Lambda\xi) = -1. \tag{3.10}$$

These conventions ensure that the function ϕ is universal and (in view of the 'two scale factor universality' discussed in § 2.2) that $c \equiv c(2^l/\Lambda\xi)$ is also universal.

Utilising (3.8) through (3.10) together with our recursion formula calculations of f_l we have determined the scaling function ϕ for a number of different values of the ratio $2^l/\Lambda\xi$. The results are shown in figure 5(a). The specific case where the coarse-graining length is chosen to equal ξ is characterised by the function

$$\phi^*(x) \equiv \phi(x, 1). \tag{3.11}$$

The recursion formula result for this function is shown in figure 5(b); this result was obtained by choosing $\delta r \equiv r_0 - r_{0c}$ such that $2^l/\Lambda\xi$ is unity for a particular l. Figure

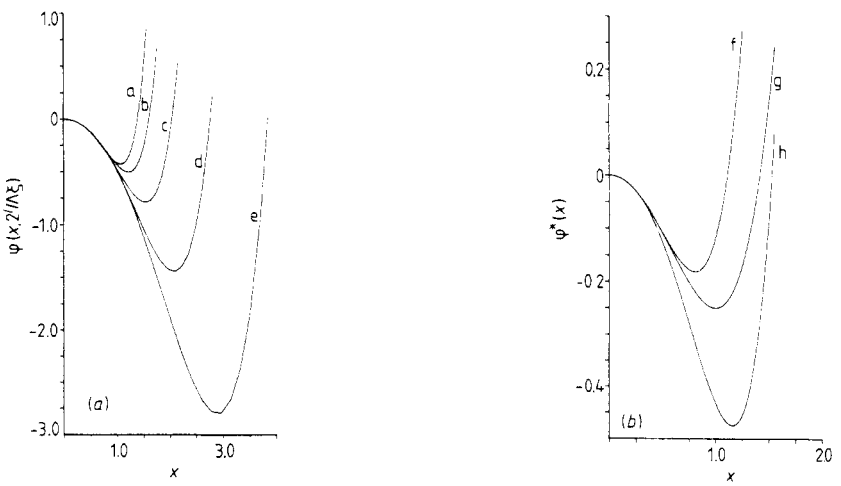

Figure 5. The coarse grained free energy function (a) for a variety of coarse graining lengths; the values of $2^l/\Lambda\xi$ are: a, 1.64; b, 0.818; c, 0.409; d, 0.204; e, 0.102. (b) for a coarse graining length $2^l/\Lambda = \xi$: f, Kawasaki *et al* (1981); g, Langer *et al* (1975); h, results from Wilson's approximate reecursion formula.

5(*b*) also displays two previously proposed forms of this function. The form suggested by Langer *et al* (1975) is simply the Landau quartic form uniquely prescribed by the normalisation conditions (3.10) augmented by the Landau (mean field) requirement that $\phi'(1)=0$ (i.e. that the minimum of the CGHF coincides with the bulk order parameter). This ansatz lacks the higher-order powers of x which will certainly be present in general (as noted by Langer *et al*) and which show up clearly in the recursion formula result in the enhanced steepness of $\phi(x)$ for large x. The result of Kawasaki *et al* (1981) was obtained on the basis of a renormalisation group calculation utilising a perturbation expansion to first order in $\varepsilon=4-d$. We note that this result has its minimum at a value of $x<1$, which is at variance with the expectation (discussed earlier, and realised in our results: cf figures 5(*a*, *b*)) that the minimum in the CGHF should approach the equilibrium magnetisation monotonically from *above*). It is possible that this anomaly (if, indeed, it is such) is a reflection of the breakdown of the $O(\varepsilon)$ renormalisation group equations which Kawasaki *et al* (1981) note are clearly evident at larger l-values.

The values of the normalisation constant $c^*=c(2^l/\Lambda\xi=1)$ also differ significantly in the three calculations. We find $c^*\sim 3.5$; Langer *et al* matched their CGHF to truly macroscopic data to find $c^*\sim 5.77$, while Kawasaki *et al* report $c^*=4.14$.

Given the clear deficiencies of the large-l behaviour of the recursion formula in the ordered phase we cannot be certain that the new result presented in figure 5(*b*) represents an improvement on its predecessors. However in the light of the qualitative deficiencies of the latter, identified above, and in view of the striking reliability of the recursion formula to describe configurations in the $2^l/\Lambda\xi \ll 1$ limit (cf the discussion of the block PDF in §§ 1 and 4) it seems not unreasonable to expect that it will in fact prove to be so.

