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LETTER TO THE EDITOR

Phenomenological renormalisation of Monte Carlo data

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Abstract. A method, akin to phenomenological renormalisation, for analysing Monte Carlo data in the critical region is proposed. The method is illustrated by an analysis of the structure factor of the two-dimensional axial next-nearest neighbour Ising model.

Phenomenological renormalisation (Nightingale 1976, 1979) has proven to be a very powerful method of probing critical behaviour. (For a recent review, see Barber (1982).) In this approach, the correlation lengths $\xi_l(T)$ and $\xi_{l'}(T)$ of the system of interest are computed in two different finite domains of (linear) size l and l'. (Usually, the domains are $l\times\infty$ strips.) A renormalisation $T\to T'$ of the temperature is then inferred by setting

$$\xi_l(T)/l=\xi_{l'}(T')/l'. \tag{1}$$

The fixed point $T=T'=T^*=T^*(l, l')$ of this transformation yields an estimate of the critical temperature T_c, while the exponent ν can be estimated from the usual formula

$$(\mathrm{d}T'/\mathrm{d}T)_{T=T^*}=b^{1/\nu}=(l/l')^{1/\nu}. \tag{2}$$

These estimates of T_c and ν depend upon l and l' but in practice converge rather rapidly as l and l' are increased. (For a discussion of the rate of convergence, see Derrida and De Seze (1982), Binder (1981b).)

Phenomenological renormalisation is a consequence (Barber 1982) of finite-size scaling (Fisher 1971, Fisher and Barber 1972), (1) following by demanding an *exact* scaling between $\xi_l(T)$ and $\xi_{l'}(T')$. Given this origin, it is natural to conceive (see also dos Santos and Sneddon 1981, Binder 1981a, b) of defining an analogous renormalisation using some other quantity that satisfies finite-size scaling but is more accessible than the correlation length, particularly from the point of view of Monte Carlo calculations.

Let $P_l(T)$ be some quantity that in the bulk limit ($l\to\infty$) behaves near T_c as

$$P_\infty(T)\sim C_\infty|t|^{-\rho}, \qquad t\to 0, \tag{3}$$

where $t=(T-T_c)/T_c$ and for finite l scales as (see Barber 1982)

$$P_l(T)\sim l^{\omega}Q(l^{\theta}t) \tag{4}$$

with $\theta=1/\nu$ and $\omega=\rho/\nu$. In analogy with phenomenological renormalisation we now infer a mapping $T \to T'$ via

$$P_l(T) = b^{\omega} P_{l'}(T') \tag{5}$$

with $b = l/l'$. We shall refer to this transformation as 'generalised phenomenological renormalisation'.

Choosing $P_l(T)$ to be $\xi_l(T)$, we recover (1) with $\omega = 1$. The problem in the generalised case is that the exponent ω is *not* known *a priori*. Further information beyond simply $P_l(T)$ for two values of l is required to estimate jointly† T_c and ω. A similar problem arises in transfer matrix studies of directed percolation (Kinzel and Yeomans 1981) where two correlation lengths $\xi_\perp$ and $\xi_\parallel$ need to be distinguished with $\xi_\perp \sim \xi_\parallel^\theta$ at T_c.

We can easily adapt the method employed by Kinzel and Yeomans to our problem (see also dos Santos and Sneddon 1981). Define

$$\zeta_{l,l'}(T) = \ln[P_l(T)/P_{l'}(T)]/\ln(l/l'). \tag{6}$$

Then the intersection of $\zeta_{l,l'}(T)$ and $\zeta_{l',l''}(T)$ as functions of T is approximately (T_c, ω). Figure 1 illustrates this procedure using Monte Carlo data for the second moment $\tilde{\chi}_l = \langle m^2 \rangle_l = N^{-2} \Sigma_{i,j} \langle \sigma_i \sigma_j \rangle = \chi_l / N$ of the $d = 2$ Ising model on $l \times l$ squares ($N = l^2$) with periodic boundary conditions (χ_l is the susceptibility above the critical temperature). Hence ω in (3) has the value $-2\beta/\nu = -\eta$. The curves for $\zeta_{4,8}$ and $\zeta_{8,16}$ clearly intersect very close to the exact values ($T_c = 2.269\ldots$, $-\eta = 0.25$). A more detailed and refined analysis involving various other system sizes, along the lines used by Binder (1981a, b), would undoubtedly yield very accurate estimates of T_c and $\omega = -\eta$.

