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Real-space dynamic renormalization group: Systematics for $T \geqslant T_c$

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In this paper we systematize the real-space dynamic-renormalization-group method we developed elsewhere. We treat the two-dimensional kinetic Ising model with relaxational dynamics defined on a square lattice. We show how one can set up a systematic perturbation-theory expansion which treats the coupling between cells of spins as a small parameter. The novel feature of the expansion is that it provides a method for determining the appropriate effective interaction between spins in a set of uncoupled cells. By obtaining a good zeroth-order approximation for a set of uncoupled cells, one finds that the effective interaction between cells is reduced. Similar ideas are also applied to the dynamics of the problem and we indicate how one can obtain a good zeroth-order approximation in terms of the dynamics of uncoupled cells. We couple these perturbation theory ideas to the real-space dynamic-renormalization-group method and carry out explicit calculations of a variety of observable quantities including the magnetic susceptibility, specific heat, static structure factor, time-dependent spin-autocorrelation function, and the dynamic structure factor. In every case we obtain excellent results in keeping with the scaling behavior near the phase transition and the high-temperature limit.

I. INTRODUCTION

The potential advantages of the real-space renormalization-group (RSRG) method have been recognized since its beginning.[1] Because one can work directly with the actual Hamiltonian of a system (rather than with an effective Hamiltonian as in the momentum-space technique) it can be used for the calculation of nonuniversal quantities in any temperature range. It is then possible to obtain phase diagrams[2] or thermodynamic quantities.[3] Furthermore, the RSRG formalism can be extended to dynamic phenomena[4,5] and as we have been able to show recently, to the evaluation of static and dynamic correlation functions[6] over a very wide range of wavelengths, frequencies, and temperatures.

There is, however, a formal aspect of the RSRG method which deserves further attention: except in one dimension, where the decimation transformation can be used and the problem solved exactly, the approximation methods needed in order to carry out RSRG method have not been very controlled. Typically, one divides the system into cells and applies block spin methods, treating the intercell couplings as small parameters. Bond-moving techniques are also used, sometimes in combination with the cell methods. Naturally the accuracy of such methods is open to question.

Let us consider, in particular, the correlation-function formalism introduced in Ref. 6. It was shown there, that in order to ensure the proper asymptotic exponential decay with distance of the static correlation functions, the recursion relations in the very high- and low-temperature limits must have certain specific forms. We found that these conditions were not satisfied by many of the standard approximation schemes, like the cumulant expansion. Those schemes cannot, then, lead to even qualitatively correct results for the correlation functions. While the required asymptotic forms for the recursion relations were satisfied by the transformation used in Ref. 6, the method used there was still plagued by the quantitative uncertainties which beset the RSRG procedure. In particular, the single-cell static and dynamic parameters K_0 and J_2 were determined in a somewhat ad hoc way by means of two adjustable parameters chosen in a rather arbitrary fashion. The procedure was clearly unsystematic and difficult to generalize. It was justified first because the assumption $K_0 \sim 2K$ (the cell coupling for a square lattice is just twice the bulk coupling) makes good physical sense, secondly because we preserved the correct asymptotic behavior of the resulting recursion relations and finally because of the impressive quantitative accuracy of the results obtained. There were additional consistency problems, as we shall discuss later, in satisfying the detailed balance condition at any given order and in the way the cell spin-flip characteristic time was determined. The latter problem can be shown to lead to erroneous results in the dynamic correlations at high temperatures.

In the present work, we wish to address ourselves to this problem of a systematic expansion. We shall develop a new expansion procedure, valid for both static and dynamic problems. Our expansion method is consistent, generalizable (it does, of course, correct the above-mentioned difficulties) and remarkably, it retains the advantages of the ad hoc procedure of the previous work: correct asymptotic behavior and good numerical results at first order. Indeed, the numerical results are even improved.

In the present paper we consider the $T \geqslant T_c$ temperature range. Below the transition the analysis is a bit more complicated because of the presence of symmetry-breaking effects. Those effects are very interesting in their own right and we shall discuss them separately in future work. We shall carry out our systematic calculations consistently to first order in an effective coupling between cells and we shall indicate how they can be extended.

This paper is divided into four sections. After this introduction we discuss the static properties in Sec. II, and the dynamics in Sec. III. The numerical results and conclusions are presented in Sec. IV.

II. STATIC CALCULATIONS

A. General considerations

To develop our systematic procedure we start out by considering the Ising Hamiltonian (multiplied by $-\beta$)

$$H[\sigma] = \tfrac{1}{2} K \sum_{\langle ij \rangle} \sigma_i \sigma_j \ , \tag{2.1}$$

where K is the coupling, the sum is restricted to nearest neighbors, and i and j are site indices. For the purposes of this work it is convenient to relabel the sites by dividing the lattice into cells. We shall use the same notation as in Ref. 6, assigning to each site a cell index i and a site within the cell index $a = 1, 2, 3, 4$. We also introduce primitive lattice vectors $\vec{\delta}_a$ in the original lattice and $\vec{\delta}'_a$ in the cell lattice. We can rewrite the Hamiltonian in the form

$$H[\sigma] = K_c V_0[\sigma] + K_I V_I[\sigma] \ , \tag{2.2}$$

where

$$V_0[\sigma] = \sum_{i,a} \sigma_{i,a} \sigma_{i,a+1} \ , \tag{2.3a}$$

$$V_I[\sigma] = \tfrac{1}{2} \sum_{i,a} \sigma_{i,a} (\sigma_{i+\delta'_a,a-1} + \sigma_{i+\delta'_{a-1},a+1}) \ . \tag{2.3b}$$

We shall call K_c the intracell coupling and K_I the intercell coupling. Of course, before we artificially divide the lattice into cells, we have $K_I = K_c = K$. Our goal will be to develop an expansion where we treat the "effective" coupling between cells as a small parameter. The identification of this effective coupling and the associated expansion requires a few rearrangements. Let us first recall that a straightforward cumulant expansion assumes that K_I is small and that uncoupled cells parametrized by the coupling $K_c = K_I$ represent a good zeroth-order approximation to the problem. A bit of reflection indicates that this does not make good physical sense. In the square lattice case the physics of the situation can be clearly seen: the spin at site i directly feels bonds of strength $4K$. When breaking up the system into cells, however, the same spin at lowest order, where we ignore couplings between cells, feels bonds of strength $2K_c^{(0)} \equiv 2K_0$. If $K_0 = K$, the error in the interaction felt at site i is large. We would in fact expect that a much better approximation for K_0 is that is should be close to $2K$.

The basic physics indicates that we should arrange our expansion such that the zeroth-order value of the cell coupling is different from the bulk value of the coupling. Thus we let

$$K_c \rightarrow K_c(\lambda) + \lambda[K_c - K_c(\lambda)] \ ,$$

where $K_c(\lambda)$ possesses a power-series expansion in the ordering parameter λ. In a similar fashion we expect that the coupling between cells should be modified due to these effects. In particular since some of the correlations between cells are taken into account through the choice of the effective cell coupling $K_0 \sim 2K$, we expect that the interaction between cells will be reduced over the bulk coupling. We can again write

$$K_I \rightarrow K_I(\lambda) + \lambda[K_I - K_I(\lambda)] \ .$$

Introducing these representations in the Hamiltonian we obtain

$$H[\sigma] = \{K_c(\lambda) + \lambda[K_c - K_c(\lambda)]\} V_0[\sigma] + \lambda \{K_I(\lambda) + \lambda[K_I - K_I(\lambda)]\} V_I[\sigma] \ , \tag{2.4}$$

and our perturbation expansion is developed in powers of λ. We assume that $K_c(\lambda)$ and $K_I(\lambda)$ possess expansions of the form

$$K_c(\lambda) = K_0 + \sum_{n=1}^{\infty} \lambda^n K_n^0 \ , \tag{2.5a}$$

$$K_I(\lambda) = K_R^0 + \sum_{n=1}^{\infty} \lambda^n K_n^R \ , \tag{2.5b}$$

and the parameters K_0, K_n^0, K_R^0, and K_n^R are to be determined through the imposition of constraints on an order by order basis.