4. Probability density functions for coarse-grained coordinates

4.1. Theoretical background

In this section we turn to consider the manner in which the coarse-grained coordinates $u_{\Lambda_1}(x)$ (3.1*b*) are distributed. Specifically we consider the probability density function P_{Λ_1}, of a single coordinate u_{Λ_1}, defined by

$$P_{\Lambda_1}(u)\equiv\langle\delta(u_{\Lambda_1}(x)-u)\rangle. \tag{4.1}$$

This distribution reflects the effective local potential, f_l, seen by the coarse-grained coordinates; however it is not simply prescribed by this potential, since the average (4.1) must be evaluated in the ensemble of interacting coarse-grained coordinates characterised by the full coarse-grained free energy functional (3.1*a*). Though harder to calculate than the coarse-grained potential functions the coarse-grained probability density functions are potentially more interesting: specifically; they are directly observable in computer simulations, their moments define quantities which may be probed by scattering experiments, and their form expresses (to a degree that more conventional observables do not) the nature of the coarse-grained configuration spectrum.

The work we describe here represents an extension of earlier studies (Bruce *et al* 1979, Bruce 1981a, 1982) to which the reader is referred for a discussion of the original motivation underlying this programme, and for a fuller presentation of the relevant theory, which we present here in summary form only.

We begin with a brief discussion of the moments of the PDF (4.1). The moments about the origin and about the mean are defined, respectively, by

$$\tilde{M}^{(n)}_{\Lambda_1} \equiv \int_{-\infty}^{\infty} \mathrm{d}u\, u^n P_{\Lambda_1}(u) \tag{4.2a}$$

and

$$M^{(n)}_{\Lambda_1} \equiv \int_{-\infty}^{\infty} \mathrm{d}u (u - M_s)^n P_{\Lambda_1}(u). \tag{4.2b}$$

In writing (4.2*b*) we have explicitly recognised the equivalence of the *mean* of the distribution (4.1) (the first moment in the series (4.2*a*)) and the equilibrium order parameter:

$$M_s = \tilde{M}^{(1)}_{\Lambda_1} \tag{4.3}$$

which holds independently of the coarse graining scale Λ_1. The *variance* of the distribution (the second moment in the sequence (4.2*b*)) is directly related to the propagator (2.21):

$$M^{(2)}_{\Lambda_1} = (2\pi)^{-d} \int_{|\boldsymbol{q}|<\Lambda_1} \mathrm{d}^d q\, g(\boldsymbol{q}) \tag{4.4}$$

In the limit in which $\Lambda_1 \xi$ is small compared to unity we may replace $g(\boldsymbol{q})$ in (4.4) by the macroscopic susceptibility $\chi = g(0)$. Thus we identify

$$\chi = \lim_{\Lambda_1 \xi \to 0} \frac{d(2\pi)^d}{S_d} \Lambda_1^{-d} M^{(2)}_{\Lambda_1}. \tag{4.5}$$

The *shape* of the distribution (4.1) is succinctly characterised by the dimensionless parameter

$$G_{\Lambda_1} \equiv [3(M^{(2)}_{\Lambda_1})^2 - M^{(4)}_{\Lambda_1}]/2(M^{(2)}_{\Lambda_1})^2 \tag{4.6}$$

which ranges between the value $G = 0$ for a Gaussian distribution and $G = 1$ for a symmetric double δ-function distribution. The *universal scaling properties* of the PDF have been discussed in detail in earlier work (Bruce 1981a, Binder 1981). They may be summarised in the assertion that the PDF may be written in the form

$$P_{\Lambda_1}(u) \approx a^{-1}_{\Lambda_1} P^{\pm}(a^{-1}_{\Lambda_1}(u - M_s), (\Lambda_1 \xi)^{-1}). \tag{4.7}$$

This form presupposes values of Λ_1^{-1} and ξ which are large compared to microscopic lengths. The scale factor a_{Λ_1} is introduced to absorb the non-universality of the ordering coordinate scale. We adopt the convention that the scale factor should be such that the PDF $P^{\pm}$ has unit variance in the 'critical' ($\Lambda_1 \xi \to \infty$) limit. With this (arbitrary) convention the functions P^+ and P^- (appropriate, respectively, in the $T \to T_c^{\pm}$ limits) should be universal. Finally we remark that the factor of M_s appearing in (4.7) is not strictly necessary: with the choice of scale factor a_{Λ_1} to be made below the combination M_s / a_{Λ_1} could in fact be subsumed into the second argument of the function $P^-(u, z)$. The factor of M_s is included explicitly for convenience: thus defined the function $P^-(u, z)$ has its maximum at a finite (zero!) value in both large and small z limits.

