Temperature quenches in the disordered phase of a spin system

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(Received 26 April 1982)

The problem of a sudden temperature quench of a spin system is studied for the case of a two-dimensional spin-flip kinetic Ising model in zero external field. The analysis is carried out for the case where both the initial and final temperatures are in the disordered phase. The problem is analyzed with the use of a generalization of the real-space dynamic renormalization-group method. The interesting features found in studying the time-dependent structure factor are the following: (i) a nonmonotonic time dependence at finite wave numbers corresponding to "structure pulses"; (ii) a slow shift and decay in the peak of the structure factor for fixed wave number as a function of temperature; (iii) a slow approach to the final exponential relaxation to equilibrium.

I. INTRODUCTION

The description of the response of a thermodynamic system to a strong external perturbation takes one outside the linear-response region in which we have a well-defined statistical-mechanical description.[1] One is confronted in this case with new difficulties both in terms of exotic phenomena to be understood (turbulence, nucleation, spinodal decomposition) and in terms of an appropriate formal description.[2] In this paper we will analyze a strongly nonequilibrium situation somewhat simpler than those mentioned above. We consider the time evolution of a system of two-dimensional Ising spins in zero external magnetic field driven by a spin-flip kinetic Ising[3] dynamics after a sudden temperature quench. In this work we restrict the analysis to the situation where the initial and final temperatures are in the disordered phase.

Recently[4] the one-dimensional analog of this same problem was solved exactly. Rather interesting nonmonotonic "structure pulses" were found in the time evolution of the wave-number-dependent structure factor for a range of wave numbers. The same pulses are found in the two-dimensional case. We also find another interesting effect associated with temperature dependence of the structure factor for fixed wave number and time after quench. As will be seen in Fig. 3 the peak in the structure factor as a function of temperature moves slowly to higher temperatures and loses weight as time progresses. If one quenches to a temperature near the critical point one does find that the final asymptotic decay is described by dynamical scaling, but one must wait a rather long time before this description is appropriate (this is discussed more fully in Sec. V).

The technique used in the analysis here is a generalization of the recently developed real-space dynamic renormalization-group (RSDRG) method.[5] The method is capable of treating more general situations than the specific example discussed here. The inclusion, for example, of effects due to spontaneous symmetry breaking, finite magnetic fields, and conservation laws complicate the analysis somewhat and will be discussed elsewhere.

II. PROBLEM STUDIED

Consider a set of N ferromagnetic Ising spins $\{\sigma\}$ located at sites $\vec{R}_i$ on a square lattice with spacing c. In thermal equilibrium, at a temperature T, the probability distribution governing these spins is

$$P[\sigma,K]=\exp(H[\sigma,K])/Z(K)\ , \tag{2.1}$$

where $H[\sigma,K]$ is the nearest-neighbor Ising Hamiltonian characterized by a coupling $K=J/k_BT$, J is the exchange constant, and $Z(K)$ is the partition function.

We assume that the dynamics of the Ising spins are driven by a heat bath via a pseudo-Liouville operator $D_\sigma(K)$ that depends on the temperature of the bath. We assume, for definiteness, that we have a single spin-flip operator (SFO) of the form

$$D[\sigma \mid \sigma';K]=\frac{-\alpha}{2}\sum_i \Lambda^{[i]}_{\sigma,\sigma'} W_i[\sigma',K]\sigma_i\sigma_i' \ , \tag{2.2}$$

where α is a high-temperature relaxation rate,

$$\Lambda^{[i]}_{\sigma,\sigma'}=\prod_{k(\neq i)}\delta_{\sigma_k,\sigma_k'} \tag{2.3}$$

tells us that the matrix D_σ is almost diagonal,[6] and we choose

$$W_i[\sigma,K]=1+A(K)\sigma_i \times\sum_a \sigma_{i+\delta_a}+A^2(K) \times\sum_a \sigma_{i+\delta_a}\sigma_{i+\delta_{a+1}} \ , \tag{2.4}$$

which is proportional to the probability of a spin flip, with

$$A(K)=-\tfrac{1}{2}\tanh(2K) \ . \tag{2.5}$$

The δ_a in (2.4) are the vectors connecting a site to its four nearest neighbors. Thermal equilibrium between the bath and Ising spins requires that $P[\sigma,K]$ be invariant under time translations generated by $D_\sigma(K)$; thus

$$e^{D_\sigma(K)t}P[\sigma,K]=P[\sigma,K] \ , \tag{2.6}$$

and this condition requires that $A(K)$, in (2.4), be given by (2.5). We have chosen to work with the particular form for W given by (2.4) because it is the most "local" probability one can construct.[7]

