Journal of Statistical Physics, Vol. 35, Nos. 1/2, 1984

Construction of Simple Approximants for the Structure Factor and Magnetization for the Simple Cubic Ising Model

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Received July 25, 1983

A renormalization group method is used to construct approximants for the magnetization, m, and the static structure factor, $\tilde{C}(\mathbf{q})$, for the simple cubic Ising model. Using the "best" values for the thermal critical index, the transition temperature, and the nearest-neighbor correlation function as input, we obtain recursion relations for m and $\tilde{C}(\mathbf{q})$ which lead to reasonable results over a wide range of temperatures and wave numbers.

KEY WORDS: Simple cubic Ising model; real space renormalization group; static structure factor; magnetization.

1. INTRODUCTION

It has recently been shown that the real space dynamic renormalization group (RSDRG) method can be very useful in developing simple approximants for the equilibrium properties(1),[2] of one- and two-dimensional Ising models. This is, of course, unnecessary for the one-dimensional case where everything can be determined exactly. It is also not crucial for the zero field thermodynamic properties of the two-dimensional model, where analytic solutions again exist.(2) However, for spatial correlations or time-dependent nonequilibrium problems there are few exact results in two dimensions. One must then resort to approximation techniques to determine these

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[2] Typically, real space renormalization group methods have been concerned with the study of critical properties as discussed in other articles in Ref. 1. We are concerned with a more global description in this paper.

0022-4715/84/0400-0001$03.50/0

quantities. The importance of the RSDRG formalism is that it can be directly applied in these situations to construct approximants which are reliable over a wide range of wave numbers and temperatures.

Of particular interest is the structure factor $\tilde{C}(\mathbf{q})$. In the study of dynamic phenomena, for example, it is important that equilibrium properties like $\tilde{C}(\mathbf{q})$ be treated properly, because they form the basis for the calculation of time-dependent quantities. Previously,(1) the RSDRG was used to develop simple recursion relations for both $\tilde{C}(\mathbf{q})$ and the magnetization for the two-dimensional square lattice. The iterated solutions of these recursion relations provide accurate approximants for these observables. We describe here the results of the extension of this technique to three dimensions for the simple cubic Ising model.

In the following section the model and the basic RSDRG formal structure will be briefly described. Zeroth-order recursion relations are then constructed for the magnetization, the susceptibility, and the structure factor. These recursion relations involve several parameters, whose determination is discussed in Section 3. Low-temperature calculations require special consideration, which is given in Section 4. The results of an analysis of the recursion relations are then presented in Section 5, and a comparison made with other approximation methods.

2. MODEL AND RSDRG ANALYSIS

Our model[3] consists of a set of N spins $\sigma_i = \pm 1$ on a simple cubic lattice, where the subscript i refers to the lattice site at $\mathbf{r}_i$. The equilibrium properties are governed by a nearest-neighbor Hamiltonian $H[\sigma]$ characterized by a ferromagnetic coupling K ($\geqslant 0$). The basics of the RSDRG method have been covered in detail elsewhere.(1,3) The main point is that there exists a coarse-graining transformation function $T[\mu \mid \sigma]$ which maps a set of σ spins onto block Ising spins $\{\mu\}$ defined on a new lattice with a larger lattice spacing. The probability distribution governing the new spins is given by

$$P[\mu] = \sum_{\sigma} T[\mu \mid \sigma] P[\sigma] \tag{2.1}$$

where $P[\sigma]$ is the probability distribution governing the σ spins. For any function $A[\sigma]$ we can identify its counterpart on the coarse-grained lattice by

$$A[\mu] = \langle T[\mu \mid \sigma] A[\sigma] \rangle / P[\mu] \tag{2.2}$$

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[3] We follow, where possible, the notation of Ref. 1.

where $\langle\ \rangle$ indicates an average over $P[\sigma]$. Using the normalization condition $\sum_\mu T[\mu \mid \sigma] = 1$, we then see that

$$\langle A[\mu]\rangle' = \langle A[\sigma]\rangle \tag{2.3}$$

where the prime indicates an average over $P[\mu]$. Equation (2.3) is in the form of a recursion relation relating observables on the different lattices.

To implement this transformation, we divide up our simple cubic lattice into cells of eight spins each, as in Fig. 1. These cells will also form a simple cubic lattice. Each cell will be labeled by an index i, and each lattice site within the cell will have an index a. The three nearest intracell neighbors of a site labeled a are displaced from it by a single primitive lattice vector, and therefore any one of them will be denoted by $a + 1$ (for our purposes, we do not need to distinguish between them). Similarly, the three next-nearest neighbors are labeled $a + 2$, and the opposite site is $a + 3$.