Thus far the discussion has been very general. Now let us again revert to the recursion formula framework. In our earlier work (Bruce 1981a) it was shown that, within this framework, there exists a recurrence relationship between the PDFs for

coarse graining lengths $\Lambda_l = \Lambda/2^l$ and $\Lambda_l = \Lambda/2^{l+1}$. Specifically, denoting $P_{\Lambda/2^l}$ by P_l we have, in the present notation (note the difference between equation (3.16) and (2.3*b*) of Bruce 1981a)

$$P_l(u) = \alpha^{-l} \int_{-\infty}^{\infty} \mathrm{d}v\, P_{l+1}(v) P_c(\alpha^{-l}v, \alpha^{-l}(u-v)) \tag{4.8a}$$

where α is the scale factor prescribed in (2.8) while the conditional probability function P_c is determined in terms of the renormalised potentials V_l and V_{l+1}:

$$P_c(v_1, v_2) = \frac{\exp[2^{-d}V_{l+1}(\alpha^{-1}v_1) - v_2^2 - \frac{1}{2}V_l(v_1+v_2) - \frac{1}{2}V_l(v_1-v_2)]}{\int_{-\infty}^{\infty} \mathrm{d}y \exp[-y^2 - V_l(y)]}. \tag{4.8b}$$

Before turning to the numerical exploration of these equations two further remarks are in order.

The first remark concerns the critical limit, where $\Lambda\xi/2^l \gg 1$. In this limit, where the renormalised potentials appearing in (4.8b) may be replaced by the fixed point form V^*, one readily finds that (4.8a) is consistent with the scaling ansatz (4.7) provided one chooses the scale factor $a_l \equiv a_{\Lambda_l}$ to be of the form

$$a_l = a_0 2^{-l/2}. \tag{4.9}$$

Recalling (4.4), and the '$\eta = 0$' approximation inherent in the recursion formula one can easily check that this form is consistent with the requirement that the universal function (4.7)

$$P^*(u) \equiv P^{\pm}(u, 0) \tag{4.10}$$

has unit (l-independent) variance.

The second remark concerns the limit $\Lambda\xi/2^l \ll 1$, and is of a more technical nature. Consider specifically the $T > T_c$ situation; a similar analysis, with certain refinements, can be given in the ordered phase. For large l (cf (2.15)) the potential V_l is a quadratic form and the distribution P_l may be determined explicitly as the Gaussian

$$P_l(u) = (2\pi W_l(m))^{-1/2} \exp\{-u^2/2W_l(m)\} \tag{4.11a}$$

where

$$W_l(m) = \frac{1}{(2\pi)^d} \int_{|q|<\Lambda/2^l} \mathrm{d}^d q \frac{\Omega}{2(m^2 + q^{-2}q^2)}. \tag{4.11b}$$

Now the distribution $P_{l+1}(u)$ may be determined in two ways. Firstly it may be inferred directly from (4.11) as a Gaussian of variance $W_{l+1}(m)$. Alternatively, it may be obtained from the integral equation (4.8). It transpires that the two determinations are in accord with one another only if the integral (4.11*b*) is evaluated in a fashion consistent with the approximations inherent in the recursion formula (cf § 2.1). The rules dictate (and consistency is assured by) the approximation

$$W_l(m) = \frac{\alpha^{2l}}{2} \sum_{n=0}^{\infty} \frac{2^{-(d-2)n}}{1 + 4^{l+n}m^2}. \tag{4.12}$$

It is reassuring to note that, in the large l limit, (4.11*a*) and (4.12) imply for the variance of the distribution P_l,

$$M_l^{(2)} = W_l(m) \approx 2^{-dl}/2m^2(1-2^{-d}) = [(S_d(\Lambda/2^l)^d/d(2\pi)^d]\chi \tag{4.13}$$

where, in the last step we have made use of (2.25*a*) and (2.4*a*). Equation (4.13) is clearly in accord with the expectation (4.5).