The course that we shall pursue is to determine the coefficients in these expansions in such a way as to ensure rapid convergence of the series expansion in λ. To first order in λ we have

$$H = H_0[\sigma] + \lambda H_1[\sigma] \ , \tag{2.6}$$

$$H_0[\sigma] = K_0 V_0[\sigma] \ , \tag{2.7a}$$

$$H_1[\sigma] = \Delta K_1 V_0[\sigma] + K_R^0 V_I[\sigma] \ , \tag{2.7b}$$

$$\Delta K_1 \equiv K - K_0 + K_1^0 \ . \tag{2.7c}$$

The first-order expansion for $H[\sigma]$ leads to the result for the partition function Z to first order

$$Z = \sum_\sigma e^{H[\sigma]} = Z_0[1 + \lambda \Delta K_1 N r + O(\lambda^2)] \ , \tag{2.8}$$

where N is the total number of spins. Z_0 is the partition function for uncoupled cells

$$Z_0 = \sum_\sigma e^{H_0[\sigma]} = [4(3 + \cosh 4K_0)]^{N/4} \ , \tag{2.9}$$

r is the nearest-neighbor correlation function for a cell,

$$r = \langle \sigma_{i,a} \sigma_{i,a\pm1} \rangle_0 = \frac{u_0(1+u_0^2)}{1+u_0^4} \ , \tag{2.10}$$

where $u_0 = \tanh K_0$ and $\langle \ \rangle_0$ denotes the zeroth-order thermal average. Another useful quantity is the next-nearest-neighbor correlation function for a cell

$$s = \langle \sigma_{i,a} \sigma_{i,a\pm2} \rangle_0 = \frac{2u_0^2}{1+u_0^4} \ . \tag{2.11}$$

The equilibrium probability distribution can also be expanded to this order:

$$P[\sigma] = \frac{e^{H[\sigma]}}{Z} = P_0[\sigma]\{1 + \lambda \delta H_1[\sigma] + O(\lambda^2)\} \ , \tag{2.12}$$

where

$$P_0[\sigma] = e^{K_0 V_0[\sigma]}/Z_0 \ , \tag{2.13}$$

and

$$\delta H_1[\sigma] = \Delta K_1(V_0[\sigma] - \langle V_0[\sigma] \rangle_0) + K_R^0 V_I[\sigma] \ . \tag{2.14}$$

B. First-order static renormalization

The fundamental idea of the RSDRG is the introduction of a coarse graining transformation $T[\mu|\sigma]$ which maps the original set of spins, σ, onto a new set, μ, defined on the cell lattice. This mapping is then used to obtain coarse-grained variables. Thus the equilibrium probability distribution for the σ lattice $P[\sigma]$ is mapped onto the probability distribution $P[\mu]$ for the μ lattice via

$$P[\mu] = \sum_\sigma T[\mu|\sigma] P[\sigma] \ . \tag{2.15}$$

Similarly if $A[\sigma]$ is some variable defined on the σ lattice, then the corresponding variable defined on the μ lattice can be defined as

$$A[\mu] P[\mu] = \sum_\sigma P[\sigma] T[\mu|\sigma] A[\sigma] \ . \tag{2.16}$$

The proper normalization of $P[\mu]$ requires that the mapping function $T[\mu|\sigma]$ satisfied the constraint

$$\sum_\mu T[\mu|\sigma] = 1 \ . \tag{2.17}$$

It is rather natural when thinking about the coarse graining procedure to introduce a projection operator which picks out of a σ-dependent quantity the component "along" the block spin degrees of freedom

$$\mathcal{P} A[\sigma] \equiv \sum_\mu T[\mu|\sigma] \sum_{\bar\mu} \tilde G^{-1}[\mu|\bar\mu] \times \sum_{\bar\sigma} P[\bar\sigma] T[\bar\mu|\bar\sigma] A[\bar\sigma] \ , \tag{2.18}$$

where

$$\tilde G[\mu|\mu'] \equiv \sum_\sigma P[\sigma] T[\mu|\sigma] T[\mu'|\sigma] \ , \tag{2.19}$$

$$\sum_{\bar\mu} \tilde G[\mu|\bar\mu] \tilde G^{-1}[\bar\mu|\mu'] = \delta_{\mu,\mu'} \ , \tag{2.20}$$

$$\delta_{\mu,\mu'} = \prod_{i=1}^{N'} \delta_{\mu_i,\mu_i'} \ , \tag{2.21}$$

and N' is the total number of cells. It is easy to see that $\mathcal{P}$ really is a projection operator

$$\mathcal{P}^2 A[\sigma] = \mathcal{P} A[\sigma] \tag{2.22}$$

through the use of Eq. (2.20). The appearance of the $\tilde G^{-1}$ matrix in the definition of $\mathcal{P}$ complicates matters significantly. We have found that the analysis is simplified and the physical interpretation of the coarse graining as a simple block spin transformation is maintained if we require that the constraint

$$\tilde G[\mu|\mu'] = \langle T[\mu|\sigma] T[\mu'|\sigma] \rangle = \delta_{\mu,\mu'} P[\mu] \tag{2.23}$$

be satisfied. We have then that

$$P[\mu] \tilde G^{-1}[\mu|\mu'] = \delta_{\mu,\mu'} \tag{2.24}$$

and the projection operator becomes

$$\mathcal{P} A[\sigma] = \sum_\mu T[\mu|\sigma] P^{-1}[\mu] \sum_{\bar\sigma} P[\bar\sigma] T[\mu|\bar\sigma] A[\bar\sigma] \ , \tag{2.25}$$

which agrees with our definition in Ref. 6.

If we work to zeroth order in λ and wish to satisfy Eqs. (2.17) and (2.23) then we see that T is given by a product of contributions from uncoupled cells

$$T_0[\mu|\sigma] = \prod_i T^i[\mu|\sigma] \ , \tag{2.26}$$

where T^i is given by

$$T^i[\mu|\sigma] = \tfrac{1}{2}(1 + \mu_i \psi(\sigma_i)] \ , \tag{2.27a}$$

where $\psi(\sigma_i)$ is a function of the four spins in cell i, subject to the restrictions

$$\langle \psi(\sigma) \rangle_0 = 0 \ , \tag{2.27b}$$

$$\langle [\psi(\sigma)]^2 \rangle_0 = 1 \ . \tag{2.27c}$$

Symmetry considerations imply that

$$\psi(\sigma_i) = N_1(\sigma_i^s + f\,\sigma_i^T) \ , \tag{2.28a}$$

$$\sigma_i^s = \sum_a \sigma_{i,a} \ , \tag{2.28b}$$

$$\sigma_i^T = \sum_a \sigma_{i,a}\sigma_{i,a-1}\sigma_{i,a+1} \ . \tag{2.28c}$$

The normalization N_1 is determined by Eq. (2.23) [or Eq. (2.27c)].

Some discussion of the role of the parameter f was given in our previous work. Ultimately we will choose f by noting that certain functions of the spin variables are less susceptible to change under perturbations due to thermal fluctuations than all others. It is sensible to map the block spin variables onto these "slowly" varying degrees of freedom. The quantification of these ideas is easiest carried out in the context of our dynamic considerations. It is worth noting that the identification of the slow degrees of freedom with the solution of an eigenvalue equation for the spin-flip operator $\tilde{D}_\sigma$ can also be thought of as purely statistical statement associated with a Monte Carlo sampling procedure. We will show later, in Sec. III, that our discussion of dynamics leads naturally to the choice $f = 0$. Let us say here that the choice $f = 0$ seems reasonable from two qualitative considerations. First, the choice $f = 0$ indicates that the slow mode in a cell is just the order parameter for that cell. Since the order parameter is the slow degree of freedom of the system this makes sense. Secondly, if we choose $f \neq 0$ we find that at first order in λ that the coarse grained variable associated with the spin $\sigma_{i,a}$ is proportional to $\mu_i + C\mu_i^T$ where μ_i^T is the symmetric sum of three spins similar to σ_i^T given by Eq. (2.28c). At this level we see that the physical interpretation of μ_i as a block spin is blurred by the appearance of the triplet term μ_i^T. It is not difficult to show that the coefficient C is proportional to f and the choice $f = 0$ eliminates the triplet term from the mapping $\sigma_{i,a} \to \mu_i$ and leads to a clear separation of the slow and fast modes in the system. We will return to this point later.

Once $f = 0$ we can determine the normalization N_1 from Eq. (2.28c) giving

$$N_1^2 = [4(1 + 2r + s)]^{-1} \ . \tag{2.29}$$

Thus far we have been discussing the zeroth-order value of the mapping function $T_0[\mu|\sigma]$. It is to be expected that one should have higher-order corrections to T and we have discussed the determination of these higher-order contributions elsewhere.[4,6] Here we are primarily interested in a first-order calculation, hence we consider only $T_1[\mu|\sigma]$, the contribution to $T[\mu|\sigma]$ that is of first order in λ. We construct T_1 in a two-step process. The first step is to construct the quantity $\bar{T}[\mu|\sigma]$ as the solution to the eigenvalue problem discussed in Sec. III. We can write

$$\bar{T}[\mu|\sigma] = T_0[\mu|\sigma] + \lambda \bar{T}_1[\mu|\sigma] + O(\lambda^2) \ . \tag{2.30}$$

For our purposes in this section the main property of $\bar{T}_1$ is that it is orthogonal to T_0 to zeroth order

$$\langle \bar{T}_1[\mu|\sigma] T_0[\mu'|\sigma] \rangle_0 = 0 \ . \tag{2.31}$$

The second step in the determination of T is to rotate $\bar{T}[\mu|\sigma]$ in μ space such that the constraint Eq. (2.23) is satisfied. That is we perform a rotation to diagonalize the quantity.

$$\langle \bar{T}[\mu|\sigma] \bar{T}[\mu'|\sigma \rangle \equiv \bar{G}[\mu|\mu'] \ . \tag{2.32}$$