Our basic approximation is very similar to that described in Ref. 1. We will give its motivation here. The first assumption is that in constructing "collective" variables using (2.2) it is reasonable to take the average to be

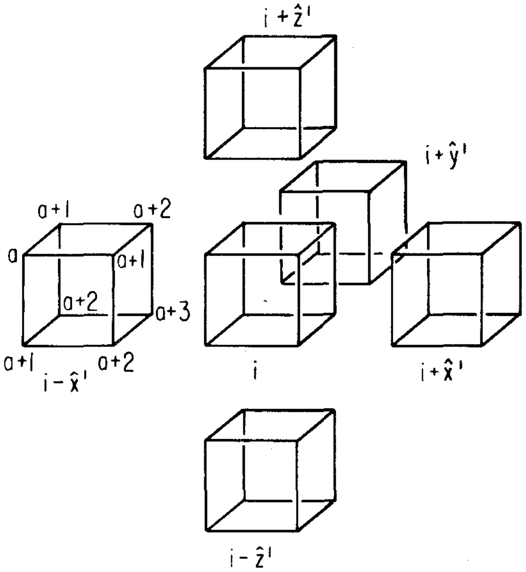

Fig. 1. Lattice broken into cells of eight spins each. Cell i is separated from its nearest neighbors by coarse-grained primitive lattice vectors $\hat{x}', \hat{y}', \hat{z}'$. Within a cell, a spin a has three nearest neighbors $a + 1$, three next-nearest neighbors $a + 2$, and a third-nearest neighbor $a + 3$.

over a set of uncoupled cells as long as the effective coupling K_0 governing those cells is chosen appropriately. The second assumption is that the renormalized Hamiltonian $H[\mu]$ is again characterized by a single coupling K', and that we have nonperturbative methods for constructing a good approximant for the thermal recursion relation $K' = K'(K)$. Given the thermal recursion relation, one can use the recursion relation satisfied by a short-range correlation function to determine $K_0 = K_0(K)$.

The first step in this analysis is the choice of the mapping function. This problem in the two-dimensional case is discussed in detail in Ref. 3. In direct analogy with the analysis there we choose the mapping function

$$T[\mu \mid \sigma] = \prod_{i=1}^{N/8} \tfrac{1}{2}\left[1 + \mu_i \psi_i(\sigma)\right] \tag{2.4}$$

where $\psi_i(\sigma)$ is the normalized[4] order parameter for a cell,

$$\psi_i(\sigma) = \frac{1}{8\nu_1} \sum_a \sigma_{i,a} \tag{2.5}$$

$$\nu_1 = \langle \sigma_{i,a} \psi_i(\sigma) \rangle_0 = \left[\tfrac{1}{8}(1 + 3r + 3s + t)\right]^{1/2} \tag{2.6}$$

and $\langle\ \rangle_0$ indicates an average over a set of uncoupled cells. The parameters in (2.6) are the zeroth-order correlation functions

$$r = \langle \sigma_{i,a} \sigma_{i,a+1} \rangle_0 = \frac{u_0(1 + u_0^2 + 11u_0^4 + 3u_0^6)}{(1 + u_0^2)(1 - 2u_0^2 + 9u_0^4)} \tag{2.7a}$$

$$s = \langle \sigma_{i,a} \sigma_{i,a+2} \rangle_0 = \frac{2u_0^2(1 + 2u_0^2 + 5u_0^4)}{(1 + u_0^2)(1 - 2u_0^2 + 9u_0^4)} \tag{2.7b}$$

$$t = \langle \sigma_{i,a} \sigma_{i,a+3} \rangle_0 = \frac{2u_0^3(3 + 3u_0^2 + 9u_0^4 + u_0^6)}{(1 + u_0^2)^2(1 - 2u_0^2 + 9u_0^4)} \tag{2.7c}$$

where $u_0 = \tanh K_0$.

We are now able to construct recursion relations between observable quantities defined for the two different lattices. We consider the magnetization first. Using (2.2), the coarse-grained function corresponding to a single spin $\sigma_{i,a}$ is found to be

$$M_{i,a}[\mu] = \nu_1 \mu_i \tag{2.8}$$

in agreement with the two-dimensional case, and the magnetization is then

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[4] The normalization condition $\langle \psi_i^2 \rangle_0 = 1$ is required by the condition $\langle T[\mu \mid \sigma] T[\mu' \mid \sigma] \rangle = \delta_{\mu\mu'} P_0[\mu]$ (see Ref. 1).

given by

$$m = \nu_1 m' \tag{2.9}$$

where we have used (2.3).

The spin–spin product $\sigma_{i,a}\sigma_{j,b}$ has a coarse-grained counterpart

$$M_{i,a;j,b}[\mu] = \nu_1^2 \mu_i \mu_j + \delta_{ij}\left[\delta_{a,b} + r\delta_{a,b+1} + s\delta_{a,b+2} + t\delta_{a,b+3} - \nu_1^2\right] \tag{2.10}$$

so that the spin–spin correlation function has a recursion relation given by

$$C_{i,a;j,b} = \langle \delta\sigma_{i,a}\delta\sigma_{j,b}\rangle = \nu_1^2 C'_{ij} + \delta_{ij}\left[\delta_{a,b} + r\delta_{a,b+1} + s\delta_{a,b+2} + t\delta_{a,b+3} - \nu_1^2\right] \tag{2.11}$$

where $\delta\sigma_{i,a} = \sigma_{i,a} - m$. We may also use (2.10) to calculate recursion relations for correlation functions of the form

$$\epsilon(m,n,p) = \frac{1}{N}\sum_{\mathbf{r}} \langle \sigma_{\mathbf{r}}\sigma_{\mathbf{r}+m\hat{x}+n\hat{y}+p\hat{z}}\rangle \tag{2.12}$$