4.2. Results

When taken in conjunction with the recursion formula itself, (4.8*a*) and (4.8*b*) define a closed recurrence relation prescribing the PDF for blocks of scale size $2^{l+1}/\Lambda$ in terms of the PDF for blocks of scale size $2^l/\Lambda$. In our earlier study of this problem (Bruce 1981a) these equations were solved to give the fixed point distribution P^* (4.10) describing the form of the block PDF in the limit in which $2^l/\Lambda \ll \xi$ (with l, nevertheless, large). The form of P^* obtained (in $d = 3$) is reproduced in figure 6 as a benchmark for the further results to be presented below. The non-Gaussian character of the distribution is reflected in the value of the associated cumulant ratio (4.6)

$$G^* = \lim_{2^l/\Lambda\xi \to 0} G_l \approx 0.33. \tag{4.14}$$

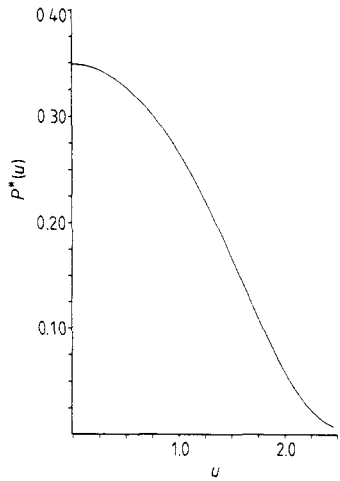

Figure 6. The universal distribution $P^*(u) \equiv P^{\pm}(u, 0)$.

Subsequent Monte Carlo calculations by Binder (1981) proved to be in excellent accord with these results, yielding in particular $G^* = 0.32 \pm 0.02$. This accord strongly substantiates the claimed universality of the distributions: the Monte Carlo study was based on a nearest-neighbour fixed-length-coordinate Ising model, in contrast to the continuous coordinate model ((2.1), (2.11)) underlying the results shown in figure 6. The level of accord also seems to indicate a surprising insensitivity of the results to the specific way in which the coarse-grained coordinates are defined: the Monte Carlo study utilised block cordinates defined, in the original Kadanoff fashion, with a direct space cut off (i.e. as in equation (2.3*a*) of Bruce 1981a) in contrast to the reciprocal space cut off (cf (3.1*b*)) employed in our renormalisation group studies. Although the limiting PDF is (given the coordinate scaling (4.9)) expected to be independent of the *length-scale* of the coarse graining (i.e. the block size or inverse cut off $2^l/\Lambda$) there is no reason, *a priori*, to expect such independence of the *form* of coarse graining.

The fixed point from P^* describes the block coordinate distribution only in the limit in which the block size is small compared to the correlation length. When the block size is large compared to the correlation length the block distribution is widely expected to be Gaussian (see e.g. Cassandro and Jona-Lasinio 1978). In what follows we examine the *crossover behaviour* whose occurrence is implied by these remarks.

To define our strategy, consider first the situation where the temperature is close to but above its critical value (i.e. $\delta r \equiv r_0 - r_{0c}$ is small and positive). In this case the renormalised potential V_l evolves from its (non-universal) local form V_0, though a regime where it lies close to the fixed point potential V^*, and ultimately into a regime where it has a single minimum, with the quadratic form (2.15). In this regime the distribution is clearly Gaussian, with the explicit form prescribed in (4.11). Given this large l limiting form, together with the sequence of potentials V_l, the recurrence relation (4.8*a*) may be used to determine the sequence of distributions P_l (for the chosen δr). A check on the consistency of this procedure is afforded by the requirement that the sequence of distributions which it yields should be insensitive to the particular ('large') value of l at which the distribution is matched to the Gaussian form (4.11).

We now discuss qualitatively the sequence of distributions P_l which emerge from this procedure. The local distribution $P_{l=0}$ is prescribed by the local Hamiltonian and is, of course, non-universal: for the particular choice (2.11) (and $r_0 \geqslant r_{0c}$) P_0 has a symmetric double-peaked form. As l increases to l_0 (where $V_l \approx V^*$) P_l (more precisely the distribution of the *scaled* variable $a_l u$, with a_l given by (4.9) and a_0 prescribed by the unit variance condition) evolves to the form P^* and remains close to this form for a range of l values. The closer the system is to criticality the larger is the range of l values for which the block PDF remains close to P^*. Eventually the distributions depart from the fixed point form and become progressively more Gaussian.