To first order one finds easily that, because of Eq. (2.31), $\bar{T}_1$ in fact drops out of the calculation of $\bar{G}[\mu|\mu']$. The first-order correction comes, then, only from the first-order Hamiltonian Eq. (2.14). We find after straightforward algebra

$$\bar{G}[\mu|\mu'] = \delta_{\mu,\mu'} \bar{P}[\mu] + \lambda \bar{\Delta}[\mu|\mu'] + O(\lambda^2) \ , \tag{2.33}$$

where

$$\bar{P}[\mu] = P_0[\mu]\{1 + \lambda 2\nu_1^2 K_R^0 H_1[\mu] + O(\lambda^2)\} \ , \tag{2.34a}$$

$$P_0[\mu] = 1/2^{N/4} \ , \tag{2.34b}$$

$$\nu_1 = \langle \sigma_{i,a} \psi(\sigma_i) \rangle_0 = \tfrac{1}{2}(1 + 2r + s)^{1/2} \ , \tag{2.34c}$$

and

$$H_1[\mu] = \tfrac{1}{2} \sum_{i,a} \mu_i \mu_{i+\delta_a'} \ , \tag{2.35}$$

$$\bar{\Delta}[\mu|\mu'] = P_0[\mu] \sum_i \Lambda^{[i]}_{\mu,\mu'} \mu_i \mu_i' \Delta K_i \left[\frac{1 + 4r + s}{1 + 2r + s} - 2r \right] \ , \tag{2.36}$$

$$\Lambda^{[i]}_{\mu,\mu'} = \prod_{k(\neq i)} \delta_{\mu_k, \mu_k'} \ . \tag{2.37}$$

We see that $\bar{G}[\mu|\mu']$ is not diagonal so we must obtain $T[\mu|\sigma]$ from $\bar{T}[\mu|\sigma]$ via a rotation S

$$T[\mu|\sigma]=S[\mu|\bar{\mu}]\bar{T}[\bar{\mu}|\sigma] \quad , \tag{2.38}$$

preserving the condition Eq. (2.23). In Eq. (2.38) a sum over barred configurations is implied. The calculation is quite straightforward. We assume S to be symmetric and find that $\tilde{G}$ differs from $\bar{G}$ only by the absence of the off-diagonal term in Eq. (2.33). One then has

$$P[\mu]=\bar{P}[\mu][1+O(\lambda^2)] \quad , \tag{2.39}$$

which implies, together with Eq. (2.34a), that the new coupling characterizing the μ probability distribution is given by

$$K'=2\nu_1^2 K_R^0 \quad . \tag{2.40}$$

The first-order contribution to $T_1[\mu|\sigma]$ due to the rotation can then easily be obtained.

C. Zeroth-order collective variables and recursion relations

We can now derive the recursion relations for the static correlation functions. With the probability distribution $P[\mu]$ taken at first order, we need to consider the coarse-grained variables at zeroth order only. From Eq. (2.15) we easily find, for $T=T_0$, the coarse-grained variables corresponding to $\sigma_{i,a}$, $\sigma_{i,a}\sigma_{j,a'}(i\neq j)$, and $\sigma_{i,a}\sigma_{i,a'}$. These we call, respectively, $M_{i,a}[\mu]$, $\Pi^{l}_{i,a;ja'}[\mu]$, and $\Pi^{c}_{i,aa'}[\mu]$ and are given by

$$M_{i,a}[\mu]=\nu_1\mu_i+O(\lambda) \quad , \tag{2.41}$$

$$\Pi^{l}_{i,a;j,a'}[\mu]=\nu_1^2\mu_i\mu_j+O(\lambda) \quad , \tag{2.42}$$

$$\Pi^{c}_{i,aa'}[\mu]=\delta_{a,a'}+r(\delta_{a',a+1}+\delta_{a',a-1})+s\delta_{a',a+2}+O(\lambda). \tag{2.43}$$

Using the projection operator procedure developed in Ref. 6 we can work out the recursion relation for the static correlation functions for

$$\tilde{C}_{i,a;j,a'}=\langle\delta\sigma_{i,a}\delta\sigma_{j,a'}\rangle \quad , \tag{2.44}$$

with

$$\delta\sigma_{i,a}=\sigma_{i,a}-\langle\sigma_{i,a}\rangle \quad ,$$

we obtain [using Eq. (4.26) in Ref. 6]

$$\tilde{C}_{i,a;j,a'}=\nu_1^2\tilde{C}'_{ij}+\delta_{ij}[\delta_{a,a'}+r(\delta_{a',a+1}+\delta_{a',a-1}) +s\delta_{a',a+2}-\nu_1^2] \quad , \tag{2.45}$$

where a prime signifies the quantity defined in terms of the coarse-grained μ variables.

For the magnetic susceptibility we find in this case, making use of Eq. (2.34c) the extremely simple result

$$\chi=4\nu_1^2\chi' \quad . \tag{2.46}$$

The Fourier transform of Eq. (2.45) yields the recursion relation for the q-dependent structure factor

$$\tilde{C}(q)=1+2rg_1(q)+sg_2(q) -\nu_1^2 f(q)+\nu_1^2 f(q)\tilde{C}'(2q) \quad , \tag{2.47}$$

where the f and g functions are essentially cell structure factors

$$f(q)=1+\cos q_x+\cos q_y+\cos q_x\cos q_y \quad , \tag{2.48a}$$

$$g_1(q)=\tfrac{1}{2}(\cos q_x+\cos q_y) \quad , \tag{2.48b}$$

and

$$g_2(q)=\cos q_x\cos q_y \quad . \tag{2.48c}$$

All wave vectors are measured in terms of the inverse lattice constant which is taken to be unity [notice the rescaling in the last term of Eq. (2.47)]. At $q\to 0$ Eq. (2.47) reduces to Eq. (2.46). Notice that in the limit $q\to 0$ the "inhomogeneous" term in Eq. (2.47) vanishes. Note that in the case $f\neq 0$ then $4\nu_1^2-1-2r-s\neq 0$ and there is an inhomogeneous contribution to the recursion relation for the susceptibility. This has the consequence that only for $f=0$ do we map all of the slow mode onto a $q=0$ mode.

It is also of interest to write down the recursion relations for the short-range correlation functions of the form

$$\epsilon(m,n)=\frac{1}{N}\sum_i\langle\sigma_i\sigma_{i+m\hat{x}+n\hat{y}}\rangle \quad . \tag{2.49}$$

We find for the first few such quantities

$$\epsilon(1,0)=\tfrac{1}{2}r+\tfrac{1}{2}\nu_1^2\epsilon'(1,0) \quad , \tag{2.50}$$

$$\epsilon(2,0)=\nu_1^2\epsilon'(1,0) \quad , \tag{2.51}$$

$$\epsilon(1,1)=\tfrac{1}{4}[s+2\epsilon'(1,0)+\epsilon'(1,1)] \quad . \tag{2.52}$$

General formulas depend on whether m and n are even or odd and we will not write them down here.

Finally we can write down a recursion relation for the specific heat

$$C_v=K^2k_BC \quad , \tag{2.53}$$

where

$$C=\frac{1}{N}\langle[\delta E(\sigma)]^2\rangle \quad , \tag{2.54}$$

where

$$E(\sigma)=H[\sigma]/K \ , \tag{2.55}$$

and $H[\sigma]$ is given by Eq. (2.1). The lowest order recursion for C is given by

$$C=2+3(s-r^2)+8\nu_1[\nu_1+2N_1(s+r)-2\nu_1 r]\epsilon'(1,0)$$
$$+\nu_1^2(s-1)\epsilon'(2,0)+\nu_1^4(C'-2) \ . \tag{2.56}$$

D. Determination of the parameters

It is not possible to proceed any further without specifying the required parameters in the expansions of K_c and K_l, Eqs. (2.5).

It follows from Eqs. (2.28) and (2.24) that, to first order, we need to specify only two quantities K_0 and K_R^0. Because of Eq. (2.40), specifying K_R^0 is equivalent to specifying $K'(K)$, once K_0 is known as a function of K. Obviously, to higher order more parameters are needed, but these can be specified by generalization of the procedure developed here.

We are guided by two important physical principles. One is that the following two conditions must be satisifed in order to ensure[6] that $\tilde{C}_{ij}$ decays to zero exponentially at large distances

$$K'\propto K^2 \quad (K<<1) \ , \tag{2.57a}$$

$$K'=2K \quad (K>>1) \ . \tag{2.57b}$$

The second physical point is that dividing the system into cells, cutting bonds, etc., will lead, in principle, to very large errors in the determination of the short-range correlations. Once $K'(K)$ has been obtained in a satisfactory way, the remaining parameters (K_0 to this order) must be obtained from short-range considerations.

Consider first $K'(K)$. The simplest relation between K' and K, not involving cell parameters through ν,r,s, which we can obtain from our recursion relations is

$$\frac{\epsilon(4,0)}{\epsilon(2,0)}=\frac{\epsilon'(2,0)}{\epsilon'(1,0)} \ . \tag{2.58}$$

The exact solution to this equation satisfies the conditions Eq. (2.57) as may be seen from the series expansion of $\epsilon(m,n)$. We showed in Ref. 6 that an approximate solution $K'(K)$ which is a good approximation to Eq. (2.58) and very convenient to use is given by the relation:

$$\phi'=\phi^2 \ , \tag{2.59}$$

where $\phi=e^{2K}\tanh K$. The function $K'(K)$ obtained from Eq. (2.59) leads to very nearly the same numerical results as the more laborious series method solution of Eq. (2.58). This point is further discussed in Ref. 6. More importantly we know that the recursion relation given by Eq. (2.59) gives the exact value of the transition temperature and the proper flows to the high- and low-temperature limits under iteration. It is completely consistent and certainly a simplification to simply assume that $K'=K'(K)$ is given by Eq. (2.59). This corresponds to a specific choice for the zeroth-order form of K_R^0 via Eq. (2.40): $K_R^0=K'(K)/2\nu_1^2$.

