Dynamical Correlation Functions in the Two-Dimensional Kinetic Ising Model: A Real-Space Renormalization-Group Approach

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A real-space dynamic renormalization-group scheme is used to evaluate static and dynamic correlation functions for a kinetic Ising model on a two-dimensional square lattice. The critical exponents obtained from the correlation functions calculated using this method satisfy the proper static and dynamic scaling relations and are in excellent agreement with known values.

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The calculation of static and dynamic correlation functions in systems that undergo a phase transition is a problem of great interest. These functions can be measured in scattering experiments and exhibit a wide variety of phenomena in the region near the phase transition. Recently,[1,2] a real-space dynamic renormalization-group (RSDRG) method was introduced for the investigation of lattice dynamical models. In this Letter we apply this method to the kinetic Ising (KI) model on a square lattice and show how, within the formalism, one can calculate space- and time-dependent correlation fucntions.

The KI model[3] describes the stochastic time evolution of a set of Ising spins $\{\sigma\}$. The equilibrium properties are governed by the nearest-neighbor Ising-model Hamiltonian, H_σ, characterized by a coupling K. The time evolution of this model is assumed to be generated by a single-spin-flip operator (SFO):

$$\tilde{D}[\sigma|\sigma'] = -\tfrac{1}{2}\alpha \textstyle\sum_i \Lambda_{\sigma,\sigma'}^{[i]} W_i[\sigma]\sigma_i\sigma_i', \quad (1)$$

where α is a relaxation rate, i is a site index, $\Lambda_{\sigma,\sigma'}^{[i]}$ sets all $\sigma_k=\sigma_k'$ except for site i, and the simplest $W_i[\sigma]$, consistent with detailed balance and which reproduces itself under RG iterations, is of the "minimal-coupling" form:

$$W_i[\sigma] = 1 + A_1\sigma_i\sigma_i^T + A_2\sigma_i^{(n)}, \quad (2)$$

where $A_1 = -\frac{1}{2}\tanh(2K)$, $A_2 = A_1^2$, σ_i^T is the sum of the four nearest neighbors about the spin at site i, and $\sigma_i^{(n)}$ is the symmetric sum of the products of two nearest-neighbor spins about the spin at site i.

As a first step in our RSDRG analysis we divide the system into cells of four spins and the dynamical operator into intracell and intercell parts: $\tilde{D}_\sigma = \tilde{D}_\sigma^0 + \epsilon\tilde{D}_\sigma^I$. The intracell part is of the form

$$\tilde{D}^0[\sigma|\sigma'] = \textstyle\sum_i \Lambda_{\sigma,\sigma'}^{[i]}\tilde{D}_i^0[\sigma|\sigma'], \quad (3)$$

where i now labels cells, $\Lambda_{\sigma,\sigma'}^{[i]}$ sets all $\sigma_k=\sigma_k'$ at all cells except i, and $\tilde{D}_i^0$ depends only on the spins in the ith cell:

$$\tilde{D}_i^0[\sigma|\sigma'] = -\tfrac{1}{2}\alpha_0 \textstyle\sum_a \Lambda_{\sigma,\sigma'}^{[i,a]}\sigma_{i,a}\sigma_{i,a}' W_0^{[i,a]}[\sigma], \quad (4)$$

$$W_0^{[i,a]}[\sigma] = 1 + J_1\sigma_{i,a}(\sigma_{i,a+1}+\sigma_{i,a-1}) + J_2\sigma_{i,a+1}\sigma_{i,a-1}, \quad (5)$$

where the index a labels the four spins in the ith cell. The detailed balance condition for the uncoupled cells gives the condition $J_1 = -\frac{1}{2}(\tanh 2K_0)\times(1+J_2)$, where K_0 is the nearest-neighbor coupling for the uncoupled cells.

As discussed in Ref. 2, the RSDRG method corresponds to choosing a mapping function $T[\mu|\sigma]$, relating our original problem to a similar one on a lattice with a larger lattice constant, as the solution to the eigenvaluelike equation:

$$\textstyle\sum_{\bar{\sigma}} \tilde{D}[\sigma|\bar{\sigma}]T[\mu|\bar{\sigma}] = \sum_{\bar{\mu}} D[\mu|\bar{\mu}]T[\bar{\mu}|\sigma], \quad (6)$$

where the block-spin variables are denoted by μ and the "eigenvalue" D_μ is the SFO operating in μ space. This choice of T ensures[2] that non-Markovian effects are eliminated. The renormalized probability distribution is as usual[4] $P[\mu] = \langle T[\mu|\sigma]\rangle$.