Binder's method of analysis is actually very similaı to that proposed here (e.g. his function W_β^* is identical to $\zeta_{l,l'}$ with $P_l = \langle m^2 \rangle_l$), but does differ in two features. Firstly,

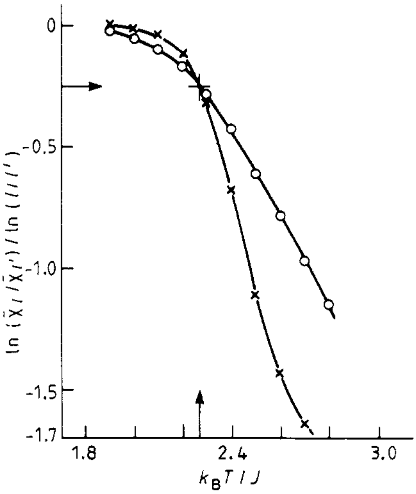

Figure 1. Plot of the functions $\zeta_{l,l'} = \ln(\tilde{\chi}_l/\tilde{\chi}_{l'})/\ln(l/l')$ against T for $l = 2l' = 16$ (×) and $l = 2l' = 8$ (○). Hence $\tilde{\chi}_l$ is the second moment of the Ising model on a $l \times l$ square lattice with periodic boundary conditions. The arrows locate the exact values of $k_B T_c/J$ and $-\eta$.

† Once T_c and ω are known, ν can be estimated from (2). However, this is probably difficult with Monte Carlo data in view of the derivative required.

in general Binder estimates $\langle m^2\rangle_l$ for $l\times l$ blocks embedded in a larger system. Secondly, his method of determining T_c involves a joint scaling of $\langle m^2\rangle_l$ and the fourth moment so that data from *two* different block sizes suffice. Estimating the fourth moment by Monte Carlo methods is however difficult. It is thus significant that a comparably accurate estimate of T_c can be obtained from the second moment alone.

An alternative method, using data from *four* sizes, is as follows. Let

$$R_{l,l'}(T)=P_l(T)/P_{l'}(T); \tag{7}$$

then $R_{l_1,l_2}(T)$ and $R_{l_3,l_4}(T)$ should intersect at (T_c, b^{ω}) provided

$$l_1/l_2=l_3/l_4=b. \tag{8}$$

For the $d=2$ Ising model on $l\times l$ squares with periodic boundary conditions, this method yields estimates of T_c and η of a similar accuracy to those in figure 1. In this case, the systems are small ($4\leqslant l\leqslant 16$) and the Monte Carlo statistics are very good using moderate amounts of computer time. We have found, however, that $\zeta_{l,l'}(T)$ is very susceptible to fluctuations in the data whereas $R_{l,l'}(T)$ is less so.

To illustrate this second method we have performed a scaling analysis of the structure factor $\chi(q)$ of the $d=2$ axial next-nearest neighbour Ising (ANNNI) model (Fisher and Selke 1980). This model has received considerable attention as the simplest Ising model exhibiting an incommensurately modulated phase (see e.g. Selke and Fisher 1980, Selke 1981, Villain and Bak 1981, Rujan 1981, Barber and Duxbury 1981, 1982, Duxbury and Barber 1982, Huse and Fisher 1982 and further references cited in these papers). From this work a fairly clear picture of the phase diagram has emerged. For weak antiferromagnetic next-nearest neighbour coupling ($\kappa<\frac{1}{2}$, see below) the system orders ferromagnetically at low temperatures and melts into the paramagnetic phase, where a disorder line separates regions of purely exponentially decaying correlations from ones with oscillatory modulated correlations. For $\kappa>\frac{1}{2}$ the (2, 2) antiphase state melts into a modulated or floating incommensurate phase. The remaining questions concern mainly the extent of this modulated phase.

On an infinite lattice, the onset of the modulated phase is heralded (Redner and Stanley 1977) as the temperature T is lowered by a divergence in $\chi(q)$ at a critical q value, q_c, dependent on the anisotropy parameter $\kappa=|J_2|/J_1$. Here J_1 (J_2) is the nearest (next-nearest) neighbour interaction in the x direction ($J_1>0$, $J_2<0$). (We follow Selke (1981) and write $J_1=(1-\alpha)J_0$, $J_2=-\alpha J_0$, where J_0 (>0) is the nearest neighbour interaction in the y direction. Hence $\kappa=\alpha/(1-\alpha)$.) As T is lowered further, $\chi(q)$ remains infinite but at a different value of q which approaches $\pi/2$ as the antiphase boundary is approached.

On a finite lattice, $\chi_l(q)$ remains finite but inside the modulated phase we would expect a finite-size scaling ansatz of the form

$$\chi_l(q)\sim l^x Q(l^{\theta}t;q), \tag{9}$$

where $t=[T-T_c(q)]/T_c(q)$ and q is such that $\chi_\infty(q)$ diverges. The value of the exponent x is unclear (see below).