Given $K'=K'(K)$ we can determine the cell parameter K_0 from the short-range behavior of the system. The shortest range recursion relation available is Eq. (2.50). In terms of $\epsilon(0,1)$ and $\epsilon'(0,1)$ Eq. (2.50) yields the result for K_0

$$a_0\equiv\tanh 2K_0=(-2-\epsilon'(1,0)+\{[2+\epsilon'(1,0)]^2-16\epsilon(1,0)[\epsilon'(1,0)-8\epsilon(1,0)]\}^{1/2})/8\epsilon(1,0) \tag{2.60}$$

from which one can obtain $K_0(K)$ provided that $\epsilon(0,1)$ is known as a function of K [and likewise $\epsilon'(0,1)$ as a function of K']. In the present case $\epsilon(0,1)$ is known exactly,[7] but this is not very important: the solution to Eq. (2.44) with the exact expression for $\epsilon(0,1)$ shows that K_0 is a very smooth function of K. We plot in Fig. 1 K_0-2K vs $\tanh K$. We see that this quantity is small over the entire temperature scale. This result could have been deduced from high- and low-temperature–series-expansion results had exact results not been available.

With all parameters determined, the various static correlation functions can be evaluated. We postpone the discussion of the numerical results thus obtained to Sec. IV. We point out here that, when more expansion parameters are needed (for higher-order calculations), they can simply be determined as functions of K, like K_0, by use of Eqs. (2.51), (2.52), etc. It seems likely that it is not necessary to use the exact expressions for $\epsilon(m,n)$ as a knowledge the asymptotic high- and low-temperature behavior may suffice.[4] We now move on to the more complicated and interesting problem of the dynamics.

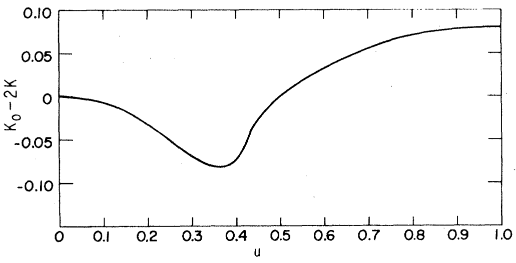

FIG. 1. K_0-2K vs $u=\tanh K$.

III. DYNAMIC CALCULATIONS

A. General considerations

We now turn our attention to the dynamics. We wish to show how the ideas elaborated in the previous section can be used just as well for the dynamics. In particular, we will show how the cell parameters in the dynamical operator can be determined.

As is well known,[4] the dynamics of the kinetic Ising model are given by a stochastic spin-flip operator (SFO) which can be written in the form

$$\tilde{D}[\sigma|\sigma'] = -\frac{\alpha}{2}\sum_i \Lambda^{[i]}_{\sigma,\sigma'}\sigma_i\sigma'_i\, e^{-\sigma_i E_i[\sigma]}V_i[\sigma] , \quad (3.1)$$

where α is the characteristic spin-flip rate and

$$E_i[\sigma] = K\sum_a \sigma_{i+\delta_a} , \quad (3.2)$$

where the sum is over the nearest neighbors of i. The function $V_i[\sigma]$ depends on the neighbors of σ_i, but not on σ_i itself. Expanding the exponential, we can write[6]

$$\begin{aligned} W_i[\sigma] &= V_i[\sigma]e^{-\sigma_i E_i[\sigma]} \\ &= 1 + A_1\sigma_i\sigma_i^s + A_2\sigma_i^n \\ &\quad + \bar{A}_2\sigma_i^{nn} + A_3\sigma_i\sigma_i^T + A_4\sigma_i^c , \end{aligned} \quad (3.3)$$

where

$$\begin{aligned} &\sigma_i^n = \sum_a \sigma_{i+\delta_a}\sigma_{i+\delta_{a+1}},\quad \sigma_i^s = \sum_a \sigma_{i+\delta_a} , \\ &\sigma_i^{nn} = \sum_a \sigma_{i+\delta_a}\sigma_{i+\delta_{a+2}},\quad \sigma_i^T = \sigma_i^c\sigma_i^s , \\ &\sigma_i^c = \prod_a \sigma_{i+\delta_a} , \end{aligned} \quad (3.4)$$

and the A_i parameters are constrained by the stationarity condition that requires that $W_i[\sigma]P[\sigma]$ be independent of σ_i. Upon iteration of $\tilde{D}[\sigma|\sigma']$ under the action of the RG, it is found, to first order, that $\bar{A}_2$, A_3, and A_4 vanish after one iteration. Hence, these must be higher-order quantities. This result is in fact obvious since these parameters couple third-nearest neighbors. The SFO determined by

$$\tilde{D}[\sigma|\sigma'] = -\frac{\alpha}{2}\sum_i \Lambda^{[i]}_{\sigma,\sigma'}W_i[\sigma]\sigma_i\sigma'_i , \quad (3.5)$$

$$W_i[\sigma] = 1 + A_1\sigma_i\sigma_i^s + A_2\sigma_i^n , \quad (3.6)$$

is the so-called "minimal-coupling operator." We have from stationarity

$$A_1 = -\tfrac{1}{2}\tanh 2K , \quad A_2 = A_1^2 , \quad (3.7)$$

and it is the operator that we shall use throughout the present work.

B. Cell decomposition of the SFO operator

Our goal in this section is to decompose the minimal coupling operator in a way consistent with the decomposition of the Hamiltonian given by Eq. (2.2), and the expansions of K_c and K_l. Once we have, to a certain order in λ, K_c and K_l, we must expand $\tilde{D}[\sigma|\sigma]$, (or $W_i[\sigma]$) in a consistent way, so that the detailed balance and stationarity conditions

$$D[\sigma|\sigma']P[\sigma'] = D[\sigma'|\sigma]P[\sigma] , \quad (3.8a)$$

$$D[\sigma|\bar{\sigma}]P[\bar{\sigma}] = 0 , \quad (3.8b)$$

hold at any order.

Again using the cell-site labeling, we have in general

$$\begin{aligned} W_{i,a}[\sigma] = 1 &+ \sigma_{i,a}[B_1(\sigma_{i,a+1}+\sigma_{i,a-1}) + B_2(\sigma_{i+\delta'_a,a-1} + \sigma_{i+\sigma'_{a-1},a+1})] \\ &+ B_3\sigma_{i,a+1}\sigma_{i,a-1} + B_4(\sigma_{i,a+1}\sigma_{i+\delta'_a,a-1} + \sigma_{i,a-1}\sigma_{i+\delta'_{a-1},a+1}) + B_5\sigma_{i+\delta'_a,a-1}\sigma_{i+\delta'_{a-1},a+1} , \end{aligned} \quad (3.9)$$

where we have decomposed σ_i^s and σ_i^n into intracell and intercell pieces. At $K_c = K_l = K$ we require

$$B_1 = B_2 = A_1,\quad B_3 = B_4 = B_5 = A_2 \quad (3.10)$$

[see Eq. (3.7)]. Upon decomposing $E_i[\sigma]$ in the way indicated by Eq. (2.3) and imposing the stationarity condition, a system of equations relating the B_i's to K_c and K_l is found. Taking into account the limit Eq. (3.10) the system has a solution which is, with $a_c \equiv \tanh 2K_c$ and $a_l \equiv \tanh 2K_l$

$$B_1 = \frac{a_c}{2(a_c+a_l)}[a_l a_c(a_l - a_c) - (a_c + a_l)] , \quad (3.11a)$$

$$B_2 = \frac{a_l}{2(a_c+a_l)}[a_l a_c(a_c - a_l) - (a_c + a_l)] , \quad (3.11b)$$

$$B_3 = \frac{a_l a_c^3}{(a_l+a_c)^2} , \quad (3.11c)$$

$$B_4 = \frac{1}{2}\frac{a_l a_c(a_l^2 + a_c^2)}{(a_l+a_c)^2} , \quad (3.11d)$$

$$B_5 = \frac{a_c a_l^3}{(a_l+a_c)^2} . \quad (3.11e)$$

We see that only B_1 contributes at zeroth order, that is, only B_1 appears in the expression for $W_i^0[\sigma]$. This is in contrast with the assumption made in Ref. 6, where both B_1 and B_3 were included at zeroth order. That assumption leads to inconsistencies. It is the requirement that $B_{3'}^0=0$ that determines that $f=0$ in Eq. (2.28a). We see that B_2, B_3, and B_4 must be included at first order, but B_5 starts at third order.