For example,

$$\epsilon(1,0,0) = \frac{r}{2} + \frac{\nu_1^2}{2}\epsilon'(1,0,0) \tag{2.13a}$$

$$\epsilon(2^n,0,0) = \nu_1^2\epsilon'(2^{n-1},0,0) \tag{2.13b}$$

Equation (2.11) can be used to find the recursion relation for the static structure factor:

$$\begin{aligned}\tilde{C}(\mathbf{q}) &= \frac{1}{N}\sum_{i,a;j,b} e^{i\mathbf{q}\cdot(\mathbf{r}_{i,a}-\mathbf{r}_{j,b})}C_{i,a;j,b}\\ &= 8\nu_1^2 f(\mathbf{q})\left[\tilde{C}'(2\mathbf{q}) - 1\right] + 1 + 3rg_1(\mathbf{q}) + 3sg_2(\mathbf{q}) + tg_3(\mathbf{q})\end{aligned} \tag{2.14}$$

where

$$f(\mathbf{q}) = \tfrac{1}{8}\left[1 + 3g_1(\mathbf{q}) + 3g_2(\mathbf{q}) + g_3(\mathbf{q})\right] \tag{2.15a}$$

$$g_1(\mathbf{q}) = \tfrac{1}{3}\left[\cos q_x + \cos q_y + \cos q_z\right] \tag{2.15b}$$

$$g_2(\mathbf{q}) = \tfrac{1}{3}\left[\cos q_x \cos q_y + \cos q_y \cos q_z + \cos q_z \cos q_x\right] \tag{2.15c}$$

$$g_3(\mathbf{q}) = \cos q_x \cos q_y \cos q_z \tag{2.15d}$$

All wave vectors $\mathbf{q}$ are measured in terms of the inverse lattice constant. Note that this results in a rescaling by a factor of 2 of the wave vector in the coarse-grained structure factor in (2.14). If we now let $\mathbf{q}\to 0$ and use (2.6), we obtain the recursion relation for the magnetic susceptibility χ, which has the particularly simple form

$$\chi = 8\nu_1^2\chi' \tag{2.16}$$

3. DETERMINATION OF THE PARAMETERS K' AND K_0

The recursion relations we developed in Section 2 depend on temperature through the parameters K, K', and K_0. Therefore, given K we need to be able to determine K' and K_0. The approach we have developed(1,4) has been to invert the recursion relations (2.13) for the short-range correlation functions. Thus, we could use the ratio

$$\frac{\epsilon(4,0,0)}{\epsilon(2,0,0)} = \frac{\epsilon'(2,0,0)}{\epsilon'(1,0,0)} \tag{3.1}$$

derived from (2.13b), to determine $K' = K'(K)$ given the best available approximations for $\epsilon(2^n,0,0;K)$. $K_0 = K_0(K)$ may be found in a similar manner using (2.13a).

In this paper we will be less ambitious than to invert (3.1), and instead use a phenomenological thermal recursion relation which builds in a large amount of known information. As discussed in Ref. 4, there are several restrictions which we can place on the form of this relation. Briefly, a consideration of the exponential decay requirements of long-range correlation functions tells us that at high and low temperatures, the recursion relation must have the forms

$$K' \propto K^2 \qquad (K \ll 1) \tag{3.2a}$$

$$K' \approx 2K \qquad (K \gg 1) \tag{3.2b}$$

The correct relation should interpolate smoothly between these two limits, and have a fixed point at finite $K = K' = K_c$. In addition, the relation should satisfy $(\partial K'/\partial K)_{K_c} = 2^{y_T}$, where $y_T = 1/\nu$ is the associated thermal index, and give the proper flow to the high- and low-temperature fixed points under iteration.

A simple recursion relation which satisfies all of these requirements and which is convenient to use is given by

$$\varphi' - \frac{1}{\varphi'} = 2^{y_T - 1}(\varphi^2 - \varphi^{-2}) \tag{3.3a}$$

where

$$\varphi = \frac{u/u_c}{y/y_c} \tag{3.3b}$$

and

$$u = \tanh K \tag{3.4a}$$

$$y = e^{-4K} \tag{3.4b}$$

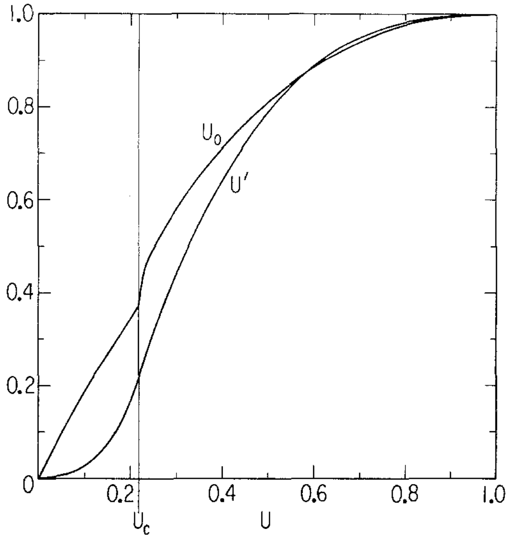

Fig. 2. The renormalized coupling $u' = \tanh K'$ and intracell coupling $u_0 = \tanh K_0$ as a function of $u = \tanh K$.

are the usual high- and low-temperature variables, respectively. Equation (3.3) is a generalization of a thermal recursion relation used in two dimensions in Refs. 1, 3, and 4, which follows from the recursion relation satisfied by the correlation length ξ:

$$\xi' = \xi/2 \tag{3.5}$$

To use (3.3), however, we need to know K_c and ν in three dimensions. We will simply use their best known values:

$$\begin{aligned} K_c &= 0.221692^{(5)} \\ \nu &= 0.6300^{(6,7)} \end{aligned} \tag{3.6}$$

The resulting relation $u' = u'(u)$ is shown in Fig. 2.

