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1987 J. Phys. A: Math. Gen. 20 6371

(http://iopscience.iop.org/0305-4470/20/18/036)

J. Phys. A: Math. Gen. 20 (1987) 6371-6390. Printed in the UK

Time coarse graining near critical points

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Received 22 June 1987

Abstract. We investigate the statistical properties of local variables, coarse grained in time, in systems undergoing continuous phase transitions. A general theory is developed which suggests universal scaling behaviour in the limit of large coarse-graining times. The predictions are substantiated with Monte Carlo studies of two-dimensional scalar models. A simple fractal model of the time profile of the ordering variable is developed which captures and illuminates its timescale-invariant character. The theory is used to study the critical behaviour of local resonance lineshapes. In the two-dimensional case studied explicitly the critical slowing down is shown to drive a crossover to a split slow-motion lineshape.

1. Introduction

The distinctive behaviour of a system near a critical point originates in the existence of configurational structure persisting over lengths and times long on microscopic scales. Experimentally such structure is most naturally probed with the aid of scattering studies tuned to the relevant regions of reciprocal space. In the theoretical context the important structure is customarily exposed with the aid of spatial coarse-graining methods which monitor either coupling constant flow (in the standard implementation of the renormalisation group method: Wilson and Kogut (1974)) or configuration flow (in complementary realisations of the renormalisation group, focusing on the expectation values of the operators: Binder (1981)). In this paper (a brief preliminary report of which has already appeared: Nicolaides and Bruce (1986)) we examine an alternative way of probing the important configurational structure, which rests upon a *temporal* rather than a *spatial* coarse graining.

The basic idea is simple. It is most easily presented in the context of a droplet picture of an Ising model near its critical point (Bruce and Wallace 1983), although, we believe, the idea is of more general validity than this particular imagery. Within the droplet picture the configuration of the system, at any instant, consists of a hierarchy of droplets of the two phases, nested inside one another, and with a range of length scales extending up to a maximum set by the correlation length ξ. We consider, then, within this framework, the behaviour of a single spin represented by a local coordinate ϕ. At any instant this spin will be found in one or other of its two states. The state will change (the spin will flip) when the spin is traversed by a droplet boundary. The predominant structure of the time profile of the local coordinate will reflect the time evolution of *small* length scale structure: thus, in particular, the majority of spin flips will be associated with the passage of the relatively small droplets whose abundance is greatest, and the typical time, τ_l, between spin flips will (like the concentration of the smallest droplets) be largely insensitive to the phase transition. However, the time profile of the local coordinate must also reflect the existence and behaviour of large length scale structure: in particular, although at any *instant* the coordinate must assume one or other of two values, it will have a *predisposition* to one state or the other according to the nature of the largest droplet within which it is embedded. More generally, it should be possible in principle to discern, in the behaviour of the local coordinate, a whole hierarchy of timescales, intermediate between the 'inner' timescale τ_i and an 'outer' limit τ_0 (of order ξ^z where z is the dynamic critical index) reflecting the influence of the whole hierarchy of droplets of different length scales. In practice it is not easy to discern the effects of the larger length scale structure, superimposed, as it is, on the more rapid fluctuations associated with the smallest droplets. To see the former one needs to suppress the latter. This aim is realised in the study of a coordinate M_τ measuring the mean of the local variable ϕ over some averaging time τ; the time profile of M_τ then represents a time-coarse-grained form of the profile of ϕ itself. For averaging times τ large compared to τ_i the effects of the short length scale structure will be averaged away, exposing the contributions of the large length scale structure. It is well known that the large length scale structure has universal features (Bruce 1981). Consequently one may expect that the large timescale structure of the local variable, revealed in this way, will also have universal characteristics.

This picture is more directly relevant to experimental studies of phase transitions than it might appear. In particular local resonance (EPR or NMR) studies explore the behaviour of local variables, time averaged by motional narrowing effects (see, e.g., Kubo 1962). Indeed it is this phenomenon which provided the original insight and motivation for the present study (Bruce *et al* 1979).

The ideas sketched above are developed in a more concrete fashion in the sections which follow. We will focus on the behaviour of the moments $M_\tau^{(n)} \equiv \langle M_\tau^n \rangle$ of the time-coarse-grained variable, and the associated distribution $P(M_\tau)$. In § 2 we develop a general scaling theory for the moments, implying a universal scaling structure for the distribution $P(M_\tau)$, in close analogy with its counterpart $P(M_l)$, characterising the distribution of the ordering field *spatially* coarse grained over a region of linear dimension l (Binder 1981, Bruce 1981). In § 3 we present the results of Monte Carlo studies of two-dimensional scalar models, designed to test and extend the scaling theory. The results substantiate the predicted scaling behaviour of the moments, provide an estimate for the dynamic critical index z consistent with (though not as precise as) the most recent and detailed study using *spatial* coarse-graining techniques (Williams 1985), and substantiate the claimed universality of the distribution $P(M_\tau)$, to within minor discrepancies which we attribute to finite-size effects. It transpires that this distribution is remarkably similar to its spatial counterpart, $P(M_l)$ (Binder 1981), clear testimony in support of the basic thesis that the time-coarse-graining process allows access to large length scale (universal) configurational structure. In § 4 we develop a simple fractal model of the time profile of the time-coarse-grained variables, in the spirit of the droplet theory (Bruce and Wallace 1983). The model accounts for the essential structure of the M_τ distribution. In § 5 we use the theory of the time-coarse-grained variable to explore the behaviour of local resonance lineshape functions near a critical point. We express the lineshape function in terms of the M_τ distribution. In the 'fast' motion regime the lineshape is dominated by the behaviour of the M_τ distribution for coarse-graining times large compared to the outer timescale. In this regime the distribution is Gaussian and the lineshape is Lorentzian. In the 'slow' motion regime the lineshape is controlled by the behaviour of the M_τ distribution for coarse-graining times small compared to the outer timescale; in this regime the distribution is non-Gaussian and the lineshape is non-Lorentzian. The simulation results for the M_τ distribution in this regime are used to compute the slow motion lineshape function: for the two-dimensional universality class studied here a split-line structure emerges. Our results and conclusions are summarised in § 6.

2. Theory of the time-coarse-grained distribution

2.1. Definitions

We will develop our arguments in the context of a system exhibiting a phase transition associated with the ordering of a set of L^d scalar coordinates $\phi_j(t)$ $(j=1\ldots L^d)$ occupying the sites of a d-dimensional lattice of linear dimension L. With the exception of isolated (multicritical) points in the space of model parameters such a system is in general expected to exhibit the equilibrium critical behaviour of the Ising universality class. We will suppose, moreover, that neither the total energy nor the order parameter is a conserved quantity: the implied dynamic behaviour should then fall into the universality class of the kinetic Ising models whose study, by Monte Carlo simulation, is the subject of the following section.

We define a time-coarse-grained local variable by

$$M_{\tau j}=\frac{1}{\tau}\int_0^\tau \phi_j(t)\,\mathrm{d}t. \tag{2.1}$$

We will refer to τ as the coarse-graining time. In general we will be concerned with the behaviour of a single coarse-grained variable and the site index j in (2.1) can be omitted without ambiguity.

The statistics of the time-coarse-grained variables are reflected in the *moments*

$$M_\tau^{(n)}\equiv\langle M_\tau^n\rangle \tag{2.2a}$$

or, in an alternative and sometimes more convenient form, in the *connected moments* or cumulants (see, e.g., Cramer 1946)

$$J_\tau^{(n)}\equiv\langle M_\tau^n\rangle_{\mathrm{c}} \tag{2.2b}$$

where c denotes 'connected part'. The moments (or cumulants) together define the distribution $P(M_\tau)$ of the coarse-grained variable, through its characteristic function $\hat{P}(Y)$:

$$\begin{aligned}P(X)&\equiv\langle\delta(X-M_\tau)\rangle\\&=\frac{1}{2\pi}\int_{-\infty}^{\infty}\mathrm{d}Y\,\mathrm{e}^{\mathrm{i}YX}\hat{P}(Y)\end{aligned} \tag{2.3a}$$

$$\begin{aligned}\hat{P}(Y)&\equiv\langle\mathrm{e}^{-\mathrm{i}YM_\tau}\rangle\\&=\sum_{n=0}^{\infty}\frac{(-\mathrm{i}Y)^n}{n!}M_\tau^{(n)}\\&=\exp\left(\sum_{n=1}^{\infty}\frac{(-\mathrm{i}Y)^n}{n!}J_\tau^{(n)}\right).\end{aligned} \tag{2.3b}$$

The scaling properties of the distribution may thus be inferred from the scaling behaviour of the moments, which we now examine.