C. Dynamic renormalizaton to first order

In addition to Eqs. (2.17) and (2.23) the coarse-graining transformation, $T[\mu|\sigma]$ must also satisfy the eigenvalue equation[4,6]

$$\tilde{D}_\sigma T[\mu|\sigma]=D_\mu T[\mu|\sigma] \ . \tag{3.12}$$

To zeroth order, Eq. (3.12) is satisfied by the transformation given by Eqs. (2.26) and (2.27) provided that $\Psi(\sigma_i)$ is taken to be an eigenfunction to the zeroth-order SFO.

To construct $\tilde{D}_0$ from $\tilde{D}$, we need, first of all, to expand α in the same way as K_c, K_I are expanded in Eq. (2.4)

$$\alpha=\alpha_0(\lambda)+\lambda[\alpha-\alpha_0(\lambda)] \ . \tag{3.13}$$

It is important to realize that, while one can expand α as in Eq. (3.13) it is incorrect [and it leads to a breakdown of the condition Eq. (3.8)] to choose a different α for the cell and intercell parts of $\tilde{D}_\sigma$. Again, the ad hoc procedure of Ref. 6 does not take this into account.

Using the result from Eq. (3.11a), $B_1^0=-\frac{1}{2}a_0$ ($a_0\equiv\tanh 2K_0$), we can write the zeroth-order operator

$$\tilde{D}^0[\sigma|\sigma']=-\frac{\alpha_0}{2}\sum_{i,a}\Lambda_{\sigma,\sigma'}^{[i,a]}\sigma_{i,a}\sigma'_{i,a}W_{i,a}^0[\sigma] \ , \tag{3.14}$$

$$W_{i,a}^0[\sigma]=1-\frac{a_0}{2}\sigma_{i,a}(\sigma_{i,a+1}+\sigma_{i,a-1}) \ . \tag{3.15}$$

The eigenfunctions and eigenvalues of $\tilde{D}^0[\sigma|\sigma']$ are easily worked out. The complete set of eigenfunctions and the associated eigenvalues are given in Table I. One finds that the smallest eigenvalue corresponding to an odd eigenfunction is $\lambda^{(1)}=\alpha_0(1-a_0)$. The corresponding eigenfunction is

$$\psi_i^{(1)}(\sigma)=N_1\sigma_i^s \ , \tag{3.16}$$

with N_1 being the normalization factor, which is precisely the function we chose for our static transformation for the reasons discussed in Sec. II B. It is not surprising that the same transformation is obtained from either static or dynamic arguments. $\tilde{D}_\sigma$ basically is a measure of the propensity of a σ configuration to be changed by simple spin flips driven by thermal flucuations. Indeed, $\tilde{D}_\sigma$ generates the *static* correlation structure for this problem through the set of identities given by

$$\langle\tilde{D}_\sigma F[\sigma]\rangle=0 \tag{3.17}$$

for arbitrary $F[\sigma]$.

To zeroth order, we thus find that the SFO for the coarse-grained system is given by

$$\tilde{D}^0[\mu|\mu']=-\frac{\lambda^{(1)}}{2}\sum_i\Lambda_{\mu,\mu'}^{[i]}\mu_i\mu'_i \ . \tag{3.18}$$

Proceeding to first order we find first the operator $\bar{D}_\mu^{(1)}$ which satisfies Eq. (3.17) with $T\rightarrow\bar{T}$ [see Eq. (2.30)] and then we can obtain D_μ by the rotation indicated in Eq. (2.38). The first contribution to $\bar{D}_\mu^{(1)}$ comes from the first-order term in the expansion of α and a_0 which is clearly of the same form as the zeroth-order contribution and which when added to it merely leads to the replacement $\alpha_0\rightarrow\alpha_0+\lambda\times(\Delta\alpha_1-\Delta a_0^{(1)})$ [$\Delta\alpha_1$ and $\Delta a_0^{(1)}$ are defined as in Eq. (2.7c)]. The second contribution to first order comes from the expansion of $W_{i,a}$ that is

$$\bar{D}^{(1)}[\mu|\mu']P_0[\mu']=\langle T_0[\mu|\sigma]\tilde{D}^{(1)}[\sigma|\bar{\sigma}]T_0[\mu'|\bar{\sigma}]\rangle_0 \ , \tag{3.19}$$

where

$$\tilde{D}^{(1)}[\sigma|\sigma']=-\frac{\alpha}{2}\sum_{i,a}W_{i,a}^{(1)}[\sigma]\Lambda_{\sigma,\sigma'}^{[i,a]}\sigma_{i,a}\sigma'_{i,a} \ , \tag{3.20}$$

where α is needed only to zeroth order and

$$\begin{aligned}W_{i,a}^{(1)}[\sigma]=&B_1^{(1)}\sigma_{i,a}(\sigma_{i,a+1}+\sigma_{i,a-1})+B_2^{(1)}\sigma_{i,a}(\sigma_{i+\delta'_a,a-1}+\sigma_{i+\delta'_{a-1},a+1})+B_3^{(1)}\sigma_{i,a}\sigma_{i,a-1}\\&+B_4^{(1)}(\sigma_{i,a+1}\sigma_{i+\delta'_a,a-1}+\sigma_{i,a-1}\sigma_{i+\delta'_{a-1},a+1}) \ ,\end{aligned} \tag{3.21}$$

TABLE I. We list the solutions to the eigenvalue equation $\tilde{D}_{\sigma}^{0}\psi_i^{(n)}=-\lambda^{(n)}\psi_i^{(n)}$. The Φ's are defined as $\Phi_1(Q)=\sum_a e^{iQa}\sigma_a$, $\Phi_2^{n}(Q)=\sum_a e^{iQa}\sigma_a\sigma_{a+1}$, $\Phi_2^{nn}(Q)=\sum_a e^{iQa}\sigma_a\sigma_{a+2}$, $\Phi_3(Q)=\sum_a e^{iQa}\sigma_{a-1}\sigma_a\sigma_{a+1}$, $\sigma_c=\prod a\ \sigma_a$ with the short-hand notation $\sigma_{l,a}=\sigma_a$.

n	$\lambda^{(n)}/\alpha_0$	$\psi^{(n)}$	N_n
1	0	1	
2	$1-a_0$	$N_2\Phi_1(0)$	$\frac{1}{2(1+u_0)}\left(\frac{1+u_0^4}{1+u_0^2}\right)^{1/2}$
3	1	$N_3\Phi_1(\pi/2)$	$\frac{1}{2}\frac{(1+u_0^4)^{1/2}}{1-u_0^2}$
4	1	$N_3\Phi_1(3\pi/2)$	
5	$1+a_0$	$N_5\Phi_1(\pi)$	$\frac{1}{2(1-u_0)}\left(\frac{1+u_0^4}{1+u_0^2}\right)^{1/2}$
6	$2(1-a_0/\sqrt{2})$	$N_6\left(\Phi_2^n-4r+\frac{1}{\sqrt{2}}(\Phi_2^{nn}-4s)\right]$	$\frac{1}{2\sqrt{2}}\frac{(1+u_0^2-\sqrt{2}u_0)}{(1-u_0^2)}$
7	2	$N_7\Phi_2^n(\pi/2)$	$\frac{(1+u_0^4)^{1/2}}{2(1-u_0^2)}$
8	2	$N_7\Phi_2^n(3\pi/2)$	
9	2	$N_7\Phi_2^n(\pi)$	
10	2	$N_7\Phi_2^{nn}(\pi)/\sqrt{2}$	
11	$2(1+a_0/\sqrt{2})$	$N_{11}\left(\Phi_2^n-4r-\frac{1}{\sqrt{2}}(\Phi_2^{nn}-4s)\right]$	$\frac{1}{2\sqrt{2}}\frac{(1+u_0^2+\sqrt{2}u_0)}{(1-u_0^2)}$
12	$(3-a_0)$	$N_{12}[-a_0\Phi_1(0)+\Phi_3(0)]$	$\frac{1}{2}\frac{[(1+u_0^4)(1+u_0^2)]^{1/2}}{(1+u_0)(1-u_0^2)}$
13	3	$N_3\Phi_3(\pi/2)$	
14	3	$N_3\Phi_3(3\pi/2)$	
15	$3+a_0$	$N_{12}\left(\frac{1+u_0}{1-u_0}\right]\left[a_0\Phi_1(\pi)+\Phi_3(\pi)\right]$	
16	4	$N_{16}\left(r\Phi_2^n(0),\ -\frac{s}{2}\Phi_2^{nn}(0)-s-\sigma_c\right]$	$\frac{u_0(1+u_0^2)}{(1-u_0^2)^2}$

and we find from Eq. (3.11)

$$B_1^{(1)}=-\tfrac{1}{2}a_0^2a_l\ , \tag{3.22a}$$

$$B_2^{(1)}=-\tfrac{1}{2}a_l\ , \tag{3.22b}$$

$$B_3^{(1)}=a_la_0\ , \tag{3.22c}$$

$$B_4^{(1)}=\tfrac{1}{2}a_la_0\ . \tag{3.22d}$$

The averages indicated in Eq. (3.20) are carried out straightforwardly, and the following result is obtained:

$$\bar{D}^{(1)}[\mu|\mu']=-\frac{\alpha}{2}\sum_i\Lambda^{[i]}_{\mu,\mu'}\mu_i\mu_i'\left(R_1+R_2\mu_i'\sum_a\mu'_{i+\delta_a'}\right]\ , \tag{3.23}$$

$$R_1=-a_0^2a_l+4N_1^2(3r+s)a_0a_l\ , \tag{3.24a}$$

$$R_2=-\frac{\lambda^{(1)}}{\alpha_0}a_l\nu_1^2\ . \tag{3.24b}$$

Expanding everything consistently and introducing the quantity

$$\Delta\lambda^{(1)}=\alpha_0 R_1=\frac{\alpha_0 u_R^0 a_0^2}{1+a_0}(1-a_0) \quad , \tag{3.25}$$

we have

$$\bar{D}^{(1)}[\mu|\mu']=-\sum_i \Lambda^{[i]}_{\mu,\mu'}\mu_{i/2}\mu_i' \times\left(\Delta\lambda^{(1)}-\lambda^{(1)}2\nu_1^2 u_R^0 \mu_i' \sum_a \mu'_{i+\delta a'}\right) \quad . \tag{3.26}$$