We can proceed to solve (6) (together with normalization conditions discussed in Ref. 2) in a power series in the cell coupling. To zeroth order in ϵ, one finds that the mapping function is $T_0[\mu|\sigma] = \prod_i \frac{1}{2}[1+\mu_i \psi_i^{(1)}(\sigma)]$, where $\psi_i^{(1)}(\sigma)$ is the slowest-decaying odd eigenfunction of $\tilde{D}_i^0$. The zeroth-order expression for $\tilde{D}_\mu{}^0$ is of the same form as (1) with $A_1 = A_2 = 0$ and a new relaxation rate $\alpha' = \lambda_1$ where λ_1 is the eigenvalue associated with $\psi_i^{(1)}(\sigma)$. The first-order (in ϵ) calculation leads to a $\tilde{D}_\mu$ identical in form to (1) but with a new coupling[5] $K' = (\alpha/\alpha_0) f(K, K_0, J_2)$ and $\alpha' = \alpha \Delta_\alpha(K, K_0, J_2)$. At this stage the intracell parameters α_0, K_0, and J_2 are unspecified.

Consider a time correlation function $C_{AB}(t) = \langle B_\sigma A_\sigma(t)\rangle$ where A_σ and B_σ are spin variables of interest. Associate with A_σ a coarse-grained variable $A_\mu P[\mu] \equiv \langle T[\mu|\sigma] A_\sigma\rangle$, define the projection operator P in σ space $PA_\sigma = \sum_\mu T[\mu|\sigma] A_\mu$, and let Q be the complement of P. We can then easily obtain the relation $C_{AB}(t) = C_{AB}'(t) + \langle (QB_\sigma) \times (QA_\sigma(t))\rangle$ where $C_{AB}'(t)$ is the correlation function in the coarse-grained variables with dynamics generated by $\tilde{D}_\mu$. We expect C_{AB}' to carry the information about long distances and times, and the other term to be short ranged. More specifically, if $A_\sigma = \sigma_{i,a}$ then, to lowest order in ϵ, $A_\mu = \nu_1(a)\mu_i$ with[6] $\nu_n(a) \equiv \langle \psi_i^{(n)}(\sigma)\sigma_{i,a}\rangle_0$. We can then evaluate the term involving QA_σ to lowest order in ϵ and obtain the key result used in our calculations:

$$C_{ia,ja'}(t) = \nu_1{}^2 C_{ij}'(t) + \delta_{ij} \sum_n (1-\delta_{n,1}) \nu_n{}^*(a) \nu_n(a') \exp(-\lambda_n t), \tag{7}$$

where λ_n is the nth eigenvalue of $\tilde{D}_i^0$. Recursion relations for static two-spin correlation functions can easily be constructed from (7) by setting $t = 0$.

There are important restrictions on our procedure imposed by the asymptotic behavior of static correlation functions at large distances. Assume that the RG transformation changes the length scale by a factor b. If the spins are initially separated by a distance $R = b^n$, we find, at high temperature, after n iterations that[7] $\langle \sigma_0 \sigma_{b^n}\rangle = (\nu_1{}^2)^n \langle \mu_0 \mu_1\rangle$ where μ_0 and μ_1 are nearest neighbors interacting with coupling K_n. For n large K_n will be small and $\langle \mu_0 \mu_1\rangle = K_n$. In order to obtain exponential decay with distance we require $K_n \sim K^R \sim K^{b^n}$, hence the recursion relation must be of the form $K' \sim K^b$ for K small. The cumulant approximation[4] gives $K' \sim K$. A similar argument shows that $K' = bK$ at low T. We thus conclude that acceptable recursion relations must interpolate smoothly, as T changes, between these two behaviors. In the case of a square lattice with $b = 2$, we suggest that a natural variable to introduce is $\varphi = e^{2K} u$ ($u \equiv \tanh K$) and the recursion relation

$$\varphi' = \varphi^2 \tag{8}$$

gives the proper interpolation between large and small K and will, therefore, lead to exponential decay of the correlation functions. It is worth noting that (8) gives the exact critical coupling $u_c = \sqrt{2} - 1$ and the exact thermal exponent $\nu^{-1} = y_T = 1$. The recursion relation (8) does not come directly out of our previous analysis but it gives a large hint as to how to develop a systematic theory. If we define $\epsilon(n)$ as the two-spin static correlation function for spins separated by n lattice sites along the x or y directions, then we have from (7) that $\epsilon(2n) = \nu_1{}^2 \epsilon'(n)$ for $n > 1$. This relation depends on the details of the renormalization procedure through the factor ν_1. The ratio $\epsilon(4)/\epsilon(2) = \epsilon'(2)/\epsilon'(1)$ gives an implicit relation between K and K'. Since we cannot directly invert this equation to obtain K', we have used the known high-temperature results[8] for the $\epsilon(n)$ to determine the coefficients in the expansion