2.2. Scaling theory

In the course of this paper we shall be principally concerned with the behaviour at the critical point. In these circumstances (in fact, for all temperatures $T \geqslant T_c$) all moments $M_\tau^{(n)}$ with n odd vanish by the (supposed) symmetry of our model. We begin by studying the simplest case, namely the second moment precisely at criticality.

Appealing to the definitions (2.1) and (2.2) we see that

$$J_\tau^{(2)} = M_\tau^{(2)} = \frac{1}{\tau^2}\int_0^\tau \mathrm{d}t_1 \int_0^\tau \mathrm{d}t_2 \langle \phi_j(t_1)\phi_j(t_2)\rangle. \tag{2.4}$$

Introducing time-and-space Fourier transformed variables by

$$\phi_j(t) = L^{-d/2}\sum_{k}\int_{-\infty}^{\infty}\frac{\mathrm{d}\omega}{2\pi}\phi_k(\omega)\,\mathrm{e}^{\mathrm{i}\omega t} \tag{2.5}$$

this expression may be recast in the form

$$J_\tau^{(2)} = L^{-d}\sum_{k}\int_{-\infty}^{\infty}\frac{\mathrm{d}\omega}{2\pi}\left(\frac{\sin(\omega\tau/2)}{(\omega\tau/2)}\right)^2 C(\boldsymbol{k},\omega) \tag{2.6}$$

where $C(\boldsymbol{k},\omega)$ is the dynamic correlation function defined by

$$\langle \phi_{k_1}(\omega_1)\phi_{k_2}(\omega_2)\rangle = 2\pi\delta(\omega_1+\omega_2)\delta_{k_1+k_2}C(\boldsymbol{k}_1,\omega_1). \tag{2.7}$$

We assume now that there exists a, possibly small, region of $\boldsymbol{k}$ and ω space ($k<k_l$ and $|\omega|<\omega_l$ say) within which dynamic scaling holds. We proceed to argue that, for sufficiently large coarse-graining times, the second cumulant is dominated by contributions originating in this scaling region. Consider first the contributions arising from modes of wavevectors $k>k_l$. For such modes we may assume that there exists a maximum value for $C(\boldsymbol{k},\omega)$ which remains finite at criticality

$$C(\boldsymbol{k},\omega) \leqslant C_{\max}^{(1)} \qquad k>k_l. \tag{2.8}$$

The implied contribution to $J_\tau^{(2)}$ can then be bounded by

$$C_{\max}^{(1)}\left(L^{-d}\sum_{k>k_l}\right)\int_{-\infty}^{\infty}\frac{\mathrm{d}\omega}{2\pi}\left(\frac{\sin(\omega\tau/2)}{(\omega\tau/2)}\right)^2 = \mathrm{O}(1/\tau). \tag{2.9}$$

Now consider the contributions to (2.6) originating in portions of ω space where $|\omega|>\omega_l$. Again we assume that there exists a finite value $C_{\max}^{(2)}$ such that

$$C(\boldsymbol{k},\omega) \leqslant C_{\max}^{(2)} \qquad |\omega|>\omega_l. \tag{2.10}$$

The implied contributions to $J_\tau^{(2)}$ may then be bounded by

$$C_{\max}^{(2)}\left(L^{-d}\sum_{k}\right)\int_{|\omega|>\omega_l}\frac{\mathrm{d}\omega}{2\pi}\left(\frac{\sin(\omega\tau/2)}{(\omega\tau/2)}\right)^2 = \mathrm{O}(1/\tau^2). \tag{2.11}$$

Finally we consider the contribution from the range of $\boldsymbol{k}$ and ω space in which dynamic scaling holds. In this regime we may write (Hohenberg and Halperin 1977)

$$C(\boldsymbol{k},\omega) = k^{-(2-\eta)-z}\tilde{C}(\omega/k^z). \tag{2.12}$$

The associated contribution to (2.6) is then of the form

$$J_\tau^{(2)} \equiv M_\tau^{(2)} \approx \int_{-\omega_l}^{\omega_l}\frac{\mathrm{d}\omega}{2\pi}\left(\frac{\sin(\omega\tau/2)}{(\omega\tau/2)}\right)^2\int_{k<k_l}\frac{\mathrm{d}^d k}{(2\pi)^d}k^{-(2-\eta)-z}\tilde{C}(\omega/k^z). \tag{2.13}$$

Changing variables of integration appropriately one finds that

$$J_\tau^{(2)} = M_\tau^{(2)} \approx \tilde{J}^{(2)} \tau^{-2\lambda_\tau} \tag{2.14}$$

where

$$\lambda_\tau = \frac{d-2+\eta}{2z} = \frac{\beta}{z\nu} \tag{2.15}$$

while $\tilde{J}^{(2)}$ exists as a finite τ-independent constant provided $d<4$. In this regime $\lambda_\tau < \frac{1}{2}$ and so it is always possible to choose sufficiently large coarse-graining times that the second moment is indeed dominated by the region of $\boldsymbol{k}$ and ω space for which $C(\boldsymbol{k}, \omega)$ obeys dynamic scaling.

Now consider the nth-order cumulant. The analogue of (2.6) is

$$J_\tau^{(n)} = \left(L^{-d/2} \sum_{\boldsymbol{k}_1}\right) \ldots \left(L^{-d/2} \sum_{\boldsymbol{k}_n}\right) \int_{-\infty}^{\infty} \frac{\mathrm{d}\omega_1}{2\pi} \ldots \int_{-\infty}^{\infty} \frac{\mathrm{d}\omega_n}{2\pi} \prod_{\alpha=1}^{n} \frac{\sin(\omega_\alpha \tau/2)}{(\omega_\alpha \tau/2)}$$
$$\times L^{-(n-2)d/2} 2\pi\delta(\omega_1 + \ldots + \omega_n)\delta_{\boldsymbol{k}_1+\ldots+\boldsymbol{k}_n} C^{(n)}(\boldsymbol{k}_1 \ldots \boldsymbol{k}_n, \omega_1 \ldots \omega_n) \tag{2.16}$$

where the connected n-point correlation function $C^{(n)}$ is defined by

$$\langle \phi_{\boldsymbol{k}_1}(\omega_1) \ldots \phi_{\boldsymbol{k}_n}(\omega_n) \rangle = 2\pi\delta(\omega_1 + \ldots + \omega_n)\delta_{\boldsymbol{k}_1+\ldots+\boldsymbol{k}_n} L^{(n-2)d/2} C^{(n)}(\boldsymbol{k}_1 \ldots \boldsymbol{k}_n, \omega_1 \ldots \omega_n). \tag{2.17}$$

In the limit of large τ the sine functions in (2.16) ensure that the integrals are dominated by the region in which the frequencies $\omega_1 \ldots \omega_n$ are small $(\mathrm{O}(1/\tau))$. Let us consider the contribution arising from the regime in which, moreover, the wavevectors $k_1 \ldots k_n$ are small (compared to k_i). The correlation function (2.17) should then exhibit the dynamic scaling form implied by the homogeneity relation

$$C^{(n)}(\boldsymbol{k}_1 \ldots \boldsymbol{k}_n, \omega_1 \ldots \omega_n) = a^{\lambda_n} C(a\boldsymbol{k}_1 \ldots a\boldsymbol{k}_n, a^z\omega_1 \ldots a^z\omega_n) \tag{2.18a}$$

where

$$\lambda_n = (n-1)z + (n-1)d - nz\lambda_\tau. \tag{2.18b}$$

The implied contribution to the nth-order cumulant follows as

$$J_\tau^{(n)} \approx \tilde{J}_\tau^{(n)} \tau^{-n\lambda_\tau}. \tag{2.19}$$

As suggested by the notation we believe that this contribution does indeed dominate the asymptotic (large τ) behaviour of the cumulants. However the complexity of the n-point functions makes it hard to justify this claim analytically. Thus we will regard (2.19) as a hypothesis to be checked against the simulations reported in the following sections.