Figures 2 and 3 show plots of $\tilde{\chi}_l(q;T)/\tilde{\chi}_{l'}(q,T)$ for the indicated values of l and q for two different values of the anisotropy: $\alpha=0.376$ ($\kappa\simeq0.6$) and $\alpha=0.6$ ($\kappa=1.5$), respectively. Here

$$\tilde{\chi}_l(q;T)=N^{-2}\sum_{xy,x'y'}\exp[iq(x-x')]\langle\sigma_{xy}\sigma_{x'y'}\rangle=N^{-1}\chi(q), \tag{10}$$

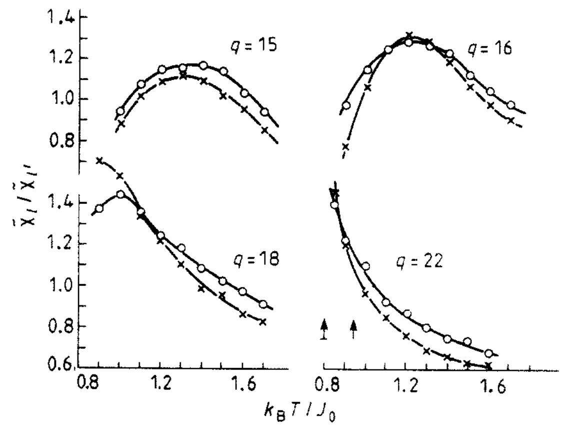

Figure 2. Plot of the functions $R_{l,l'} = \tilde{\chi}_l(q; T)/\tilde{\chi}_{l'}(q; T)$ for the ANNNI model with $\alpha = 0.376$ ($\kappa \simeq 0.6$) on $88 \times l$ lattices for $l = 2l' = 6$ (○) and $l = 2l' = 8$ (×) and the indicated q-values (q measured in units of $2\pi/88$). The arrows locate the estimates of the antiphase transition temperature T_a within the free-fermion approximation (lower temperature) and the Pesch/Kroemer approximation.

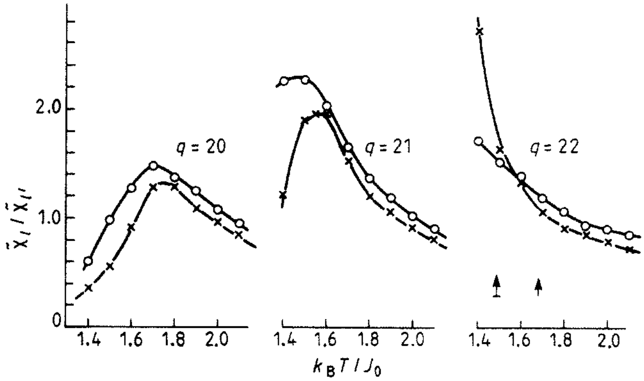

Figure 3. As in figure 2 except at $\alpha = 0.6$ ($\kappa = 1.5$).

where the lattices used were $88 \times l$, i.e. $N = 88l$ spins, with the 'long' dimension in the direction of the competition. The wavevector q is measured in units of $2\pi/88$ and is, of course, discretised by the finite size.

Because of long relaxation and fluctuation times due to the large susceptibilities and energy barriers associated with the walls created in the modulated phase, very extended Monte Carlo runs are needed to get reasonable statistics (Binder 1979, Selke 1981, Selke and Yeomans 1982, Morgenstern 1982). The data, displayed in figures 2 and 3, were obtained by averaging over several runs of 2×10^4 to 4×10^4 Monte Carlo steps per site.

Figure 2, for $\alpha = 0.376$ ($\kappa \simeq 0.6$), clearly shows that $q = 15$ is never critical, whereas $\chi(q)$ for $16 \leqslant q \leqslant 22$ become critical at successively lower temperatures as the modulated phase is crossed. For $\alpha = 0.6$ ($\kappa = 1.5$) only the antiphase susceptibility $\chi(\pi/2)$ ($q = 22$) becomes critical.

From our analysis one may estimate the antiphase transition temperature T_a, the critical wavevector q_c, the transition temperature to the paramagnetic phase T_c, the temperature dependence of q in the modulated phase and the critical exponent η. In the following, we shall briefly compare our results on these quantities with the ones found in the literature.

The estimates for T_a, i.e. the temperature where the antiphase susceptibility becomes critical, are in between the ones obtained from the free-fermion approximation (Villain and Bak 1981) and those calculated via the vanishing of an (approximate) interface free energy (Kroemer and Pesch 1982). Additional data for systems of size 88×12 (not displayed in figure 2) confirm our estimate.