$$\varphi' = \varphi^2 + \sum_{n=3}^{\infty} a_n \psi^n,$$

where $\psi = e^{-4K} u$. This form clearly interpolates between the appropriate high- and low-temperature results for K'. Using terms up to a_6 we obtain a recursion relation with fixed point properties $u_c = 0.4150$ and $\nu^{-1} = y_T = 1.011$. Since these results are very close to the exact results, we will, for simplicity, use the simple recursion relations given by (8) in our numerical calculations.

We must now reconcile the recursion relation (8) with the result given by the direct analysis leading to D_μ. It turns out to be quite convenient to demand that the relation $K' = (\alpha/\alpha_0) f(K, K_0, J_2)$ be used to fix $\alpha_0 = \alpha_0(K, K_0, J_2)$ with K' given by (8). Conceptually this is nice because it decouples the determination of the static recursion relation

from the dynamics.

We have to specify the quantities K_0 and J_2. An analytic investigation of the recursion relation for $\epsilon(1)$ at high and low temperatures shows that we must require $K_0 = 2K$ in *both* limits. This "bond doubling" is physically appealing since one cut two bands to each spin in decoupling the cells. The parameter J_2 should go as K_0^2 for small K_0 and if we require, which is physically sensible, that $T_0[\mu|\sigma]$ reduce to the "majority rule"[4] at low temperatures then $J_2 \to 1$ as $K \to \infty$. We have used a very simple interpolation formula for K_0 and J_2 between these high- and low-temperature limits: $K_0 = 2K - u^2/8q$ and $J_2 = \tanh^2(2pK_0)$. The temperature-independent parameters q and p were determined to be 0.38 and 0.434 by simultaneously demanding that the $\epsilon(1)$ calculated from the recursion relations agree with the exact result at the critical temperature $\epsilon_c(1) = 1/\sqrt{2}$ and that α_0 be as close to α as possible for $K = K_c$.

Using these results we obtain, to lowest order in ϵ, the magnetic eigenvalue $\lambda_h = 4\nu_1 = 3.676$ which yields $\beta = 0.1219$ (exact value is 0.125). This value is considerably better than those yielded by cumulant expansion analysis at a similar order. The associated calculation of the magnetization leads to excellent agreement with the exact result, for all temperatures. The largest error is for $u = 0.43$ and is 2.4%. The "dynamic" recursion relation relating α' and α leads to the dynamic exponent $z = -\ln(\Delta_\alpha)/\ln b = 1.791$ which is larger than the known[9] lower bound ($z = 1.75$). (The results for β and z obtained by using the full recursion relation for φ are $\beta = 0.1215$ and $z = 1.796$.) There is a wide range of quoted values of z from numerical analysis.[10]

We have calculated the magnetic susceptibility and compared our results with very reliable series results.[8,11] Our results are excellent, giving detailed agreement for all $T > T_c$ and a critical exponent $\gamma = 1.756$.

In Fig. 1, we give results for the wave-number–dependent static correlation function as a function of temperature for various wave numbrs and make a comparison with the results of Ref. 11. Our calculations correctly reproduce the maximum at $T > T_c$ for $q \neq 0$. This a subtle effect corresponding to a significant correction to the Ornstein-Zernike form for the static correlation function. We have also calculated $C(q, T = T_c)$ and extracted the exponent $\eta = 0.248$ (0.25 exact).

In Fig. 2 we plot the "same-site" correlation function $C_{ii}(t) = \langle \sigma_i \sigma_i(t) \rangle$ for various temperatures. The figure clearly displays critical slowing down for $K \sim K_c$. For $K > K_c$, $C_{ii}(t)$ decays to the nonzero magnetization density squared for long times, as expected. The time Fourier transform $C_{ii}(\omega)$ shows a narrow peak near $\omega = 0$ for $K \sim K_c$. The quantity $C_{ii}(\omega = 0)$ diverges as $|K - K_c|^{-n}$ and we find $n = 1.54$ in agreement with the scaling relation $n = \nu(z + 2 - d - \eta)$. Also, $C_{ii}(\omega)$ at $K = K_c$ diverges like $\omega^{-\mu}$ with $\mu = 0.86$, again in agreement with scaling.[12] We have also calculated the dynamic structure factor for a wide range of frequencies, wave numbers, and temperatures.