The scaling hypothesis is readily extended to allow for the existence of an outer length scale, L_0, for the critical fluctuations, originating either in the finite system size L or in a finite correlation length ξ. Explicitly we anticipate that (provided the length scales ξ and L are well separated)

$$J_\tau^{(n)} \approx \tilde{J}_\tau^{(n)}(\tau/L_0^z)\tau^{-n\lambda_\tau} \tag{2.20}$$

where L_0 is to be identified with L or ξ according to whether $L \ll \xi$ or $L \gg \xi$ (different scaling functions being appropriate in the different regimes).

The scaling behaviour of the distribution $P(M_\tau)$ now follows readily. Combining (2.3) and (2.2) we find that

$$P(M_\tau;\,\tau,\,L_0)\approx b\tau^{\lambda_\tau}\tilde{P}(b\tau^{\lambda_\tau}M_\tau;\,\tau/\tau_0) \tag{2.21a}$$

with

$$\tau_0 = cL_0^{z}. \tag{2.21b}$$

We have introduced constants b and c with which to absorb the non-universality of the scale of the ordering variable and the timescale of the dynamics. Modulo the arbitrariness of the conventions used to choose b and c we then expect that the scaling function $\tilde{P}(m, \bar{\tau})$ will be universal. For *large* $\bar{\tau}\equiv\tau/\tau_0$ it is clear that, since M_τ is then a sum of essentially uncorrelated variables, the distribution will have a Gaussian form (centred on $m=0$ for $T>T_c$ and, given appropriate boundary conditions, on a non-zero value of m for $T<T_c$). In the *small* $\bar{\tau}$, critical, limit on the other hand *all* the cumulants (2.19) clearly play a role, and the distribution $P^*(m)\equiv\tilde{P}(m,0)$ must in general have some non-trivial non-Gaussian form reflected in some non-trivial fixed-point value, G_τ^*, of the cumulant ratio

$$G_\tau \equiv -J_\tau^{(4)}/2(J^{(2)})^2 \equiv (3\langle M_\tau^2\rangle^2-\langle M_\tau^4\rangle)/2\langle M_\tau^2\rangle^2 \tag{2.22}$$

in contrast to the trivial fixed point values (0, 1) appropriate in the Gaussian ($T>T_c$, $T<T_c$) regimes. In the following section we check out these expectations with the aid of computer simulation.

3. Monte Carlo studies of time-coarse-grained variables

In this section we report the results of extensive Monte Carlo (MC) studies of the behaviour (basically the statistics) of time-coarse-grained variables near critical points. We have chosen to examine systems with $d=2$ space dimensions. There are two reasons for focusing on this 'low'-dimensional case. Firstly it is clear on very general grounds that the critical point statistics of the time-coarse-grained variables will differ more significantly from the classical (Gaussian) limit the lower the space dimension. Secondly, and more specifically, we may anticipate that the nested droplet picture (Bruce and Wallace 1983), which rests heavily upon low-dimensional approximations, should provide a qualitatively reasonable framework in which to interpret the observed behaviour.

We have studied two $d=2$ scalar models: the spin-$\frac{1}{2}$ Ising model at, and near, the Onsager critical point coupling $K_c^{(1/2)}=0.4404\ldots$; and the spin-1 Ising model at the value of the critical coupling, $K_c^{(1)}=0.590\,48$ indicated by the most recent series expansion studies (Adler and Enting 1984). (We remark that, in recent independent work, we have actually refined this estimate somewhat: Nicolaides and Bruce (1988).) Our MC procedure employed a standard Metropolis algorithm implemented in parallel on an ICL Distributed Array Processor. For a general discussion of parallel coding strategy the reader is referred to Hockney and Jessope (1981). The claim that the dynamics thus generated falls into the anticipated universality class (that of the kinetic Ising model with neither energy nor order-parameter conservation) has been substantiated in earlier studies by Williams (1985).

Our studies were conducted on systems of $N=L^2$ spins with L values ranging from 8 to 128. In each case the system was equilibrated for a number, τ_E, of timesteps (MC steps per spin) ranging from $\tau_E = 2\times10^5$ for $L = 8$ to $\tau_E = 10^6$ for $L = 128$. Values of the coarse-graining variables $M_{\tau,i}$ were obtained by monitoring the values of the local variables ϕ_i at a number N_s of well separated sites ($N_s = 1$ for $L = 8$, $N_s = 8$ for $L = 128$) over the appropriate interval τ, updating the system without further observation for some interval τ_I (ranging from $\tau_I = 10$ for $L = 8$ to $\tau_I = 2\times10^3$ for $L = 128$) and repeating the procedure, thus building up a distribution of coarse-grained variable values. For each parameter set (characterised by a given K, L, τ and model type) 64 such distributions were constructed, checked for their statistical independence and utilised to determine the mean values and associated uncertainties which we now present.

We begin by exploring the dependence of the coarse-grained variable statistics upon the coupling strength. Figure 1 shows the cumulant ratio G_τ (equation (2.22)) as a function of the coarse-graining time τ for a spin-$\frac{1}{2}$ system with $L = 128$, at the critical coupling K_c and at two non-critical couplings $K_c + \Delta K$ and $K_c - 2\Delta K$ with ΔK chosen to give a correlation length of approximately eight lattice spacings. In the high-temperature regime ($K < K_c$) G_τ falls towards zero with increasing τ, consistent with a distribution approaching the limiting form of a Gaussian centred on zero. In the low-temperature ($K > K_c$) region G_τ quickly rises towards unity, consistent with a limiting ordered phase distribution composed of two Gaussians, symmetrically disposed about zero, and narrow (vanishingly so, asymptotically) on the scale of their separation. Finally, precisely at the critical point ($K = K_c$) the cumulant ratio quickly settles to an intermediate value in the vicinity of 0.86 independent of the coarse-graining time (on the scale of the figure), indicating a timescale-invariant fixed-point distribution.

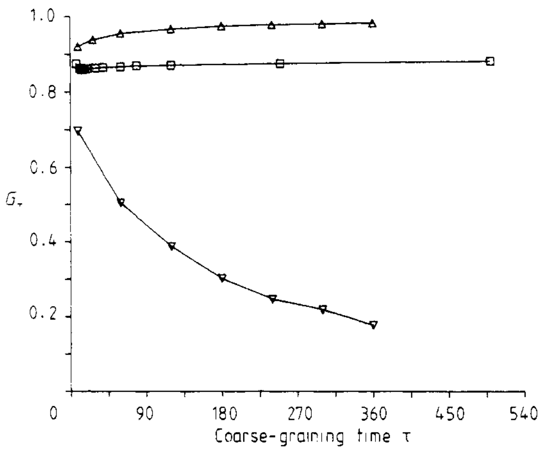

Figure 1. The cumulant ratio G_τ (equation (2.22)) as a function of coarse-graining time τ for the $d = 2$ spin-$\frac{1}{2}$ Ising model, of side $L = 128$ lattice spacings, at couplings K_c (□), $K_c + \Delta K$ (△) and $K_c - 2\Delta K$ (▽) where ΔK is chosen so that the correlation length for the two non-critical systems is approximately eight lattice spacings.