This behaviour is expressed quantitatively in figures 7(*a*) and 7(*b*). Figure 7(*a*) shows the universal scaling function $P^+(u, 2^l/\Lambda\xi)$ for a number of values of $2^l/\Lambda\xi$, in the regime ($l > l_0$) in which the mapping to the universal form (4.7) is valid. The crossover between the critical (P^*) and Gaussian forms is more explicitly expressed

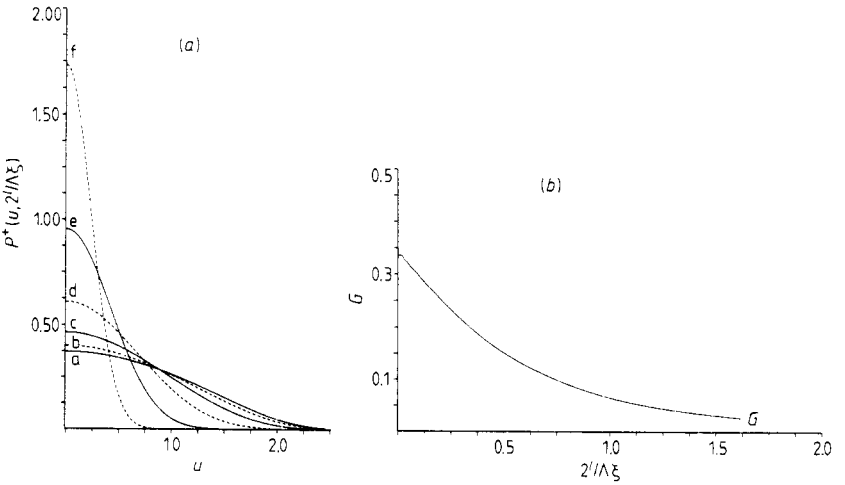

Figure 7. (*a*) The universal distribution $P^+(u, z)$ for a number of values of $z = 2^l/\Lambda\xi$: a, 8.06×10^{-2}; b, 1.77×10^{-1}; c, 3.55×10^{-1}; d, 7.09×10^{-1}; e, 1.42; f, 2.84. (*b*) The cumulant ratio G as a function of $2^l/\Lambda\xi$ for $T < T_c$.

in figure 7(b), where we show the evolution of the cumulant ratio G (4.6) from its critical fixed point value (4.14) to its Gaussian limit, $G = 0$.

Now let us consider the crossover behaviour occuring in the ordered phase. The strategy we adopt is similar to that discussed above. There are, however, two preliminary issues to be addressed.

Firstly we must now consider carefully the boundary conditions for the calculation. We shall suppose that our system, of volume V, is subject to an ordering field h with the 'thermodynamic' ($V \to \infty$) and 'infinitesimal field' ($h \to 0^+$) limits taken in such a way that hVM_s is *large* (on the scale of $k_B T_c$). As discussed by Binder and Landau (1984) the block PDF is then expected to converge, for large block size, to a *single* Gaussian centred on the order parameter M_s. (If, in contrast, the limits are taken such that hVM_s is *small* the block PDF is always a symmetric function, converging, for large block size, to *two* Gaussians centred on $\pm M_s$.) Explicitly, then, with the stipulated (notional) boundary conditions, we impose the condition that the large l behaviour of $P_l(u)$ match on to a Gaussian of the form (4.11a), but centred on $u = M_s$.

Secondly we should recall at this point that in the Gaussian regime *below* T_c the recursion formula is not wholly trustworthy. However, as we have seen, the results it yields do appear to be sensible as regards the position and curvature of the deepest minimum in the renormalised potential. Since the behaviour of $P_l(u)$ (for the larger values of l where the recursion formula is problematic) is dominated by this minimum, and by these characteristics in particular, we believe that the recursion formula results for P_l should be not unreasonable in the ordered phase.