Clearly, then, $\bar{D}[\mu|\mu']$ is of the form (3.6), to this order. We can identify the new coupling

$$u'=2\nu_1^2 u_R^0 \quad , \tag{3.27}$$

which is consistent with Eq. (2.40). The most important point is that the form of the SFO is preserved. The new relaxation rate is given by

$$\alpha'=\lambda^{(1)}+\lambda\left(\Delta\lambda^{(1)}+\frac{\Delta\alpha_1}{\alpha_0}\lambda^{(1)}-\Delta a_0^{(1)}\alpha_0\right) \quad , \tag{3.28a}$$

$$\alpha'\equiv\Delta\alpha \quad . \tag{3.28b}$$

Explicit evaluation of the rotation taking $\bar{T}\rightarrow T$ shows that it has no effect on $\bar{D}[\mu|\mu']$ and so we obtain to first order in λ the result $D[\mu|\mu']=\bar{D}[\mu|\mu']$.

D. Memory functions and exact results

Before proceeding with the recursion relations for the dynamic correlation functions, it is necessary and important to discuss some of their general properties. The time-dependent correlation functions are defined as

$$C_{ij}(t)=\langle\delta\sigma_j e^{\tilde{D}_\sigma t}\delta\sigma_i\rangle \quad , \tag{3.29}$$

where $\delta\sigma_i=\sigma_i-\langle\sigma_i\rangle$ is just σ_i above T_c. The Fourier-Laplace transform of $C_{ij}(t)$ is

$$C(q,z)=\langle\sigma_{-q}R(z)\sigma_q\rangle \quad , \tag{3.30a}$$

$$\sigma_q=N^{-1/2}\sum_i e^{i\vec{q}\cdot\vec{R}_i}\sigma_i \quad , \tag{3.30b}$$

$$R(z)=(z-i\tilde{D}_\sigma)^{-1} \quad , \tag{3.30c}$$

where $R(z)$ is the resolvent operator. It is very convenient to introduce the memory function $\phi(q,z)$ by the equation

$$[z+i\phi(q,z)]C(q,z)=\tilde{C}(q) \quad , \tag{3.31}$$

where $\tilde{C}(q)\equiv C(q,t=0)$. By judicious use of the operator identity

$$zR(z)=1+R(z)i\tilde{D}_\sigma \tag{3.32}$$

one can find an expression for ϕ in terms of $R(z)$. As usual[8] $\phi(q,z)$ decomposes into a static and a dynamic part. The static, or mean field, part being independent of z

$$\phi(q,z)=\phi^{(s)}(q)+\phi^{(d)}(q,z) \quad , \tag{3.33}$$

$$\phi^{(s)}(q)\tilde{C}(q)=-\langle\sigma_{-q}\tilde{D}_\sigma\sigma_q\rangle \quad , \tag{3.34a}$$

$$\phi^{(d)}(q,z)\tilde{C}(q)=-i[\langle(\tilde{D}_\sigma\sigma_{-q})R(z)(\tilde{D}_\sigma\sigma_q)\rangle -\langle(\tilde{D}_\sigma\sigma_{-q})R(z)\sigma_q\rangle \times C^{-1}(q,z)\langle\sigma_{-q}R(z)\tilde{D}_\sigma\sigma_q\rangle] \quad . \tag{3.34b}$$

The quantity $\phi^{(s)}(q)\,\tilde{C}(q)$ is the Fourier transform of

$$\Gamma_{ij}=\langle\sigma_j\tilde{D}_\sigma\sigma_i\rangle=-\alpha\langle\sigma_i\sigma_j W_i[\sigma]\rangle \quad . \tag{3.35}$$

Since $W_i[\sigma]P[\sigma]$ does not depend on σ_i, Γ_{ij} must be diagonal. We have, as a consequence, the *exact* result for $\phi^{(s)}\tilde{C}$

$$\phi^{(s)}(q)\tilde{C}(q)\equiv\Gamma=\alpha[1+4A_1\epsilon(1,0)+4A_2\epsilon(1,1)] \quad , \tag{3.36}$$

which is a rather rapidly decreasing positive function of the temperature. Near T^c, therefore, $\phi^{(s)}(q)$ is dominated by the behavior of $\tilde{C}^{-1}(q)$. Considering the characteristic frequency of the problem for small q,z, $\omega_c=\phi(0,0)$, we have if we take, near T_c, $\omega_c\alpha\xi^{-z}$ that, when $\phi^{(d)}$ is neglected $z=z_0=\gamma/\nu$ which is the conventional result. Stability considerations, coupled with the fact that $\phi^{(d)}(0,0)$ can be shown [from its expression Eq. (3.34b)] to be nonpositive imply that z_0 is a lower bound for z, as is well known.[9] More importantly, we see that in order to obtain a value of z, $z>z_0$, it is *required* that $\phi^{(d)}(0,0)$ precisely cancels $\phi^{(s)}(0)$ as $T\rightarrow T_c$, a very subtle effect, which in any approximate method could easily be missed.

The computation of $\phi^{(d)}(q,z)\tilde{C}(q)$ is, of course, very complicated. A high-temperature series expansion, however, can be carried out. It is trivial to see that the term in $\tilde{D}_\sigma\sigma_q$ proportional to A_1 does not contribute and that hence $\Gamma^{(d)}(q,z)\equiv\phi^{(d)}(q,z)\tilde{C}(q)$ is proportional to A_2^2

$$\Gamma^{(d)}(q,z)\equiv\phi^{(d)}(q,z)\tilde{C}(q) =-iA_2^2[\langle T_{-q}R(z)T_q\rangle-\langle T_{-q}R(z)\sigma_q\rangle \times C^{-1}(q,z)\langle\sigma_{-q}R(z)T_q\rangle] \quad , \tag{3.37}$$

$$T_q=N^{-1/2}\sum_i e^{i\vec{q}\cdot\vec{R}_i}\sigma_i\sigma_i^n \quad . \tag{3.38}$$

The high-temperature series starts out at order A_2^2 that is, at *fourth* order in the standard high-temperature expansion parameter $u \equiv \tanh K$. The leading term can be calculated by replacing $R^0(z)$ for $R(z)$ in Eq. (3.37). One obtains

$$\Gamma^{(d)}(q,z) \approx -i\alpha^2 A_2^2 \frac{4}{z+3i\alpha} \quad . \tag{3.39}$$

The quantity $\Gamma^{(d)}(0,0)/\alpha$, in this approximation, remains very small in absolute value at all temperatures. We then expect $\Gamma^{(d)}$ to have very little effect on the dynamics, except possibly near T_c.

The important point, which we discuss extensively elsewhere,[10] is that the asymptotic dynamic critical region is very narrow. It appears that there is a broad region where the static behavior is controlled by its asymptotic critical behavior but where the dynamics is still conventional. It is this nonuniversal feature which has led to great difficulties in determining the asymptotic value of z for kinetic Ising models.