The behaviour away from the critical point is in accord with the qualitative expectations offered at the conclusion of the preceding section and (with a brief exception in § 5) will not be pursued further here. We proceed, rather, to investigate in more detail the behaviour at the critical coupling. The critical behaviour cannot, of course, be strictly scale-invariant in a finite system. Indeed a slight upward drift is just discernible in the 'limiting' behaviour of G_τ, at K_c, shown in figure 1. This behaviour is more clearly evident, and its origin explored, in figure 2(*a*) which displays the value of G_τ (on a greatly expanded scale) as a function of τ, at K_c, for a variety of L values. For a given τ there is a strong dependence upon L which, however, clearly diminishes as L increases. For each L, G_τ first decreases and then increases with increasing τ; the changeover point (the minimum in G_τ) occurs at a coarse-graining time $\tau_{\min}$ which increases with increasing L, and the slope of G_τ beyond $\tau_{\min}$ decreases with increasing L.

To account for these results we must recall that timescale-invariant behaviour can be realised only within a window of coarse-graining times τ satisfying

$$\tau_i \ll \tau \ll \tau_0 . \tag{3.1}$$

For times τ insufficiently large on the scale of the inner timescale τ_i (the typical spin-flip time) there will exist corrections to scaling behaviour originating in irrelevant scaling fields. In the present case it appears that these corrections are such that the scale-invariant limit is approached from above as, indeed, one might anticipate (though the inference is not guaranteed) given that in the $\tau \to 0$ limit G_τ must approach unity, since the distribution of the M_τ variables must then approach the double delta function form of the local variable distribution.

For times τ insufficiently small on the scale of the outer timescale τ_0 (here of order L^z) there will exist finite-size corrections to the bulk scaling behaviour: to the extent that the irrelevant scaling fields are negligible, the cumulant ratio will (cf (2.21)) be a function of the 'scaled' coarse-graining time $\bar{\tau} = \tau/\tau_0$. Figure 2(*b*) shows the behaviour of G_τ (for the larger system sizes) as a function of $\bar{\tau}$. We have made the assignment $z = 2.13$ (discussed below) and have chosen for the constant c appearing in equation (2.21*b*) the value $c = (128)^{-z}$ (so that $\bar{\tau} = \tau$ for $L = 128$). The figure suggests that a gradual approach, with increasing L, to a single scaling function is plausible. The qualitative character of this scaling function is also intelligible by analogy with the behaviour of the distribution of spatially coarse-grained variables M_l. Physically one might anticipate that the behaviour of the M_τ variables would mirror that of the M_l variables for coarse-graining lengths l satisfying $\tau \sim l^z$. There exists no systematic study of the dependence of the statistics of the M_l variables upon the system size L. Two limiting cases have, however, attracted considerable attention. For $l = L$ it is known (Bruce 1985, Burkhardt and Derrida 1985, Nicolaides and Bruce 1988) that the M_l critical distribution approaches (for large $l = L$) an l-independent form characterised by a fixed point cumulant ratio $G^*_{l=L} \simeq 0.91$ (in the case of the $d = 2$ Ising universality class with periodic boundary conditions). On the other hand, for l values small compared to L (Binder 1981, Bruce 1981) there is evidence for a scale-invariant limit with $G^*_{l \ll L} \simeq 0.84$. The implied increase in G_l (as a function of l/L) between these two limits is suggestively similar to the behaviour shown in figure 2. Indeed, if one attempts to use the data shown in figure 2 to assign a value to the scale-invariant limit $G^*_{\tau \ll \tau_0}$ one finds a result very close to the corresponding limit for the spatially coarse-grained variables. However, since this limit is clearly approached non-analytically as $\tau/\tau_0 \to 0$ there are substantial uncertainties in the extrapolation procedure.

The close similarity between the statistics of the M_τ and M_l variables is more fully evident in the structure of the corresponding distribution functions. Figure 3 shows the distribution of M_τ values (for positive M_τ: the distribution is symmetric about $M_\tau = 0$) for the spin-$\frac{1}{2}$ Ising model, at criticality, with $L = 128$ and for a scaled coarse-graining time $\bar{\tau} = 79$ (selected as a compromise between the two constraints expressed

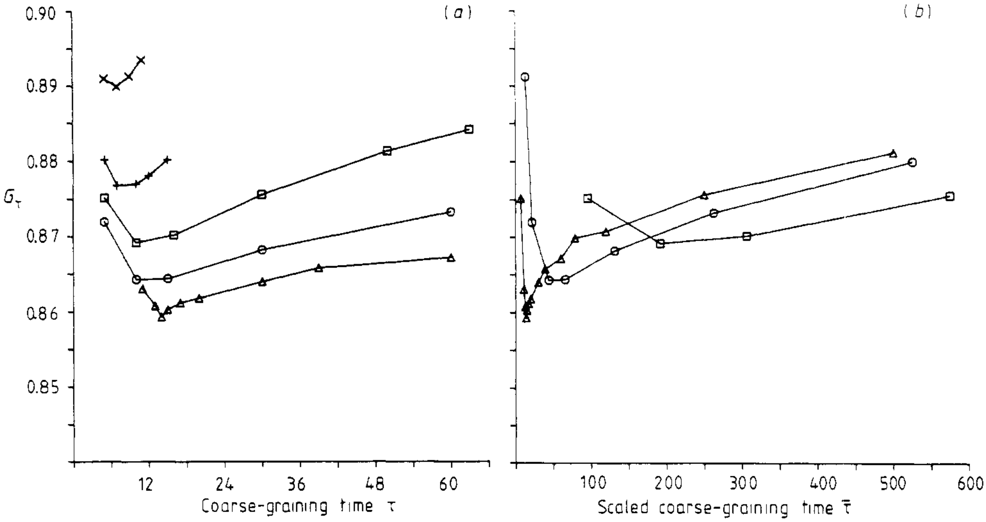

Figure 2. (*a*). The cumulant ratio G_τ for the $d=2$ spin-$\frac{1}{2}$ Ising model, at K_c, as a function of the coarse-graining time τ for a variety of system sizes L: 8 (×), 16 (+), 32 (□), 64 (○) and 128 (△). (*b*) The cumulant ratio G_τ for the $d=2$ spin-$\frac{1}{2}$ Ising model, at K_c, as a function of the *scaled* coarse-graining time $\bar{\tau}$ defined in the text, for a variety of system sizes L: 32 (□), 64 (○) and 128 (△).

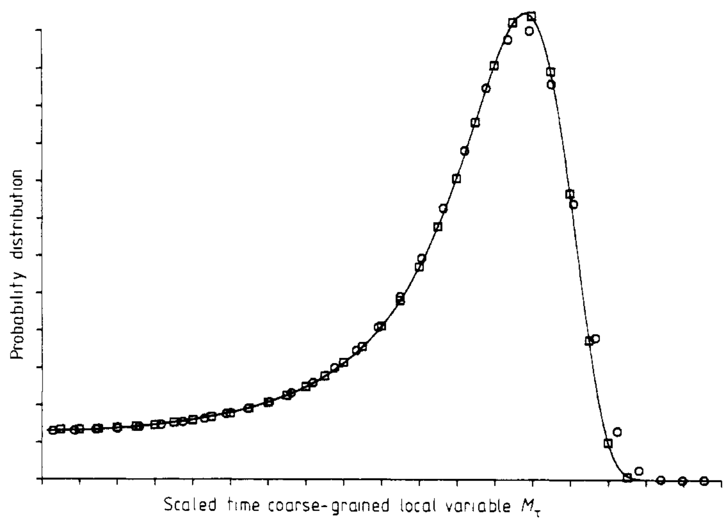

Figure 3. The distribution of M_τ variables for spin-$\frac{1}{2}$ and spin-1 Ising models with $L=128$, at criticality, for the same *scaled* coarse-graining time $\bar{\tau}$ (see text). The abscissa represents the scaled variable bM_τ where the ratio of the b values for the two models has been chosen so that the distributions have the same variance.

in the window condition (3.1)). The distribution has the same characteristic double-hump structure as its spatial counterpart (Binder 1981, Bruce 1981) indicating that the two coarse-graining procedures provide access to similar configurational structure. The figure also shows the result of a similar calculation for the spin-1 model (at criticality) for the same *scaled* coarse-graining time $\bar{\tau}$. To absorb the difference between the basic timescales of the two models we have chosen a c value for the spin-1 model (2.21b) of $c^{(1)} = 3.191 \equiv \tau_0^{(1)}/\tau_0^{(1/2)}$ where the latter ratio was determined by independent studies of the autocorrelation functions of the two models. To absorb the difference between the scales of the ordering fields of the two models we have plotted the distributions as functions of the *scaled* variables bM_τ (equation (2.21a)) with b values assigned to the two models so that the distributions have the same variance. The level of agreement between the two data sets lends support to the contention that the phenomena in question do indeed display universal features, the essential character of which we will explore further in the following section.