Again we preface the detailed results with a brief discussion of their qualitative features. The local distribution function is only weakly sensitive to the system temperature: thus, for $r_0 \leqslant r_{0c}$, $P_{l=0}$ has essentially the same the same (non-universal!) form as it does for $r_0 \geqslant r_{0c}$. Strictly, of course, the ordered phase distribution is asymmetric: its first moment defines the order parameter M_s. However, to the extent that r_0 is (arbitrarily) close to r_{0c} this first moment is (arbitrarily) small on the scale of the width of the distribution, and the asymmetry is not apparent. For $r_{0c} - r_0$ sufficiently small this statement remains true for the range of l values in which V_l approaches and remains close to V^*: thus, below the critical point, the distributions P_l again coincide with the fixed point distribution P^* for a range of l-values. This observation is simply an expression of the fact that $P^+(u, z)$ and $P^-(u, z)$ have the *same* small $z = 2^l/\Lambda\xi$ limit (namely $P^*(u)$). For larger l-values the distribution begins to depart from the fixed point form, the ratio of its width to its first moment ceases to be large and its asymmetry sbout the origin begins to be discernible; at the same time its asymmetry about the order parameter begins to decrease as the distribution (by construction) converges on a single Gaussian centred on M_s.

The (universal) aspects of these statements are expressed quantitatively in figures 8(a) and 8(b). Figure 8(a) shows the distribution $P^-(u, z)$ for a variety of values of $z = 2^l/\Lambda\xi$. Note that (cf (4.7)) this function describes the *deviation* of the coarse-grained coordinate from its mean value, M_s. Thus, for large z we see that $P^-(u, z)$ is, correctly, centred on $u = 0$. For intermediate z, $P^-(u, z)$ has its maximum at a finite positive value of u (reflecting the fact that the minimum in the coarse-grained free energy function f_l approaches its large l limit from above). For small enough z (not shown in figure 8(a)) $P^-(u, z)$ will again be centred on $u = 0$. Figure 8(b) shows the evolution from critical to Gaussian behaviour as it is reflected in the parameter G and also in the analogous ratio $\tilde{G}$ (defined as in (4.6), but in terms of the moments (4.2b) rather than (4.2a)).

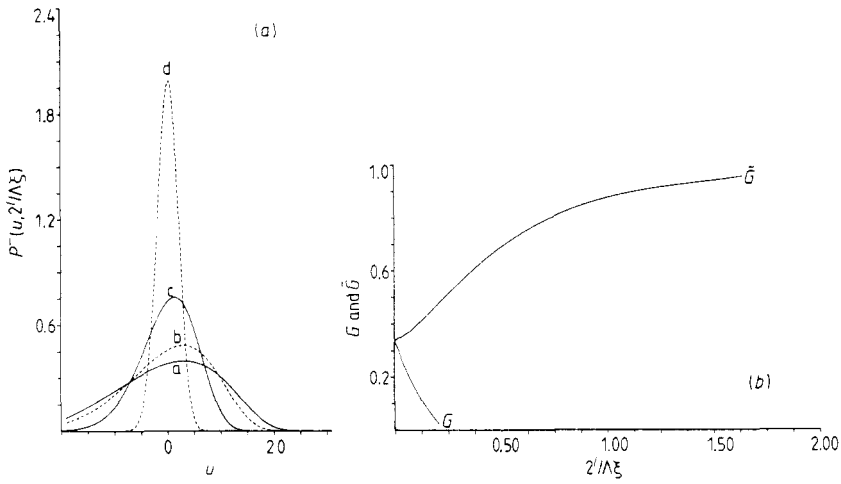

Figure 8. (*a*) The universal distribution $P^-(u, z)$ for a number of values of $z = 2^l/\Lambda\xi$: a, 5.13×10^{-2}; b, 2.05×10^{-1}; c, 8.21×10^{-1}; d, 3.28. (*b*) The cumulant ratios G and $\tilde{G}$ as functions of $2^l/\Lambda\xi$ for $T < T_c$.

4.3. Discussion

Finally we turn to discuss briefly some of the ways in which the results presented in the preceding section may illuminate, or be tested by, experiment.

The experimental technique to which the coarse-grained PDFs are most immediately accessible is certainly computer simulation. Indeed, in a series of papers, Binder has shown how Monte Carlo studies of the distributions and their moments may be used to identify critical indices and locate critical points (Binder 1981; see also Barber *et al* 1984), measure the interfacial tension (Binder 1982) and locate first-order phase boundaries (Binder and Landau 1984). In the results presented in the first of these papers (Binder 1981) the crossover behaviour discussed in the preceding section is clearly evident. We cannot make a satisfactory quantitative comparison with these results since, as noted earlier, the two studies employ different coarse-graining procedures. Although this difference appears to be unimportant in the critical limit (cf the accord on the form of P^* noted above) it cannot be evaded in the crossover regime where the form of the PDF depends explicitly on the coarse-graining length or 'block size'. Nevertheless the results of the two studies are in accord as regards the essential qualitative features of the distributions: the behaviour of the cumulant ratio $\tilde{G}$ (figures 7(*b*), 8(*b*)) which Binder exploits to locate the critical point; the dependence upon coarse-graining length of the position of the maximum in $P_l(u)$ in the ordered phase (figure 8(*a*)); and the character of the asymmetry of this function about its maximum.