E. Collective variables and dynamic recursion relations

The recursion relation for the dynamic spin-spin correlation function is given to lowest order, as shown in Ref. 6, by

$$C_{ia;ja'}(z) = \frac{\nu_1^2}{\Delta}\left(C'_{ij}(z') + \delta_{ij} \sum_n (1-\delta_{n,1}) \frac{\nu_n^*(a)\nu_n(a')}{z+i\lambda^{(n)}}\right) \quad , \tag{3.40}$$

where $\Delta = \alpha'/\alpha$, $z' = z/\Delta$ and the sum on the last term extends to all odd eigenfunctions of the operator $\tilde{D}^0_\sigma$, except for $\psi^{(1)} = \psi$. We have defined

$$\nu_n(a) = \langle \sigma_{i,a} \psi_i^{(n)}(\sigma) \rangle \quad . \tag{3.41}$$

In the equal-time limit, the completeness of the set $\{\psi\}$ can be used to show that Eq. (3.40) reduces to Eq. (2.45) [note that $\tilde{C}_{i,a;j,a'} = \lim_{z\to\infty} z C_{i,a;j,a'}(z)$]. It is sometimes convenient to use the time and space representation

$$\begin{aligned} C_{i,a;j,a'}(t) = {} & \nu_1^2 C'_{ij}(t') + \delta_{ij} \\ & \times \sum_n (1-\delta_{n,1}) \nu_n^*(a)\nu_n(a') e^{-\lambda^{(n)}t} \quad , \end{aligned} \tag{3.42}$$

or the Fourier transform

$$\begin{aligned} C(q,z) = {} & \frac{f(q)}{\Delta} \nu_1^2 C'(2q,z') \\ & + \sum_n (1-\delta_{n,1}) \frac{f_n(q)}{z+i\lambda^{(n)}} \quad , \end{aligned} \tag{3.43}$$

where

$$\begin{aligned} f_n(q) = \tfrac{1}{4} \sum_a [& \nu_n^*(a)\nu_n(a) + 2\nu_n^*(a)\nu_n(a+1) g_1(q) \\ & + \nu_n^*(a)\nu_n(a+2) g_2(q)] \quad , \end{aligned} \tag{3.44}$$

and the functions $f(q)$, $g_1(q)$, $g_2(q)$ were defined in Eq. (2.48). The recursion relation for the dynamic structure factor, $C(q,\omega)$ is obtained from Eq. (3.43) by the use of the relation

$$C(q,\omega) = -2 \,\mathrm{Im}\, C(q, z=\omega+i0^+) \quad . \tag{3.45}$$

As in the static case, in the $q=0$ limit the inhomogeneous term in the recursion relations vanishes

$$C(0,z) = \frac{4\nu_1^2}{\Delta} C'(0,z') \quad . \tag{3.46}$$

In order to proceed any further, the zeroth-order cell parameters must be specified, which we do in the next section.

F. Determination of the parameters α_0, Δ

Just as in the static case (Sec. II D) the quantities $\Delta(K)$ and $\alpha_0(\alpha,K)$ must now be determined. First of all, one must notice that these two parameters are not independent. It follows from Eq. (3.28) taken at zeroth order that

$$\alpha' = \Delta\alpha = \alpha_0(1-a_0) \quad . \tag{3.47}$$

In addition, we need a long-time condition for determining Δ. This follows directly from Eq. (3.46) which in the $z \to 0$ limit reads

$$\frac{\chi}{\phi(0,0)} = \frac{4\nu_1^2}{\Delta} \frac{\chi'}{\phi'(0,0)} \quad . \tag{3.48}$$

Taking into account Eq. (2.46) we have

$$\Delta = \frac{\phi}{\phi'} \quad . \tag{3.49}$$

A direct calculation, making use of the relation Eq. (3.37), shows that $\phi^{(d)}$ does not contribute to the ratio on the right-hand side of Eq. (3.49) to lowest order λ. We, therefore, are led to

$$\Delta \approx \Delta_0 = \frac{1}{4\nu_1^2} \left(\frac{1+4A_1\epsilon(1,0)+4A_2\epsilon(1,1)}{1+4A_1'\epsilon'(1,0)+4A_2'\epsilon'(1,1)} \right) \quad , \tag{3.50}$$

where we have taken into account Eqs. (2.46) and (3.36).

Naturally, this implies that to this order we obtain $z = \gamma/\nu$. The corrections to this result would appear only at higher orders in λ. From the fact that $\phi^{(d)}$ must indeed be very small at any $T > T_c$, it is clear that the determination Eq. (3.50) should yield good results for the correlation functions at all $T \geqslant T_c$.

Another interesting consequence of Eq. (3.50) is that the recursion relation (3.46) can be solved exactly with the result

$$C(0,z)=\frac{\chi}{z+i\phi^{(s)}(0)} \quad . \tag{3.51}$$

Therefore, the time-dependent correlations at $q=0$ are trivially obtained from χ which, of course, is obtained from its own recursion relation Eq. (2.46).

We now have all the ingredients we need to solve the static and dynamic recursion relations. This we do in the next section.

IV. NUMERICAL RESULTS

The recursion relations can now be straightforwardly iterated to obtain the physical quantities of interest. The general procedure was described in Ref. 6. We wish to focus our attention here on the differences between the results obtained by the use of the present systematic procedure, and those obtained in Ref. 6, and will not discuss in any detail those cases where there is no significant difference.

We consider first the static quantities. A very simple calculation involves the determination of the critical values of the short-range correlation functions $\epsilon(2,0)$ and $\epsilon(1,1)$ which satisfy the recursion relations (2.51) and (2.52), respectively. We easily find for $\epsilon(2,0)$ at T_c the value to be 0.5988. This compares very well with the exact value $1-4/\pi^2=0.5947$. The approximate value for $\epsilon(1,1)$ is found to be 0.6198 which is to be compared with the exact value $2/\pi=0.6366$.

In Fig. 2 we have plotted the magnetic susceptibility χ. At the scale of Fig. 2(a), our results are indistinguishable from those obtained using the best numerical estimate.[11,12] In Fig. 2(b) we show that very close to T_c a slight difference actually exists. However, the present results are appreciably closer to those of Ref. 12 than the results of Ref. 6. The maximum discrepancy between our present values of χ and the best numerical estimate is 6% in the range $0.400<u<0.413$, and it falls to less than 3% outside of that range. We find the value of the exponent γ is 1.760, in good agreement with the exact result $(\gamma=1.75)$.

In Fig. 3 we display the static structure factor $\tilde{C}(q)$ [from Eq. (2.47)] at temperatures close to T_c for several small values of q. For comparison, the results of Ref. 6 and the best numerical estimates from series expansions[12] are also exhibited. The position of the maximum in $\tilde{C}(q)$, and its variation with q are now in very close agreement with Ref. 12. Overall, the agreement is rather better than that obtained in Ref. 6, even though the value $\tilde{C}(q_{\max})$ is a little lower. The critical exponent η is now 0.240 (exact result: $\eta=0.25$). We see, then, that the agreement between the RG and the series methods is somewhat improved by the use of the systematic expansion.

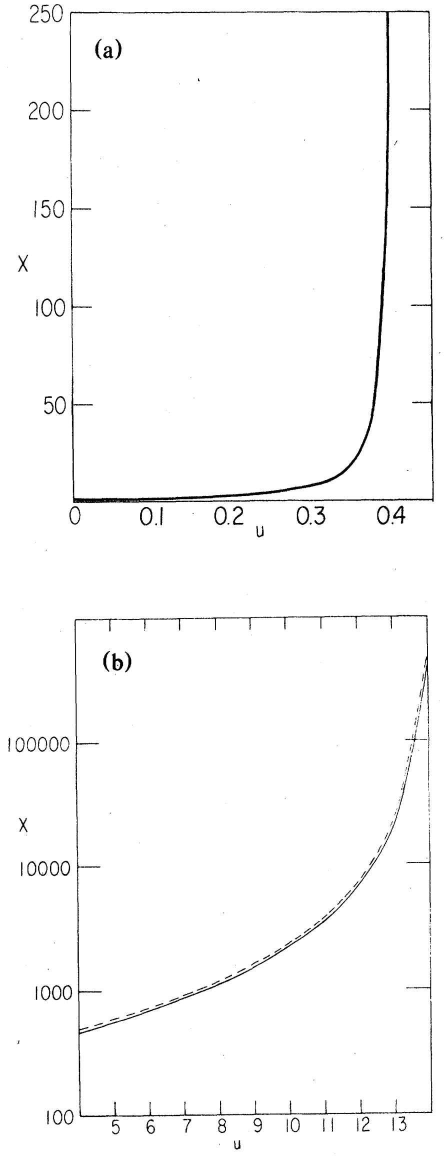

FIG. 2. χ vs $u\equiv\tanh K$ in two temperature ranges. Solid line: this work. In (b) the dashed line is the result of Ref. 11, and the u axis 5, 6, etc., indicate 0.405, 0.406, etc.

We turn next to the calculation of the specific heat using the recursion relation given by Eq. (2.56). We note immediately the C does not diverge at T_c. We obtain that $C=7.5826$ at T_c. We have then that the exponent $\alpha=0$. In Fig. 4 we plot our approximate specific heat versus the exact result. Despite the fact that our simple approximation does not reproduce the logarithmic singularity at T_c the overall agreement as a function of temperature is quite acceptable.

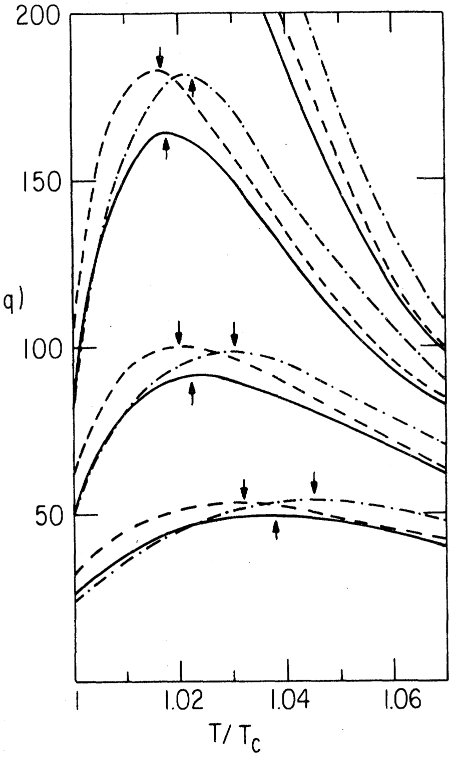

FIG. 3. Static structure factor $\tilde{C}(q)$ near T_c for different values of $q_x = q_y$. Solid line: this work, dashed line: Ref. 12, dash-dotted line: Ref. 6. From top to bottom the groups of three lines correspond to $qa = 0.03$, 0.05, 0.07, and 0.10.