The scaling behaviour of the M_τ variable distribution is more explicitly explored in figure 4. The scaled moments $\bar{M}_\tau^{(n)}$ are related to the moments $M_\tau^{(n)}$ of the M_τ distribution by

$$\bar{M}_\tau^{(n)} = L^{n\beta/\nu} M_\tau^{(n)}. \tag{3.2}$$

To the extent that the M_τ distribution satisfies the scaling form (2.21a) the scaled moments may be written in terms of the scaled time $\bar{\tau} = \tau/L^z$ as

$$\bar{M}_\tau^{(n)} = \bar{\tau}^{-n\lambda_\tau} \tilde{M}_\tau^{(n)}(\bar{\tau}). \tag{3.3}$$

Implicit in the logarithmic plots of these scaled moments, shown in figure 4, is the assignment $z = 2.13$ which we have taken from the analysis of the dynamics of spatially coarse-grained variables by Williams (1985). The extent of the data collapse shown in the figure is thus a test both of the general validity of the scaling form (3.3) and of

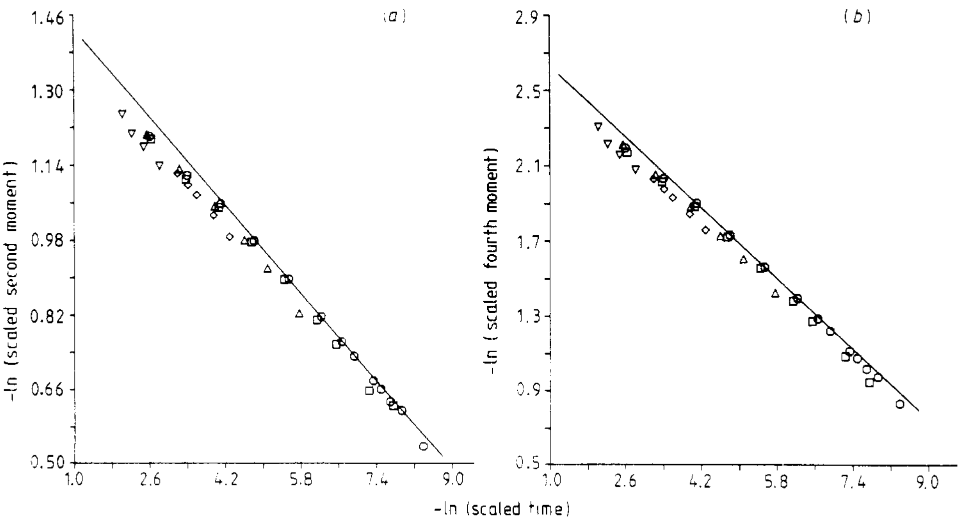

Figure 4. The logarithm of the scaled moment $\bar{M}_\tau^{(n)}$ (defined in equation (3.2)) (a) for $n = 2$ and (b) for $n = 4$ for the spin-$\frac{1}{2}$ Ising model at criticality, for a variety of system sizes L: 8 (▽), 16 (◇), 32 (△), 64 (□) and 128 (○). The abscissa is the logarithm of the scaled time $\bar{\tau}$ defined in the text. The full lines have slope $-2n\beta/z\nu$ and arbitrarily chosen intercepts.

this specific assignment. Both claims pass their respective tests: the data collapse is most satisfactory (as it should be) for the largest system sizes and for the largest timescales (towards the left-hand extreme of the data). An explicit least-squares analysis of the $L=64$ and $L=128$ data sets, keeping only the observations associated with scaled coarse-graining times $\bar{\tau}$ in excess of $\bar{\tau}=80$, yields optimum data collapse with the choice $z=2.10(5)$.

The value of z is also inherent in these results in another way. To the extent the times $\bar{\tau}$ are sufficiently small (so that $\tau \ll \tau_0$), though not so small that the lower window condition ($\tau_i \ll \tau$) is significantly violated, the scaled moments (3.3) will exhibit pure power law behaviour (with amplitudes $\tilde{M}_{\tau}^{(n)}(\tau=0)$). This exception is tested in the figures which represent the appropriate power laws (characterised by indices $n\lambda_{\tau}=n\beta/z\nu$ with $n=2$ and $n=4$ respectively) through the two straight lines. The intercepts have been chosen arbitrarily. Pure power law behaviour with the cited z value is most clearly evident for the $L=128$ system in the regime of intermediate $\bar{\tau}$ values, as one would expect.

4. A fractal model of the time profile

The general physical picture underlying the scaling theory developed in § 2 and tested in the preceding section is simple: the time profile of an ordering variable, time coarse grained to a sufficient degree, has the statistically timescale-invariant structure characteristic of a fractal (Mandelbrot 1983). The specific character of such a time profile will clearly reflect the dynamic universality class of the system. It seems hard to compute from first principles. We proceed, instead, to construct a simple phenomenological model very similar, in spirit, to the droplet model of equilibrium behaviour developed by Bruce and Wallace (1983).

Consider the time profile of some local variable ϕ over some time interval of length τ. The profile will consist of regions in which $\phi=+1$ and regions in which $\phi=-1$, separated by 'time kinks'. It is thus tempting to model the statistics of the time profile in terms of the statistics of a time kink 'gas'. However the kink representation is actually not the most tractable, since the kink variables can certainly not be regarded as being independent: a time kink represents the passage of the boundary of a droplet whose continued existence will tend to promote subsequent 'time kinks' separated by times which are some measure of the spatial extent of that droplet. The simplest way of encoding this kind of kink correlation is to view the profile as being constructed of *pairs* of time kinks, forming 'time droplets' which are nested inside one another; the kink pairs might be thought of as two spin flips associated with the passage of (in some sense) the 'same' spatial interface; the associated time droplets have temporal extents ranging from τ_i upwards, the larger members capturing the bias of the sign of the local variable induced by the presence of the spatially larger droplets.

This picture is certainly oversimplified. We use it here to motivate a phenomenology which may have a greater validity. The phenomenology may be regarded as a prescription for constructing a typical time profile of an Ising variable ϕ. We envisage first a uniform profile, say $\phi(t)=1$, $0<t<\tau$. (In the ensemble of profiles over which we must eventually average, uniform profiles $\phi=1$ and $\phi=-1$ are supposed to occur with equal likelihood.) We then envisage 'decorating' the profile with time droplets first of phase $\phi=-1$ and then subsequently of both phases, adding droplets of successively smaller temporal extent. At each stage of this decoration procedure (which is implemented differentially) the probability that in a unit time interval of $\phi=+1$ ($\phi=-1$) profile there will appear (as a result of the decoration) new time droplets of phase $\phi=-1$ ($\phi=+1$) and of temporal extent (then under consideration) $\tau_r \to \tau_r + d\tau_r$ is taken to be

$$p(\tau_r)\,d\tau_r = \frac{D}{\tau_r^2}\,d\tau_r \tag{4.1}$$

where D, the single parameter of the phenomenology, will be identified below. The specific form of this ansatz has been constructed by analogy with the equilibrium droplet theory (Bruce and Wallace 1983). Its analogue in that context is explicitly justifiable in $d=1+\varepsilon$ dimensions. Here we adopt (4.1) as the simplest prescription that can account for the anticipated scaling properties of the coarse-grained variable.