As regards experiments on real systems there are a number of potential points of contact. Firstly we note (Bruce 1982) that the second moment $\tilde{M}^{(2)}_{\Lambda_R}(2a)$ of the coarse grained distribution $P_{\Lambda_R}(u)$ is directly measurable in a neutron or x-ray scattering experiment: it represents the total (frequency-integrated) cross section in an experiment whose resolution function (prescribing the range of wavevectors contributing to the observed intensity) is a sphere of radius Λ_R centred on the condensing mode. To illustrate this point figure 9 shows the scattering intensity I (the second moment $\tilde{M}^{(2)}_{\Lambda_R}$)

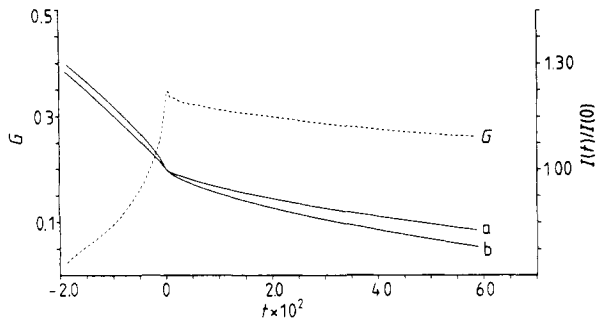

Figure 9. The normalised scattering intensity crossover function as given (*a*) by the present calculation and (*b*) by Bruce (1981b). The reduced temperature is expressed in units defined in the text. The tempeature dependence of the cumulant ratio G is also shown.

plotted as a function of reduced temperature t; the latter is measured in units of $(f_+\Lambda_R)^{1/\nu}$, where f_+ is the amplitude of the correlation length for $T > T_c$, and the intensity is normalised to unity at the critical point. With these conventions the cross section has a universal form. In the same figure we show the results of an earlier calculation of this scaling function (Bruce 1981b) based upon an expansion in $\varepsilon = 4 - d$. The level of agreement is not unreasonable given the different approximations inherent in the two calculations. We would not venture to anticipate which of the calulations is likely to prove the more reliable. The predictions are, however, testable by a suitable neutron scattering study (or, of course, by computer simulation). Indeed, recent neutron scattering studies of a $d = 2$ Ising antiferromagnet (Cowley *et al* 1984) have already borne out one implication of the existence of such a universal scaling form, namely the unique relationship it prescribes between the scattering at reduced temperatures t and $-t$ (in the 'good resolution' limit, $\Lambda_R \xi \ll 1$).

The non-Gaussian character of the critical fluctuation spectrum is of course implicit in the critical indices and thus in the temperature dependence of the scattering cross section shown in figure 9. Nevertheless, such experiments, in as much as they measured only the *second* moment of the coarse-grained PDF, are not explicitly sensitive to this non-Gaussian component, whose signature is the non-zero value of G, also displayed in figure 9. There are, however, two forms of scattering experiment which may be more informative in this regard. Firstly, it is conceivable that the *time-dependence* of the coarse grained coordinates, reflected in the frequency-dependent scattering cross section, may more fully reflect the character of the equilibrium distribution function. This possibility, touched on elsewhere (Bruce 1982) merits further study. Secondly it may be possible to devise a scattering experiment which measures the coarse-grained PDFs directly. One possibility is to study the distribution of the numbers of photons scattered from a critical volume of a fluid, in certain respects the cleanest realisation of the Ising universality class. This distribution should reflect the spectrum of density fluctuations within this volume, and can thus be related to the coarse-grained distributions studied here. The possibility of such an experiment was considered some years ago (see e.g. Tartaglia and Chen 1973) and deemed to be at or beyond the limits of the technology then available. We believe that, given subsequent advances in experimental technique, and the motivation afforded by the specific theoretical predictions available here, the feasibility of such an experimental study merits fresh scrutiny.

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