Once $K' = K'(K)$ is known, Eqs. (2.6) and (2.7) may be used to invert (2.13a) and express $K_0 = K_0(K)$ through the nearest-neighbor correlation function $\epsilon(1,0,0)$. Series expansions for $\epsilon(1,0,0)$ are known to very high order in both the high- and low-temperature regimes,$^{(8)}$ and estimates have been made of its value at the critical point,$^{(8)}$ so that simple two-point Padé approximants for $\epsilon(1,0,0)$ may be produced which are useful through the entire temperature range (see Fig. 3). Although these approximants do not incorporate a continuous derivative at the critical point, this will have only

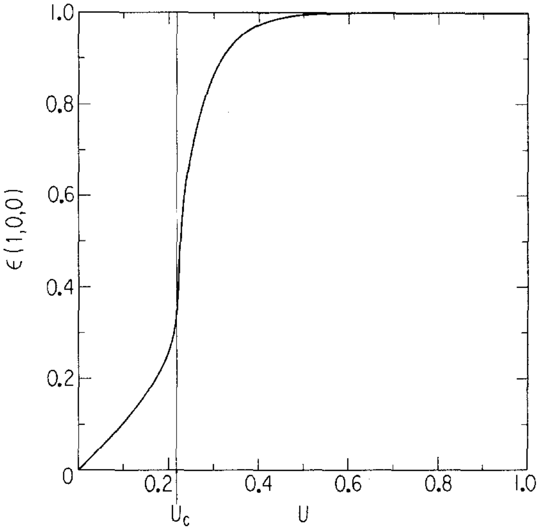

Fig. 3. High- and low-temperature Padé approximants for $\epsilon(1,0,0)$ used to calculate $u_0 = u_0(u)$.

a small effect on our results. This lack of smoothness is observable, however, in Fig. 2, where $u_0 = u_0(u)$ is plotted.

The interpretation of K_0 as an effective intracell coupling, after the bonds between cells are broken, implies that it will not be equal to K. Instead, because half of the bonds are cut, we expect that $K_0 \sim 2K$. This is found to be true across the entire temperature range, where the average percentage difference $|(K_0 - 2K)/2K|$ is 3%. The maximum difference is 12%, just above the critical point.

4. LOW-TEMPERATURE CALCULATIONS

Calculation with the results of Sections 2 and 3 generally involves straightforward iteration of the recursion relations.(1,4) This is true in the high-temperature regime, and for the magnetization recursion relation (2.9) below T_c. However, serious problems occur if (2.14) and (2.16) for the structure factor and susceptibility are used in this way in the ordered phase.(9) Analysis of (2.14) at very low temperatures quickly reveals the difficulty. At lowest order in y, $\tilde{C}(\mathbf{q}) = 4y^3$ independent of $\mathbf{q}$.(5) The thermal recursion relation (3.3) tells us that $y' \sim y^2$, so that $\tilde{C}'(2\mathbf{q}) \sim y^6$, and it may be neglected in comparison to the inhomogeneous part of (2.14). This recursion relation then becomes

$$\tilde{C}(\mathbf{q}) = 1 + 3rg_1(\mathbf{q}) + 3sg_2(\mathbf{q}) + tg_3(\mathbf{q}) - 8\nu_1^2 f(\mathbf{q}) + O(y^6) \quad (4.1a)$$

$$= \frac{64}{15}\left[1 - f(\mathbf{q})\right]y^3 + O(y^4) \quad (4.1b)$$

While we do not expect such expansions of the recursion relation to match up order by order with the series expansion, the qualitative dependence on $\mathbf{q}$ in (4.1b) is unacceptable. In particular, in the $\mathbf{q} = 0$ limit, the right side of (4.1a) vanishes identically because of (2.6), causing the susceptibility to be zero throughout the low-temperature regime.[5]

A similar problem occurs if one examines the recursion relation for the second moment of correlation $\mu_2 = (1/N)\sum_{i,j}(\mathbf{r}_i - \mathbf{r}_j)^2 C_{ij}$, which is found to become negative for low enough temperatures.(9) This is clearly an unphysical result, and can be traced to the fact that the zeroth-order correlation functions r, s, and t defined in (2.7) become smaller than the square of the magnetization as the temperature approaches zero. A systematic procedure for avoiding this behavior has been developed which also rectifies the structure factor and susceptibility difficulties described above. Basically, we require that

$$t \geqslant m^2 \quad (4.2)$$

throughout the ordered phase. This means that the method described in Section 3 for determining K_0 through (2.13a) must be modified whenever $t < m^2$. We do this by relaxing the normalization condition (see footnote 4) which results in the expression (2.6) defining ν_1. We may then determine ν_1 in this region by requiring that

$$t = m^2 \quad (4.3)$$

This relation marginally satisfies Eq. (4.2) and is well defined. Combined with Eq. (2.13a), ν_1 and K_0 will again be precisely determined.