The prescription can be implemented explicitly (to the extent that D is a small parameter: see below) in a fashion paralleling the analysis of spatial coarse graining realised in the equlibrium droplet theory (Bruce and Wallace 1983). Accordingly we shall simply present the results. We introduce the characteristic function

$$\hat{P}(Y;\tau,\tau_r) \equiv \left\langle \exp\left(i\frac{Y}{\tau}\int_0^\tau \phi_{\tau_r}(t)\,dt \right) \right\rangle \tag{4.2}$$

where $\phi_{\tau_r}(t)$ is the profile generated by decoration (as detailed above) with time droplets of all temporal scales in excess of the resolution time τ_r. The average extends over the ensemble of decorated configurations consistent with the prescription (4.1). The key result can then be expressed in the claim that this characteristic function satisfies the differential equation

$$\frac{\partial \ln \hat{P}(Y;\tau,\tau_r)}{\partial \tau_r} = \frac{D\tau}{\tau_r^2}\left[1-\cos\left(\frac{2Y\tau_r}{\tau}\right)+\sin\left(\frac{2Y\tau_r}{\tau}\right)\cdot\frac{\partial \ln P(Y;\tau,\tau_r)}{\partial Y}\right]. \tag{4.3a}$$

This equation is to be solved with boundary condition

$$\hat{P}(Y;\tau,\tau)=\cos(Y) \tag{4.3b}$$

expressing the supposedly structureless character of the undecorated time profile.

The differential equation may be solved easily by making the cumulant expansion (2.3b). Setting the resolution time $\tau_r=\tau_i$, assumed small compared to τ, one finds for the n-point cumulant (to which we now append the subscript τ_i):

$$J^{(n)}_{\tau,\tau_i} \approx \tilde{J}^{(n)}_{\tau}(\tau/\tau_i)^{-2Dn}. \tag{4.4}$$

Comparison with (2.19) shows that the phenomenological theory does indeed capture the scaling behaviour of the cumulants and identifies the time-droplet concentration parameter D as

$$D=\lambda_\tau/2=\beta/2z\nu. \tag{4.5}$$

Moreover the coefficients $\tilde{J}^{(n)}_{\tau}$ in (4.4) are, one discovers, uniquely prescribed (modulo the arbitrary overall scale assigned to the ordering field) in terms of the index D. In particular we find for the fixed point value of the cumulant ratio (2.22) the expansion

$$G^*_\tau = 1-8D/3+O(D^2). \tag{4.6}$$

The neglect of the $O(D^2)$ terms is necessary for consistency: the decoration procedure can be implemented analytically only to the extent that D is sufficiently small that the time droplets constitute a dilute gas (Bruce and Wallace 1983). For the $d=2$ universality class of interest D is indeed a small parameter. Specifically, from (4.5) we find

$D = 0.029$ so that, from (4.6), $G_\tau^* \simeq 0.916$. The result is somewhat higher than that suggested by the Monte Carlo work reported in § 3. Part of the discrepancy is due to the simplistic boundary condition (4.3*b*) which does not address the existence of time droplets of temporal extent larger than τ that may partially overlap the interval under examination. This effect can be taken into account: one finds that G_τ^* is then lowered by approximately 0.02. The remaining discrepancy doubtless reflects a more serious deficiency of the model, which encodes time kink correlations only in the simplest (and crudest) fashion consistent with a scaling picture. Nevertheless the level of accord gives reason to believe that the model captures some of the key physics of the time profile.

5. Critical behaviour of local resonance lineshapes

5.1. Background

In this section we proceed to show how the theory of time-coarse-grained variables illuminates, and is potentially testable by, electron paramagnetic resonance (EPR) or nuclear magnetic resonance (NMR) studies of systems undergoing phase transitions.

Consider, then, a system exhibiting a phase transition with the characteristics of the Ising universality class. We suppose that the system is doped with a small concentration of probe ions which, we will assume, do not perturb their environment to a significant degree. We focus on the resonant absorption of radiation associated with transitions between two specific Zeeman-split electronic or nuclear states of the probe ion. We denote by $\hbar\omega_0$ the energy level separation in the absence of interaction between the probe ion and its environment. We suppose that the ion couples to a single local degree of freedom, ϕ, of the Ising ordered field. (The arguments which follow actually transcend this restriction.) Specifically we suppose that the energy level splitting $\hbar\omega$ for a given ion is actually a *linear* function of the local variable with which it interacts:

$$\hbar\omega = \hbar\omega_0 + \mu\phi \tag{5.1}$$

where μ is some constant. Finally we make the 'adiabatic' (or 'secular') approximation that the time variation of the local field ϕ is slow on the scale of the inverse Larmor frequency ω_0^{-1}: the effect of the ϕ field is, then, simply to modulate the energy level splitting (in the fashion prescribed by equation (5.1)) rather than to induce further transitions. More formally this approximation may be regarded as involving the neglect of those terms in the Hamiltonian describing the spin-ϕ variable interaction that do not commute with the ion-spin Hamiltonian (Abragham 1961). Within these approximations the resonant absorption at frequency $\omega = \omega_0 + \Omega$ is prescribed by the lineshape function (Abragham 1961, Kubo 1962)

$$R(\Omega) = \frac{1}{\pi} \operatorname{Re} \int_0^\infty d\tau \, e^{i\Omega\tau} S(\tau) \tag{5.2a}$$

where the relaxation function $S(\tau)$ is defined by

$$S(\tau) = \left\langle \exp\left(-i\mu \int_0^\tau \phi(t) \, dt \right) \right\rangle. \tag{5.2b}$$

The physical consequences of the fluctuations in the Ising field for the lineshape function (5.2*a*) depend both upon the timescale(s) of the fluctuations and upon the parameter μ (which may itself be regarded as an inverse timescale). If μ is large enough (or, equivalently, if the timescale of the *fastest* of the ϕ fluctuations is long enough) the relaxation function (5.2b) will decay within a time short compared to that on which ϕ evolves, so that

$$S(\tau) \approx \langle e^{-i\mu\tau\phi} \rangle \tag{5.3a}$$

and

$$R(\Omega) \approx \langle \delta(\Omega - \mu\phi) \rangle = \mu^{-1} P_0(\mu^{-1}\Omega) \tag{5.3b}$$

where P_0 is the probability distribution of the ϕ field. In this regime, then, the resonance spectrum is broadened in a fashion which directly reflects the static distribution of the perturbing field set up by the local Ising variable. On the other hand, for smaller μ values, the relaxation function $S(\tau)$ will only begin to decay for times τ long enough that, in the course of a typical τ interval, the ϕ field will exhibit significant fluctuations. Physically it is then clear that the probe will 'see' only some kind of time-averaged (and thus reduced) effective value of the local Ising field. The interaction broadening will thus be reduced with respect to the large-μ limit. This is the phenomenon of motional narrowing (Abragham 1962).

It is evident that the essential consequence of motional narrowing is to suppress the effects of the faster fluctuations in the perturbing field and thus, relatively, to enhance the effects of the slower longer-lived fluctuations. Accordingly one might expect that, with a suitable choice of the control parameter μ, the resonance lineshape would provide a probe of the universal statistics of the large time-coarse-grained variables studied in the preceding sections. We now proceed to make this connection concrete, and to exploit it to provide specific predictions regarding resonance lineshape functions.