Because of the discretisation of the wavevector one can extract only bounds for q_c: $\frac{15}{44}\pi < q_c < \frac{16}{44}\pi$ at $\kappa \simeq 0.6$ and $\frac{21}{44}\pi < q_c \leqslant \frac{1}{2}\pi$ at $\kappa = 1.5$. For comparison, mean field theory (Elliott 1961) gives

$$q_c = 2\pi \cos^{-1}(1/4\kappa), \qquad \kappa > \tfrac{1}{4}, \tag{11}$$

which agrees very well at the smaller value of κ but overestimates appreciably the stability of the modulated phase at $\kappa = 1.5$. Unfortunately, we cannot definitely establish the (non-)existence of a Lifshitz point on the (2,2)antiphase side of the phase diagram. If a Lifshitz point does exist at $\kappa = \kappa_L$, then q_c is $\pi/2$ for $\kappa > \kappa_L$. Obviously, however, data from $\infty \times l$ strips are required to exclude critical q values that are arbitrarily close to $\pi/2$.

The behaviour seen here for $\chi_l(q)$ is similar (as is the method of analysis) to that found by Duxbury and Barber (1982) for the q-dependent mass gap of the quantum Hamiltonian version (Barber and Duxbury 1981, Rujan 1981) of the ANNNI model on relatively short, finite chains. Our bounds on q_c are much sharper than those found by Duxbury and Barber (1982), and we have lifted the lower bound on κ for the existence of a Lifshitz point to $\kappa_L \geqslant 1.5$. Within the different bounds on q_c our results agree quite well with the Hamiltonian conclusions.

The estimate for T_c at $\kappa = 0.6$ is surprisingly close to the position of the maximum in the specific heat, C, if extrapolated in a simple fashion to the thermodynamic limit (Selke 1981). Greater deviations might have been expected, since C is not a critical quantity for this transition which is believed to be XY-like or of Kosterlitz–Thouless character (Selke and Fisher 1980).

The most interesting aspect of our analysis seems to be the possibility to monitor wavevectors as they successively become critical in the modulated phase. Note that some wavevectors do not become critical, although the structure factor has a maximum at those q values well below the temperature where the specific heat is maximal. This shows probably the greatest advantage of phenomenological renormalisation: it yields a rather objective criterion for criticality.

Finally, we turn to the question of the exponent x entering the finite-size scaling ansatz (9). In principle this can be obtained from figures 2 or 3. However, while the estimates of $T_c(q)$ are relatively stable, the corresponding estimates of b^x are very dependent upon the accuracy of the Monte Carlo data and the values of l used. Consequently, no definite conclusions can be drawn. Theoretically, x is presumably related to the exponent $\eta = \eta(T)$, characterising the algebraic decay of the correlation function in the modulated phase (Villain and Bak 1981, Schulz 1980). The precise relation is, however, unclear. At a normal critical point such as that in the $d = 2$ Ising model, $\chi_l(0) \sim l^{2-\eta}$, which is confirmed by figure 1. This simple behaviour is a consequence of the infinite-lattice result that $\chi_\infty(T) \sim \xi^{2-\eta}$ near T_c and $\xi \sim l$. The problem for the ANNNI model† for $\kappa > \frac{1}{2}$ is that, at least near the antiphase boundary, two correlation lengths ξ_x and ξ_y need to be distinguished, with $\xi_x \sim \xi_y^\theta$ where $\theta = \frac{1}{2}$ and $\nu_x = 1$ (Schulz 1980). If we assert that

$$\chi_\infty(\pi/2) \sim (\xi_x \xi_y)^{(2-\eta)/2} \tag{12}$$

within a finite strip $\xi_y \sim l$, we obtain

$$\chi_\infty(\pi/2) \sim l^x, \qquad x = \tfrac{1}{2} - \tfrac{3}{2}\eta. \tag{13}$$

If η is small‡ this result is not inconsistent with figure 2. On the other hand, the upper transition is believed (Selke and Fisher 1980) to be XY-like or of Kosterlitz–Thouless character and one might believe that the scaling should be isotropic, implying $\chi_l(q_c) \sim l^{2-\eta}$ with $\eta = \frac{1}{4}$. This value, however, seems to be excluded by the estimates of figure 2. These are consistent with (13) and a small value of η for all T in $T_c \geq T \geq T_a$. A more detailed analysis of the critical behaviour of $\chi_l(T, q)$ across the modulated phase is certainly warranted. The method of analysis presented here would seem to make such an analysis feasible.

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† For $\kappa < \frac{1}{2}$, Monte Carlo data for $\chi_l(0)$ appear to be consistent with $\chi_l \sim l^{2-\eta}$ with $\eta = 0.25$.
‡ In the modulated phase, Villain and Bak (1981) state that $\langle\sigma_0\sigma_r\rangle \sim r^{-\tau}\cos(\pi q x)$ with $\tau = \frac{1}{2}(1-q)^2$ and $q = \frac{1}{2}$ at T_a. Hence $\eta(T_a) = \frac{1}{8}$.

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