The effect of this "ν_1 correction" on the value of ν_1 is very slight; less than a 1% change. It therefore does not alter the magnetization [calculated using (2.9)] in a significant way. Nevertheless, it has a dramatic effect on the structure factor, removing the wave-vector dependence (4.1b) at lowest order, and giving it the correct qualitative behavior throughout the ordered phase. However, for reasons which will be discussed in Section 5, its quantitative accuracy is limited.

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[5] If $\chi_{\mathrm{RSDRG}} = O(y^n)$, then $\chi'_{\mathrm{RSDRG}} = O(y^{2n})$, since $\nu_1 = 1 + O(y^3)$. This is inconsistent with (2.16), unless $n = 0$ and $\chi_{\mathrm{RSDRG}} = 0$. This can be considered a crude approximation, with $\chi_{\mathrm{RSDRG}}(T_c) = \infty$.

We may also examine this problem from a different point of view. Let us again consider (2.14) and (2.16) for the structure factor and susceptibility. Since they are zeroth-order recursion relations, we would expect that going to first order in the ordering parameter(10) would improve them in some way. In particular, the susceptibility recursion relation (2.16) would gain an inhomogeneous term which gives the correct very-low-temperature behavior, and which makes the recursion relation useable below T_c. We would also expect that any such addition will not be very important in the high-temperature regime, because (2.16) is found to give very good results as it stands (see Section 5).

A first-order calculation, however, is an involved procedure, and beyond the scope of this paper. A much easier technique to use instead is to simply model the assumed inhomogeneous term with an approximant incorporating the expected characteristics, and add it to the susceptibility recursion relation. More generally, we may replace the structure factor's inhomogeneous term

$$1 + 3rg_1(\mathbf{q}) + 3sg_2(\mathbf{q}) + tg_3(\mathbf{q}) - 8\nu_1^2 f(\mathbf{q}) \tag{4.4}$$

with a two-point approximant which builds in the first few terms of the series expansion for $\tilde{C}(\mathbf{q})$(5) and which maps smoothly into (4.4) at the critical point. Such a "low-temperature correction" of the recursion relation (2.14) will provide good results throughout the ordered phase, while retaining the original recursion relation above T_c. The approximant which is used in this paper ensures that the structure factor is correct to $O(y^6)$, and matches Eq. (4.4) and its first derivative at the critical point (see the Appendix).

5. ANALYSIS AND DISCUSSION

We may now proceed to study the recursion relations developed in Section 2. We will first extract as much information from them as we can analytically. Equations (2.9), (2.14), and (2.16) may be used to express critical exponents in terms of the critical parameter ν_1^* and derive scaling laws in the following way. Near the critical point, the correlation length and magnetization will behave as

$$\xi \sim |\tau|^{-\nu} \tag{5.1}$$

$$m \sim B|\tau|^{\beta} \sim \xi^{-\beta/\nu} \tag{5.2}$$

where

$$\tau = 1 - T_c/T \tag{5.3}$$

In addition, the correlation length will obey Eq. (3.5). The magnetization recursion relation (2.9) can then be expressed as

$$\xi^{-\beta/\nu} = \nu_1^*(\xi')^{-\beta/\nu} = \nu_1^*\left(\frac{\xi}{2}\right)^{-\beta/\nu} \tag{5.4a}$$

so that

$$\frac{\beta}{\nu} = -\frac{\ln \nu_1^*}{\ln 2} \tag{5.4b}$$

Similarly, because

$$\chi \sim C^{\pm}|\tau|^{-\gamma} \sim \xi^{\gamma/\nu} \tag{5.5}$$

(where ± refers to $T \gtrless T_c$), the susceptibility recursion relation (2.16) leads to

$$\frac{\gamma}{\nu} = d + 2\frac{\ln \nu_1^*}{\ln 2} \tag{5.6}$$

where we have noted that $8 = 2^d$ in (2.16). Equations (5.4) and (5.6) may be combined to yield the scaling law(11)

$$\gamma = d\nu - 2\beta \tag{5.7}$$

In the same way, we may use the critical relation

$$\tilde{C}^*(\mathbf{q}) \sim Dq^{-2+\eta} \tag{5.8}$$

for small q, to find the relation

$$\eta = 2 - d - 2\frac{\ln \nu_1^*}{\ln 2} \tag{5.9}$$

and the scaling law(11)

$$\frac{\gamma}{\nu} = 2 - \eta \tag{5.10}$$

The values of β, γ, and η obtained using ν_1^* from (2.6) and ν from (3.6) are displayed in Table I, along with the series(5,8) and field-theoretic(6) estimates of these exponents. We see that the agreement is satisfactory.