5.2. General scaling theory

Comparison of (5.2b), (2.1) and (2.3) shows that the relaxation function $S(\tau)$ is directly related to the characteristic function of the time-coarse-grained variables M_τ:

$$S(\tau) = \langle e^{-i\mu\tau M_\tau} \rangle = \hat{P}(\mu\tau). \tag{5.4}$$

Now, *provided* the dominant contributions to $S(\tau)$ originate in M_τ variables whose cumulants follow the scaling form (2.20), equation (5.4) shows that the relaxation function will itself exhibit the scaling behaviour

$$S(\tau) = \tilde{S}(\tilde{\mu}^{1/x}\tau, \tau_0^{-1}\tau) \tag{5.5a}$$

where

$$x \equiv 1 - \lambda_\tau \tag{5.5b}$$

$$\tilde{\mu} \equiv \mu / b \tag{5.5c}$$

while $\tilde{S}$ is a universal function, b is the scale factor introduced in (2.21a) and τ_0 is the outer timescale defined by (2.21b).

To expose the conditions under which this scaling form may in fact be expected to hold we consider the consequences of allowing for some irrelevant scaling field in the scaling ansatz (2.18). We then find that the scaling relation (5.5a) assumes the modified form

$$S(\tau) \approx \tilde{S}(\tilde{\mu}^{1/x}\tau, \tau_0^{-1}\tau, u\tau^{-\omega/z}) \tag{5.5d}$$

where u gives a measure of the correction-to-scaling field and ω (>0) is the associated index. Now for small enough μ, $\tilde{S}$ must certainly approach unity; accordingly, given (5.5c), $\tilde{S}$ can begin to exhibit significant structure (deviate from unity) only for times τ of the order of $\tilde{\mu}^{-1/x}$. For such times, $u\tau^{-\omega/z}$ will be of order $u\tilde{\mu}^{\omega/zx}$ which may in principle be made arbitrarily small by choosing μ to be appropriately small. The full scaling form (5.5a) for the relaxation function is then recovered. It then follows that, for sufficiently small μ, the lineshape function $R(\Omega)$ will itself have a scaling form:

$$R(\Omega) \approx \tilde{\mu}^{-1/x}\tilde{R}(\tilde{\mu}^{-1/x}\Omega, \tilde{\mu}^{1/x}\tau_0). \tag{5.6}$$

More explicitly, recalling equations (5.2a, b), (5.4) and (2.3a), we find that the lineshape function may be expressed in terms of the time-coarse-grained variable distribution by

$$R(\Omega) = \frac{1}{\pi}\,\mathrm{Re}\int_0^\infty \mathrm{d}\tau\, \mathrm{e}^{\mathrm{i}\Omega\tau}\int_{-\infty}^{\infty} \mathrm{d}M_\tau\, \mathrm{e}^{-\mathrm{i}\mu\tau M_\tau} P(M_\tau;\, \tau, L_0). \tag{5.7}$$

We now turn to explore the consequences of these relations.

5.3. *Explicit results*

We consider first the *fast motion* regime where the motional narrowing effect extends throughout the spectrum of critical fluctuations. This regime is identified explicitly by the condition

$$\tilde{\mu}^{1/x}\tau_0 \ll 1. \tag{5.8}$$

This condition ensures that times τ sufficiently large for the relaxation function $S(\tau)$ to differ from unity (cf (5.5a)) are also necessarily large compared to the outer timescale τ_0. In this regime (cf § 2.2) the M_τ distribution will be Gaussian:

$$P(M_\tau;\, \tau, L_0) = (2\pi M_\tau^{(2)})^{-1/2} \exp(-M_\tau^2/2M_\tau^{(2)}) \tag{5.9a}$$

with variance satisfying

$$M_\tau^{(2)} = J_\tau^{(2)} = 2A\tau^{-1}\tau_0^{1-2\lambda_\tau}. \tag{5.9b}$$

The latter result follows on matching the general scaling form (2.20) to the central-limit-theorem result that $M_\tau^{(2)} \sim \tau^{-1}$ for large τ. The parameter A is a non-universal constant whose value is in principle prescribed by the large-time behaviour of the autocorrelation function. Feeding these results into equation (5.7) we find for the lineshape function $R(\Omega)$ the Lorentzian form

$$R(\Omega) = \frac{\Delta\omega}{\pi}\,\frac{1}{\Delta\omega^2 + \Omega^2} \tag{5.10a}$$

where

$$\Delta\omega = A\mu^2\tau_0^{1-2\lambda_\tau} \tag{5.10b}$$

gives the linewidth. As criticality is approached in a macroscopic system and $\tau_0 \sim \xi^z$ increases, the motional narrowing becomes less effective and the line broadens. Introducing an index ψ such that

$$\Delta\omega \sim \tau_0^{\psi/z\nu} \sim \xi^{\psi/\nu} \sim |T - T_c|^{-\psi} \tag{5.11a}$$

we find from (5.10b) that

$$\psi = z\nu(1 - 2\lambda_\tau) = z\nu - 2\beta \tag{5.11b}$$

which corrects a result proposed by Schwabl (1972), but is consistent with an earlier claim by Gottlieb and Heller (1971).

These results are put to the test in figure 5. The data points represent the results of direct Monte Carlo measurements of the relaxation function $S(\tau)$ (equation (5.2*b*)) for the spin-$\frac{1}{2}$ Ising model at criticality, with μ and L values chosen to satisfy the fast-motion condition (5.8) (where $\tau_0 = L^z$). The full curve represents the simple exponential decay given by the Fourier transform of (5.10*a*):

$$S(\tau) = \mathrm{e}^{-\Delta\omega|\tau|} = \mathrm{e}^{-A\mu^2 L^{z-2\beta/\nu}|\tau|}. \tag{5.12}$$

The amplitude A was computed from an independent study of the autocorrelation function: the comparison thus involves no free parameters. The scaling theory clearly passes this test.

We now turn to the *slow motion* regime characterised by the condition

$$\tilde{\mu}^{1/x}\tau_0 \gg 1. \tag{5.13}$$

In this regime the outer timescale is large enough (on the scale set by the resonance probe parameter μ) that the relaxation function (5.5*a*) is *effectively* that of a system *at* its critical point. Accordingly the distribution of M_τ variables contributing to the lineshape function will assume its non-Gaussian scale-invariant form

$$P(M_\tau; \tau, L_0) \simeq b\tau^{\lambda_\tau} P^*(b\tau^{\lambda_\tau} M_\tau) \tag{5.14}$$

throughout the contributing range. The lineshape function then has the simple scaling form

$$R(\Omega) \simeq \tilde{\mu}^{-1/x}\tilde{R}^*(\tilde{\mu}^{-1/x}\Omega) \tag{5.15a}$$

The line 'width' (defined in any appropriate fashion) will vary with the resonance probe parameter μ as

$$\Delta\omega \sim \mu^{1/x} \tag{5.15b}$$

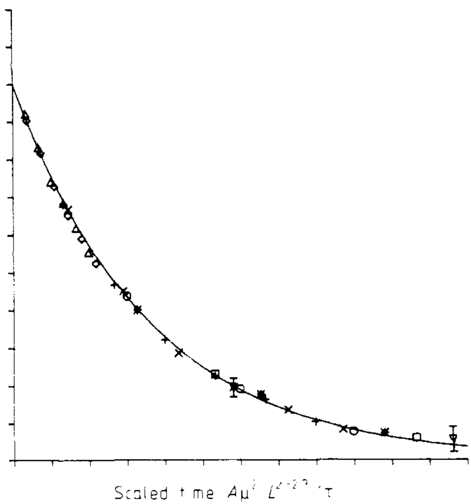

Figure 5. The relaxation function $S(\tau)$ (5.2*b*) for the spin-$\frac{1}{2}$ Ising model at criticality, for a variety of system sizes L and resonance probe parameters μ, chosen to give realisations of the *fast* motion regime (5.8): (▽) $L = 32$, $\mu = 1\times10^{-4}$; (*) $L = 32$, $\mu = 7.5\times10^{-5}$; (×) $L = 32$, $\mu = 5\times10^{-5}$; (◇) $L = 32$, $\mu = 2.5\times10^{-5}$; (□) $L = 16$, $\mu = 2\times10^{-4}$; (○) $L = 16$, $\mu = 1.54\times10^{-4}$; (+) $L = 16$, $\mu = 1\times10^{-4}$; (△) $L = 16$, $\mu = 5\times10^{-5}$. Representative error bars are indicated. The full curve is the exponential (5.12).

which is to be contrasted with the stronger μ dependence characteristic of the fast motion regime (5.10*b*). Using equations (5.7) and (5.14) we have computed the slow-motion fixed-point lineshape function (5.15*a*), taking for the fixed-point distribution P^* the form shown in figure 3, which is the best realisation available to us of the window condition (3.1). The result is shown in figure 6. In this regime the strongly non-Gaussian character of the fixed-point M_τ distribution manifests itself in a correspondingly strongly non-Lorentzian lineshape, which is actually split into two distinct components. We shall return to this feature in the concluding discussion to which we now turn.