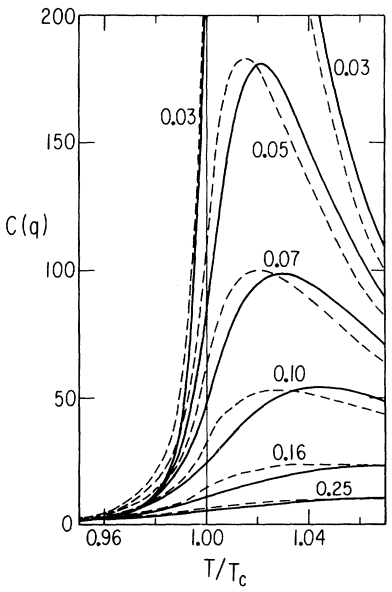

FIG. 1. The static correlation $C(q)$ for $q_x = q_y$ vs reduced temperature T/T_c for various wave numbers $(q_x a)$. The solid lines are the RG calculations and the dashed lines are taken from Ref. 11.

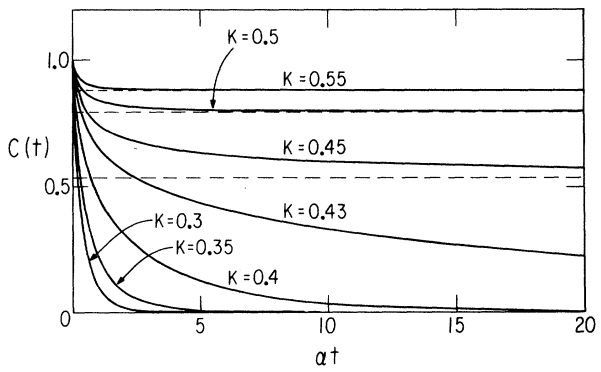

FIG. 2. The calculated site-correlation function $\langle \sigma_i \sigma_i(t) \rangle$ vs αt for various couplings K (the asymptotic values given by the magnetization squared are shown as dashed lines).

All of the various scaling relations are satisfied. A full discussion will be given elsewhere.

It should be pointed out that other approaches for applying the RSDRG to the kinetic Ising model have been suggested.[13-17] These other methods have not addressed the problem of the elimination of non-Markovian effects[2]; they have been used only to extract critical properties, and no attempt to use them as a basis for a formalism to calculate correlation functions has been made.

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[1]G. F. Mazenko, M. J. Nolan, and O. T. Valls, Phys. Rev. Lett. 41, 500 (1978).

[2]G. F. Mazenko, M. J. Nolan, and O. T. Valls (unpublished); G. F. Mazenko, in *Dynamical Critical Phenomena and Related Topics*, edited by C. P. Enz (Springer-Verlag, Berlin, 1979).

[3]R. Glauber, J. Math. Phys. (N. Y.) 4, 234 (1963).

[4]T. Niemijer and J. M. J. van Leeuwen, in *Phase Transitions and Critical Phenomena*, edited by C. Domb and M. S. Green (Academic, New York, 1976), Vol. 6.

[5]The functions f and Δ will be given elsewhere.

[6]The symbol $\langle\ \rangle_0$ denotes averaging with respect to the zeroth-order probability distribution $P_0[\sigma]$.

[7]The factor ν_1 scales to a constant value in the large- and small-K limits and does not affect our argument.

[8]M. Fisher and R. Burford, Phys. Rev. 156, 583 (1967).

[9]K. Kawasaki, in *Phase Transitions and Critical Phenomena*, edited by C. Domb and M. S. Green (Academic, New York, 1973), Vol. 2.

[10]H. Yahata and M. Suzuki, J. Phys. Soc. Jpn. 27, 1421 (1969); Z. Racz and M. F. Collins, Phys. Rev. B 13, 3074 (1976); E. Stoll, K. Binder, and T. Schneider, Phys. Rev. B 8, 3266 (1973).

[11]H. Tarko and M. Fisher, Phys. Rev. B 11, 1217 (1975).

[12]$\mu = (z+2-d-\eta)/z$. See, for example, A. M. Gottlieb and C. Hohenemser, Phys. Rev. Lett. 31, 1222 (1973).

[13]M. Suzuki, K. Sugo, I. Matsuba, H. Ikada, T. Chikama, and H. Tanaku, Prog. Theor. Phys. 61, 864 (1979).

[14]Y. Achiam, J. Phys. A 11, 975, L129 (1978).

[15]S.-k. Ma, Phys. Rev. B 19, 4824 (1979).

[16]U. Dekker, Z. Phys. B 31, 283 (1978).

[17]S. T. Chui, G. Forgács, and H. L. Frisch, Phys. Rev. B 20, 243 (1979).