Table I. Critical Exponents, as Determined by Series, Field Theoretic, and RSDRG Techniques

Method	β	γ	η
Series[a]	0.312 ± 0.005	1.250 ± 0.003	0.056 ± 0.008
Field theory[b]	0.325 ± 0.001	1.2402 ± 0.0009	0.0315 ± 0.0025
RSDRG	0.321	1.248	0.020

[a] Reference 8.

[b] Reference 6.

Table II. Critical Amplitudes, as Determined by Series and RSDRG Techniques

Method	B	C^-	C^+	D
Series[a]	1.569 ± 0.003	0.209 ± 0.003	1.0585 ± 0.0010	3.98 ± 0.02
RSDRG:				
ν_1 correction	1.81 ± 0.08	0.28 ± 0.14	0.9934 ± 0.0013	3.01 ± 0.04
Low-temperature correction	1.836 ± 0.006	0.2111 ± 0.0019		

[a] References 5 and 8.

These exponents may also be calculated numerically, by direct iteration of the recursion relations. As we would expect, they agree with the analytic results in Table I. We have also calculated the numerical values of the critical amplitudes B, $C^{\pm}$, and D as defined in Eqs. (5.2), (5.5), and (5.8). These are displayed in Table II, along with their series estimates. As with the exponents, there is reasonable agreement between the two sets of amplitudes.

We now move away from the critical region and examine our results over a wider range of temperatures. The magnetization m, calculated using our two low-temperature methods, is shown in Fig. 4, along with a Padé

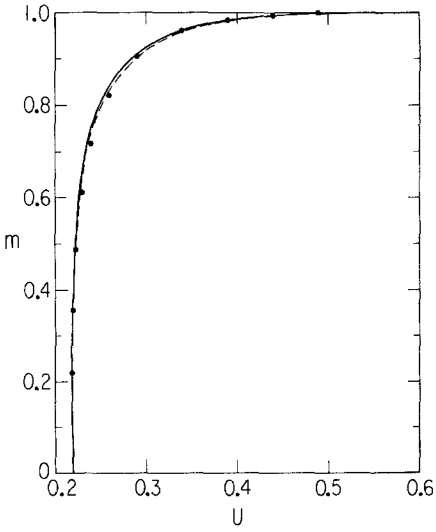

Fig. 4. The magnetization m as a function of u. Solid line, uncorrected; dashed line, ν_1 correction; dots, Ref. 12.

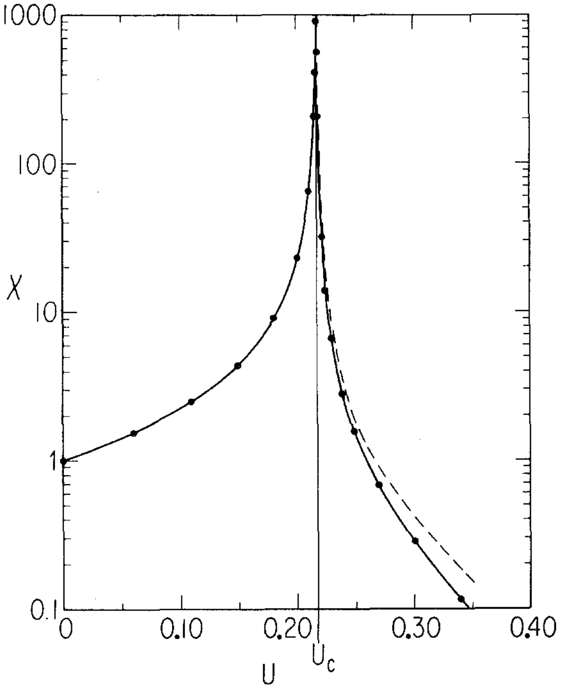

Fig. 5. The susceptibility χ as a function of u. For $u > u_c$: solid line, low-temperature correction; dashed line, ν_1 correction. Dots, Ref. 5.

approximant(12) for comparison. There is very little difference between these three approximants, except near the critical point, where the Padé approximant separates from the RSDRG results. This is due to the smaller critical amplitude in the Padé approximant. A direct comparison with series(8) shows a difference of less than 1% throughout the series' region of validity ($u \gtrsim 0.30$), for both RSDRG calculations.

The susceptibility χ is shown in Fig. 5, again with an approximant(5) for comparison. As before, there is very little difference between them, although attention must be drawn to the ν_1-corrected susceptibility. This approximant shows the correct qualitative behavior, but its amplitude is in general too large. Comparison with the series expansion of χ shows that the difference is at most 65% at $u \approx 0.42$, going to zero at $u = 1$. The low-temperature-corrected susceptibility has less than a 1% difference for $u \gtrsim 0.35$, while in the high-temperature regime, the difference is less than 1% for $u \lesssim 0.17$.