Suppose we rapidly change the temperature of the bath from T_I to T_F. We assume, in keeping with Monte Carlo studies of this problem, that this quench is instantaneous. This is somewhat unrealistic and we intend to study finite quench rate effects in future work. The Ising system will respond to this quench through its dynamic coupling to the bath via the SFO $D_\sigma(K_F)$ which drives the Ising system to equilibrium with the bath at temperature T_F. The probability distribution governing the Ising spins for times $t\geq 0$ is given then by

$$P[\sigma,t]=\exp[tD_\sigma(K_F)]P[\sigma,K_I] \ . \tag{2.7}$$

We will focus in this paper on the time-dependent "static" structure factor:

$$\tilde{C}(q,t)=\frac{1}{N}\sum_{i,j} e^{i\vec{q}\cdot(\vec{R}_i-\vec{R}_j)}\sum_\sigma \sigma_i\sigma_j P[\sigma,t] \ . \tag{2.8}$$

There has been a lot of Monte Carlo work on this model,[8] but the emphasis has been on the case where there is a magnetic field change,[9] a conservation law,[10] or a quench into the ordered phase.[11] We have not found any published Monte Carlo results for $\tilde{C}(q,t)$ in the region we have studied. We would welcome any subsequent efforts to compare our results with Monte Carlo calculations.

Most analytical work[12] has focused on the critical phenomena aspects of the problem (quenching to very near T_c and looking at the effective relaxation rate). Related work has been carried out on the time-dependent Ginzburg-Landau model.[13,14] As discussed in Ref. 4, and elsewhere,[14] this model, at least to lowest order in perturbation theory in the quartic coupling, leads to a straightforward exponential relaxation for the structure factor connecting the initial and final states.

We want to study the problem posed in this section using renormalization-group (RG) methods. There are very good reasons for believing that this is a good approach to this problem. The first reason is the most obvious. If one quenches into the critical region then a RG approach is needed to treat the critical properties. The justification here for the use of the RG is standard[15] and based on the notions of scaling and a fixed point under RG transformations. One should remember, however, that the power of the renormalization group is not only that it can treat systems near a critical point but that it can treat systems that are *self-similar* as one changes a length scale. There are a number of strongly nonequilibrium situations where there is a development in time of objects of progressively larger scale (a coarsening) which are built up of similar objects on a smaller scale. It seems, therefore, that a renormalization-group analysis is in order.

III. REVIEW OF THE RSDRG METHOD

Before constructing a theory for calculating $\tilde{C}(q,t)$ we need to quickly review our methods[5,16] for treating $\tilde{C}(q,K)$ in equilibrium. The RSDRG method involves mapping the slowly varying degrees of freedom for the σ spins onto a similar Ising model on a lattice with a lattice constant bc (the rescaling factor $b=2$ here) characterized by a set of $N'=N/b^2$ Ising "block" spins $\{\mu\}$. Central to this mapping is a transformation function $T[\sigma \mid \mu;K]$ that relates $P[\sigma,K]$ to the probability distribution governing the block spins:

$$P[\mu,K']=\sum_\sigma P[\sigma,K]T[\mu \mid \sigma;K] \ , \tag{3.1}$$

where K' is the normalized coupling. In order to guarantee that the new probability distribution is properly normalized we require that T satisfy

$$\sum_{\mu} T[\mu \mid \sigma;K]=1 . \tag{3.2}$$

For each variable $A[\sigma]$, we define an associated coarse-grained version,

$$A[\mu]P[\mu,K']=\sum_{\sigma} A[\sigma]P[\sigma,K]T[\mu \mid \sigma;K] . \tag{3.3}$$

Note that the average of $A[\sigma]$ over $P[\sigma,K]$ equals the average of $A[\mu]$ over $P[\mu,K']$ due to (3.2).

A key ingredient in our analysis is that $T[\mu \mid \sigma;K]$ is to be constructed perturbatively as a solution to the eigenvaluelike equation[16]

$$\tilde{D}_{\sigma}(K)T[\mu \mid \sigma;K]=D_{\mu}(K')T[\mu \mid \sigma;K] , \tag{3.4}$$

where $\tilde{D}_{\sigma}$ is the adjoint[17] of D_{σ} and $D_{\mu}(K')$ the SFO governing the dynamics of the μ spins. We also require that $T[\mu \mid \sigma;K]$ satisfy the normalization condition

$$\sum_{\sigma} P[\sigma,K]T[\mu \mid \sigma;K]T[\mu' \mid \sigma;K]=\delta_{\mu,\mu'}P[\mu,K'] . \tag{3.5}$$