6. Discussion and conclusions

In this paper we have explored a simple but, we believe, novel way of exposing some of the universal features of the dynamic behaviour of systems undergoing phase transitions.

At the most pedestrian level one may regard the time-coarse-graining method as a tool for the computation of the critical index z, being the natural extension to dynamic phenomena of the space-coarse-graining techniques developed by Binder (1981) for the study of equilibrium critical phenomena. However, if this is one's primary aim, one would almost certainly do better to study the time-coarse-grained properties of the order parameter (the 'magnetisation') of the system, rather than that of the local variables we have studied here: the additional (implicit) *spatial* coarse graining will then serve to minimise the role of irrelevant scaling fields.

At a somewhat deeper level there lies the nature of the time-coarse-grained configurations themselves. A number of issues remain unresolved here. We have already noted the similarity between the distributions of time- and space-coarse-grained variables, M_τ and M_l respectively, which complements the striking insensitivity of the M_l distributions to the specific manner in which the coarse graining is implemented (Binder 1981, Bruce 1981). It seems possible that the constraints imposed by the conformal invariance of critical-point configurations (Cardy 1986) may offer some insight into this issue. The fractal character of the time profile of the ordering variable also merits further attention. The model developed in § 4 is certainly a crude one. Nevertheless it may be possible to substantiate the ansatz (equation (4.1)) for the time kink concentration, at least within the kind of low-dimensional approximation within which its equilibrium counterpart (for droplet concentration) is known to hold (Bruce and Wallace 1983).

Finally we turn to the experimental level where the original motivation for this work is to be found. Our theory of local resonance phenomena shows that, with the approach to criticality, the critical slowing down of the long-wavelength contributions to the local fluctuation spectrum drives a crossover in the lineshape from the Lorentzian form, appropriate in the fast motion regime (equation (5.8)) to a non-Lorentzian form in the critical slow motion regime (equation (5.13)). We make this claim in the context of resonance probes whose Larmor frequency is *linearly* dependent upon the local ordering variable (equation (5.1)). The case of a *quadratic* shift has been studied by Mukamel *et al* (1983), although only within a cumulant expansion approximation; a qualitatively similar crossover effect is reported. In the specific case of the two-dimensional system investigated here, the slow-motion fixed-point lineshape is actually split into two distinct components (figure 6) with a form very like that of the fixed-point

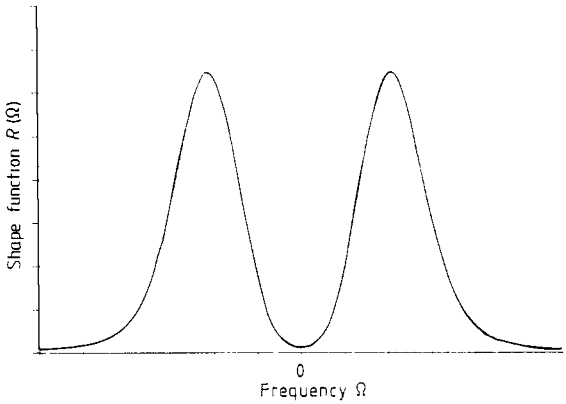

Figure 6. The lineshape function $R(\Omega)$ in the slow motion regime, computed from the fixed-point form of the M_τ distribution.

M_τ distribution itself (figure 3). This is not hard to understand. Inspection of (5.7) and (2.21*a*) shows that, in the limit in which λ_τ tends to zero, the lineshape function is, in fact, a direct image of the M_τ distribution. In two dimensions λ_τ ($\simeq 0.06$) is small enough to maintain a close correspondence between the functions. In three dimensions, where λ_τ (≈ 0.15) is significantly larger, this correspondence will be less close; moreover, in $d=3$ it is clear, by analogy with the M_l distribution studies (Bruce 1981, Binder 1981), that the fixed-point M_τ distribution will be less structured than its $d=2$ counterpart, presumably singly peaked. Accordingly, in this case, one might expect a critical point lineshape function with a single somewhat flattened peak.

One can certainly find much in the experimental literature that appears to be in at least qualitative accord with this picture. The 'accord' has to be viewed with considerable caution. Electron paramagnetic resonance studies of the 105 K structural phase transition in $SrTiO_3$ (Müller and von Waldkirch 1975, Bruce *et al* 1979) do show a crossover from a Lorentzian to a flattened 'over-Gaussian' form within a few degrees of the phase transition, qualitatively similar to the picture (of three-dimensional systems) advanced above. However it remains far from clear that the effect is characteristic of the ideal defect-free critical dynamics envisaged here.

Both EPR and NMR studies have also shown pretransitional splitting in spectral lines in a wide variety of hydrogen-bonded materials exhibiting structural phase transitions, as reviewed by Blinc (1977), Müller (1979) and Dalal (1982). In most instances, however, this 'crossover' occurs at a temperature $T^*(\mu)$ relatively far above the transition temperature T_c. Accordingly it is unlikely either that the dominant fluctuations are of long wavelength, or that the latter fluctuations have the asymptotic scaling characteristics assumed here. (In any case we would not expect that the critical fluctuation spectrum for *this* universality class would support a *split* fixed point lineshape.) For the theory developed here to be applicable, the resonance probe must be such that the parameter μ is small enough to ensure motional discrimination against the faster short wavelength modes. This condition is more likely to be fulfilled the closer the crossover temperature $T^*(\mu)$ is to the critical temperature T_c. In this respect the NMR study of the phase transition in squaric acid, reported by Mehring and Suwelack (1979) appears more promising. The ^{13}C resonance line studied begins to develop non-Lorentzian structure some two degrees above the 370 K phase transition. At the phase transition temperature itself the spectrum has a double-line form very like that shown in figure 6. Again, however, this correspondence is most probably illusory. For, although our theory would account for the *limiting* form of the lineshape, we do not believe that it would account for the manner in which the lineshape *evolves* towards this form as the phase transition is approached. The observations show that the two lines present in the spectrum at the phase transition actually first appear as *wings* on a further, central, line; the latter (the dominant feature above 372 K) disappears as the phase transition is approached. By contrast, tentative studies of the fast–slow motion crossover identified in the preceding section (exploiting the corresponding crossover displayed in the M_τ distribution: cf figure 1) suggest that, with the approach to criticality, the central line simply *splits* to give the double-line slow motion spectrum. Thus it seems more likely that the behaviour observed in squaric acid should, as suggested by Mehring and Becker (1981), be regarded as evidence that the phase transition is slightly first order.

We conclude that existing data do not offer a substantive test of the predictions made here for a fluctuation-driven crossover to a slow motion lineshape characteristic of the universality class. To provide such a test one should ideally examine a nuclear resonance of a host crystal ion (to eliminate the concerns associated with the introduction of EPR centres) in a quasi-two-dimensional system (where deviations from Lorentzian behaviour will be most pronounced) exhibiting a continuous phase transition (free of the ambiguities associated with a first-order transition) and with a coupling parameter μ sufficiently small that the line splitting occurs (if indeed it does!) as close as possible to the critical temperature.

Acknowledgments

One of us (ADB) acknowledges many helpful discussions with K A Müller when the work was conceived. The work was supported by research grant GRC 80431.

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