Figure 6 displays the structure factor $\tilde{C}(\mathbf{q})$ for several values of $\mathbf{q}$. Easily seen are the maxima which occur just above T_c. Their existence was

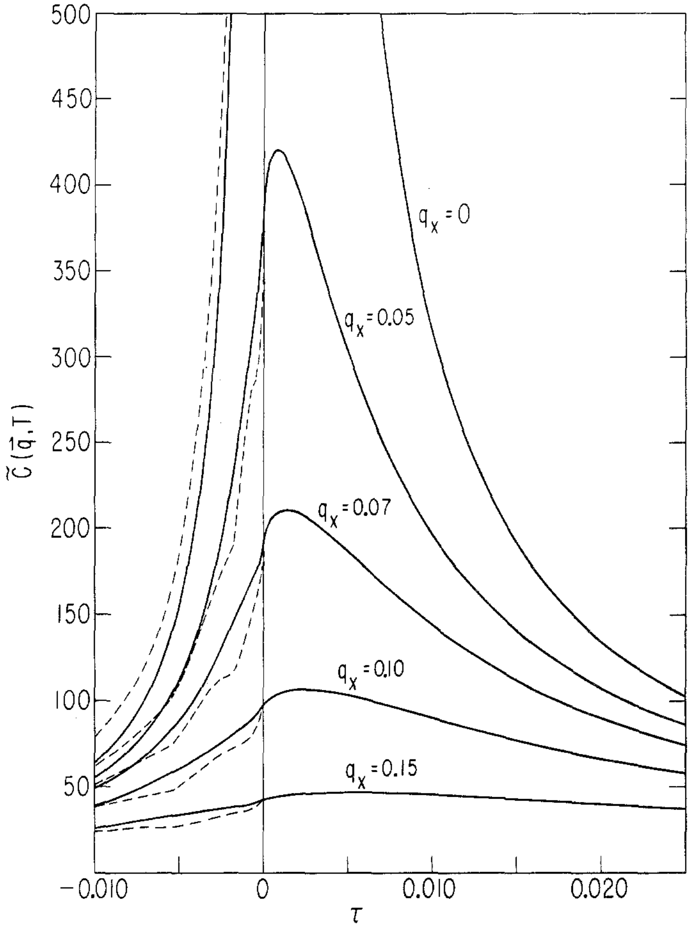

Fig. 6. The static structure factor $\tilde{C}(\mathbf{q})$ as a function of $\tau = 1 - T_c/T$. The curves are labeled by the values of $q_x = q_y = q_z$. For $\tau < 0$: solid line, low-temperature correction; dashed line, ν_1 correction.

previously predicted by Fisher and Burford,(5) and verified by neutron scattering experiments near the order–disorder transition of β-brass.(13) Just below T_c is a sharp fall-off in the scattering. The ν_1-corrected structure factor, while again showing the correct qualitative behavior, has several inflections near the critical point. These are due to the unsmooth transition to the condition (4.3), which occurs at $\tau \approx -0.15$, and the recursive nature of the calculation. These inflections are also the source of the larger uncertainties for the ν_1 correction in Table II. Both of the low-temperature approximants shown do not join perfectly smoothly to the high-temperature curve. This is because the parameter u_0 is also not smooth at T_c (see Fig. 2).

A detailed study of the structure factor near the critical point, for $q_x = 0.10$, is shown in Fig. 7. A scattering approximant from Ref. 5 is plotted along with the RSDRG result. Qualitatively, the two are very similar. Both have a maximum just above the critical point, and a rapid decay just below. However, the RSDRG structure factor has a smaller maximum value. This is related to the fact that the RSDRG susceptibility has a smaller amplitude and exponent than the series estimates on which the Ref. 5 approximant is based (see Tables I and II). The RSDRG maximum is also much farther from the critical point, occurring at $\tau_{\max} = 0.0024$, as compared to $\tau_{\max} = 0.0003$ for the maximum in Ref. 5 (the

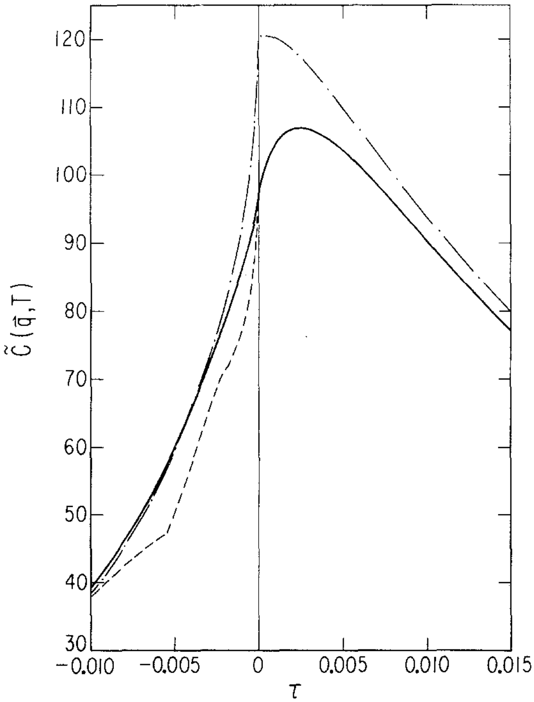

Fig. 7. The static structure factor $\tilde{C}(\mathbf{q})$ near the critical point, for $q_x = q_y = q_z = 0.10$. For $\tau < 0$: solid line, low-temperature correction; short dashed line, ν_1 correction. Dash-dotted line, Ref. 5.

latter is more in line with the experimental results(13)). In addition, the RSDRG structure factor's maximum value is about 9% larger than the critical point value, while the maximum in Ref. 5 is almost flat. Away from the critical point there is very little difference between the two.