We turn now to the dynamics. It follows from our procedure, (see Sec. III), that the exponent z is 1.76 (1.79 in Ref. 6). We find, in general, that sufficiently near T_c our results are extremely close to those of Ref. 6. Away from T_c, however, they are clearly different. We now proceed to show how and why.

It is particularly illuminating to examine the same site correlation function $C(t)$ from Eq. (3.42) (Fig. 5). At $T \gtrsim T_c$, $C(t)$ decays to zero extremely slowly, exactly as in Ref. 6. As the temperature increases, however, $C(t)$ decays to zero progressively faster, but considerably more slowly than in Ref. 6. This is particularly clear in Fig. 5 where one can see that at $u = 0.1 C(t)$ decays to zero in the present approximation more slowly than it did even at $u = 0.3$ in the previous work.

What is going on here can be ascertained from the known fact that at very large temperatures one must have $C(t) = e^{-\alpha t}$. This limit is also plotted in Fig. 5. At any finite temperature $C(t)$ must decay more slowly. It is quite clear that our present results behave correctly, while the work in Ref. 6 did not deal appropriately with the higher temperatures: the determination of α_0 used there did not take into account the relation Eq. (3.47) that must consistently be satisfied. This (which is related to the detailed balance condition) led to an excessively large value of α_0 at high temperatures. Very close to T_c, however, the results are practically unaffected: for this reason, all scaling relations between exponents were found to hold in Ref. 6 and are maintained in the present work.

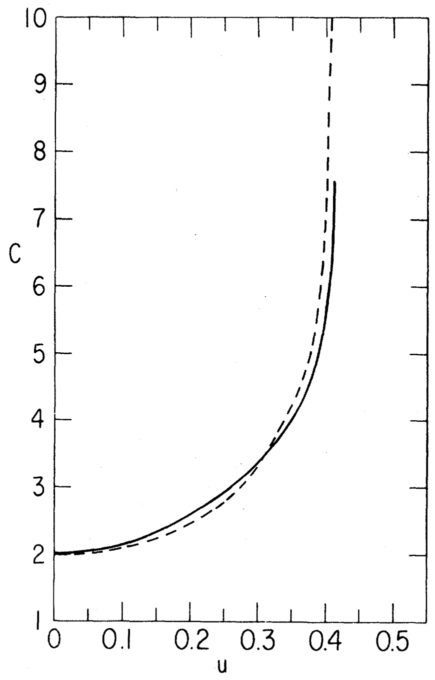

FIG. 4. Specific heat [as defined by Eq. (2.54)] vs $u = \tanh K$. The dashed lined is the exact result and the solid line results from the iterative solution of Eq. (2.56).

Finally we discuss the behavior of the dynamic correlations as the temperature changes. This is exhibited in Figs. 6(a) and 6(b), where the behavior of the dynamic structure factor $C(q,\omega)$ is plotted at

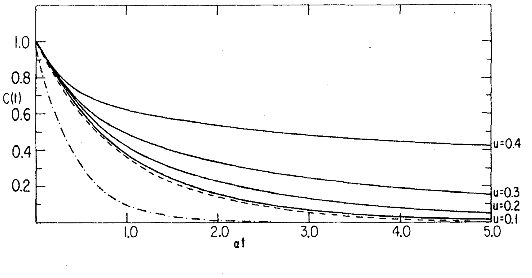

FIG. 5. Same site correlation function vs time at several temperatures. Solid line: present results. Dashed line: $u \to 0$ exact limit. Dash-dotted line: result from Ref. 6 at $u = 0.03$

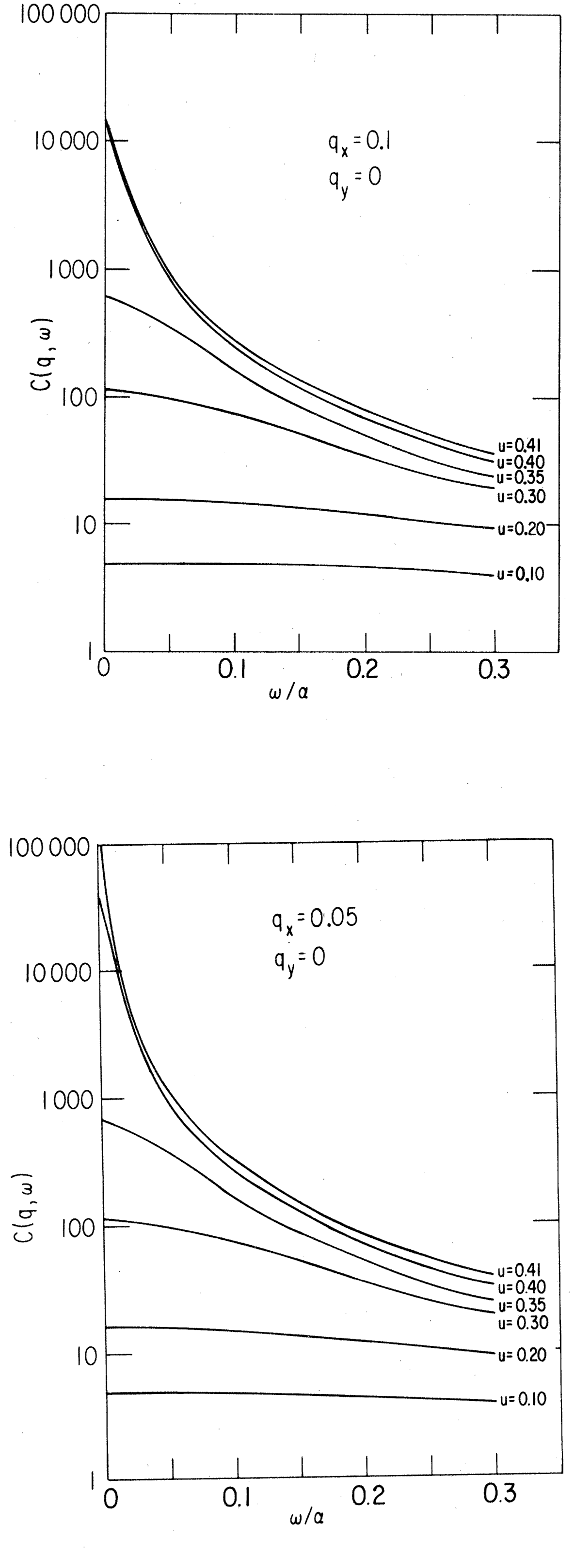

FIG. 6. Dynamic structure factor $C(q,\omega)$ at constant q vs frequency at several temperatures.

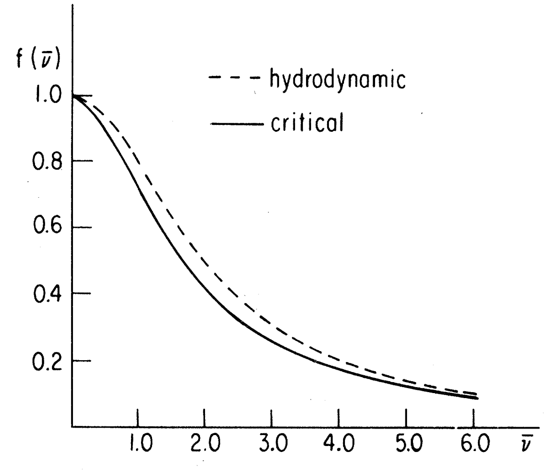

FIG. 7. Shape function defined in the usual way (Ref. 13). Solid line: present results in the critical limit. Dashed line: present results in the hydrodynamic limit.

fixed q as a function of ω for several temperatures. The analysis of the critical region is identical to that of Ref. 6. All scaling relations are satisfied. Some of them are, in fact, trivial. It follows for example from Eq. (3.51) that $C(q=0,\omega)$ at $T=T_c$ diverges as ω^{-2} in agreement with the proper scaling behavior $C(0,\omega)\alpha\omega^{-(2+z-\eta)/z}$ since $z=2-\eta$ in our case.

It is also necessary to recalculate the shape function[13] in the hydrodynamic regime. This can now be done analytically with the help, again, of Eq. (3.51) and the result, which is Lorentzian, is plotted in Fig. 7. The shape function in the critical regime (which is little changed from Ref. 6 is also plotted).

In conclusion the results of this systematic study of the RG cell expansion are extremely satisfactory. The static results appear to be extremely close to the best series-expansion results. The dynamic results satisfy all expected scaling relations and have the correct high-temperature limit. For the first time, dynamic results for the correlation functions have been obtained within a consistent expansion method.

ACKNOWLEDGMENTS

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