There is one shortcoming of the structure factor's zeroth-order recursion relation (2.14) which should be mentioned. It is expected that the scattering near the critical point should be nearly isotropic.(5) The RSDRG approximant, however, is direction dependent for $q\xi \gg 1$. This can be associated with the very slow convergence[6] of the recursion relations for $\tilde{C}(\mathbf{q})$ in the [100] direction for T near T_c. This defect does not influence the results in the [111] direction which are in good agreement with the nearly isotropic series results.

6. CONCLUSION

We have seen that the approximants developed with the RSDRG formalism in general provide a good description of the equilibrium properties of the simple cubic Ising model. They display all of the essential qualitative features we expect, such as the critical divergence of the susceptibility, and the near-critical structure factor maxima. More importantly, the quantitative results, such as the critical exponents and amplitudes, are in close agreement with other evaluations. We can therefore be confident that these results give a reasonable description of the statics when used in a nonequilibrium context.

In this paper, we have presented two methods for performing low-temperature calculations with the susceptibility and structure factor recursion relations. The ν_1 correction provides approximants with the correct qualitative behavior, but with limited quantitative accuracy. However, it has the advantage of being readily extendable to more complex situations, such as time-dependent systems, since the correction is already determined in the manner described in Section 4. The low-temperature correction, while being considerably more accurate, is a somewhat more *ad hoc* procedure. It therefore may be difficult to generalize to other situations.

ACKNOWLEDGMENTS

This work was supported by a National Science Foundation Grant No. DMR 80-20609.

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[6] There are two special sets of wave numbers, of the form $\mathbf{q} = (2m\pi/(2^n - 1))\hat{x}$ and $[(2m+1)\pi/2^n]\hat{x}$ which give finite but irregular values of $\tilde{C}(\mathbf{q})$ at the critical point.

APPENDIX: LOW-TEMPERATURE CORRECTION TO THE STATIC STRUCTURE FACTOR RECURSION RELATION

With the low-temperature correction described in Section 4, the static structure factor's recursion relation (2.14) is modified in the following way:

$$\tilde{C}(\mathbf{q}) = 8\nu_1^2 f(\mathbf{q})\tilde{C}'(2\mathbf{q}) + I(\mathbf{q}, y) \tag{A1}$$

where

$$I(\mathbf{q}, y) = a_3(\mathbf{q})y^3 + a_5(\mathbf{q})y^5 + a_6(\mathbf{q})y^6 + a_{27}(\mathbf{q})y^{27} + a_{28}(\mathbf{q})y^{28} \tag{A2}$$

$$a_3(\mathbf{q}) = 4 \tag{A3a}$$

$$a_5(\mathbf{q}) = 24\left[1 + g_1(\mathbf{q})\right] \tag{A3b}$$

$$a_6(\mathbf{q}) = -8\left[4 + 3g_1(\mathbf{q}) + 4\left(\frac{u_c}{y_c}2^{1-y_T}\right)^3 f(\mathbf{q})\right] \tag{A3c}$$

$$a_{27}(\mathbf{q}) = y_c^{-27}\left[28b_0(\mathbf{q}) - b_1(\mathbf{q})y_c - 25a_3(\mathbf{q})y_c^3 - 23a_5(\mathbf{q})y_c^5 - 22a_6(\mathbf{q})y_c^6\right] \tag{A3d}$$

$$a_{28}(\mathbf{q}) = y_c^{-28}\left[-27b_0(\mathbf{q}) + b_1(\mathbf{q})y_c + 24a_3(\mathbf{q})y_c^3 + 22a_5(\mathbf{q})y_c^5 + 21a_6(\mathbf{q})y_c^6\right] \tag{A3e}$$

$$b_0(\mathbf{q}) = 1 + 3r_c g_1(\mathbf{q}) + 3s_c g_2(\mathbf{q}) + t_c g_3(\mathbf{q}) - 8\nu_{1,c}^2 f(\mathbf{q}) \tag{A3f}$$

$$b_1(\mathbf{q}) = 3\left(\frac{dr}{dy}\right)_c g_1(\mathbf{q}) + 3\left(\frac{ds}{dy}\right)_c g_2(\mathbf{q}) + \left(\frac{dt}{dy}\right)_c g_3(\mathbf{q}) - 8\left(\frac{d\nu_1^2}{dy}\right)_c f(\mathbf{q}) \tag{A3g}$$

$$r_c = 0.498319, \qquad s_c = 0.376342, \qquad t_c = 0.322390, \qquad \nu_{1,c}^2 = 0.493297 \tag{A3h}$$

$$\left(\frac{dr}{dy}\right)_c = -7.53479, \qquad \left(\frac{ds}{dy}\right)_c = -8.86747 \qquad \left(\frac{dt}{dy}\right)_c = -9.25491,$$

$$\left(\frac{d\nu_1^2}{dy}\right)_c = -7.30771$$

This recursion relation gives the correct low-temperature behavior to the structure factor through $O(y^6)$, and $I(q, y)$ matches the inhomogeneous term (4.4) through $O(y - y_c)$ at T_c. The order of the matching terms $a_{27}(\mathbf{q}), a_{28}(\mathbf{q})$ were chosen for maximum smoothness.

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