We can construct $T[\mu \mid \sigma;K]$, $D_{\mu}(K')$, $P[\mu,K']$, and any $A[\mu]$ order by order in a perturbation theory[16] expansion in an effective coupling between cells. We assume that a system of uncoupled cells (with 4 σ spins per cell) gives a good zero-order description of the problem if the coupling in the cell is chosen properly. We can then derive recursion relations relating observables on different length scales. In particular, working at lowest order in the coupling between cells, we obtain[18] the recursion relation for the static structure factor

$$\tilde{C}(q,K)=1+2rg_1(q)+sg_2(q) -\nu_1^2 f(q)+\nu_1^2 f(q)\tilde{C}(2q,K') , \tag{3.6}$$

where r and s are the nearest- and next-nearest-neighbor correlation functions[19] for a cell, ν_1 is the projection of a given spin in a cell onto the associated block spin given by

$$\nu_1=\tfrac{1}{2}(1+2r+s)^{1/2} \tag{3.7}$$

and

$$g_1(q)=\tfrac{1}{2}[\cos(q_x c)+\cos(q_y c)] , \tag{3.8}$$

$$g_2(q)=[\cos(q_x c)\cos(q_y c)] , \tag{3.9}$$

$$f(q)=1+2g_1(q)+g_2(q) . \tag{3.10}$$

Finally $\tilde{C}(2q,K')$ is to be evaluated with the new coupling constant K'. Our recursion relation[20] determining K' is given by $\phi'=\phi^2$ where $\phi=e^{2K}u$, $u=\tanh K$. We have shown[7,16] that (3.6) can be solved upon direct iteration to obtain $\tilde{C}(q,K)$ and we obtain good results over a wide range of temperatures and wave numbers. The main point here is that this method leads to a good description for $\tilde{C}(q,K)$ and therefore should give a good description of $\tilde{C}(q,t)$ for short and very long times.

IV. TREATMENT OF THE QUENCH PROBLEM

A. General development

Our method for calculating an observable in the strongly nonequilibrium situation requires generalizing (3.1) and (3.3) to the case where $P[\sigma,t]$ has the time dependence given by (2.7), and the mapping function becomes time dependent:

$$P[\mu,t]=\sum_{\sigma} T[\mu \mid \sigma;t]P[\sigma,t] . \tag{4.1}$$

Since the normalization of the probability distribution is preserved for all time, we still require

$$\sum_{\mu} T[\mu \mid \sigma;t]=1 , \tag{4.2}$$

and to ensure that the mapping remains local,[21] we likewise demand that the normalization (3.5) be generalized to this case,

$$\sum_{\sigma} P[\sigma,t]T[\mu \mid \sigma;t]T[\mu' \mid \sigma;t]=\delta_{\mu,\mu'}P[\mu,t] . \tag{4.3}$$

Further constraints are that (4.1) should reduce to the appropriate equilibrium form in the short- and long-time limits. That is,

$$T[\mu \mid \sigma;t=0]=T[\mu \mid \sigma;K_I] , \tag{4.4a}$$

$$T[\mu \mid \sigma;t\rightarrow\infty]=T[\mu \mid \sigma;K_F] , \tag{4.4b}$$

and $T[\mu \mid \sigma;K_I]$ and $T[\mu \mid \sigma;K_F]$ satisfy (3.4) with the appropriate SFO.

The question then is the construction of $T[\mu \mid \sigma;t]$ for arbitrary times. We shall construct $T[\mu \mid \sigma;t]$ using the idea that it should evolve from $T[\mu \mid \sigma;K_I]$ to $T[\mu' \mid \sigma;K_F]$ as time progresses. Since the operator $\exp[t\tilde{D}_{\sigma}(K_F)]$ propagates quantities "forward in time," our first guess for $T[\mu \mid \sigma;t]$ might be

$$\exp[t\tilde{D}_{\sigma}(K_F)]T[\mu \mid \sigma;K_I] .$$

The problem with this choice is that $\exp[t\tilde{D}_\sigma(K_F)]$ drives the spin-dependent part of $T[\mu\,|\,\sigma;K_I]$ to zero as $t\to\infty$. We want the "slow" degrees of freedom to survive. We do this by properly propagating the degrees of freedom backward in time, thus our second guess for $T[\mu\,|\,\sigma;t]$ is

$$\tilde{T}[\mu\,|\,\sigma;t]\equiv\exp\{t[\tilde{D}_\sigma(K_F)-D_\mu(K_F')]\}\times T[\mu\,|\,\sigma;K_I]\ . \tag{4.5}$$

Note, because of the eigenvalue equation (3.4), that $T[\mu\,|\,\sigma;K_F]$ is stationary under the application of the operator in Eq. (4.5) and we therefore expect $\tilde{T}[\mu\,|\,\sigma;t]$ to be proportional to $T[\mu\,|\,\sigma;K_F]$ in the long-time limit.

While $\tilde{T}[\mu\,|\,\sigma;t]$ will satisfy (4.2), it will not, in general satisfy (4.3). We will be able to satisfy (4.3) if we rotate $\tilde{T}$ in the μ space with a matrix M:

$$T[\mu\,|\,\sigma;t]=\sum_{\mu'}M[\mu\,|\,\mu';t]\tilde{T}[\mu'\,|\,\sigma;t]\ . \tag{4.6}$$

Once M is chosen such that (4.3) is satisfied, then the mapping function for the nonequilibrium case is determined. The generalization of (3.3) to the nonequilibrium case is simply

$$A[\mu,t]P[\mu,t]=\sum_\sigma A[\sigma]T[\mu\,|\,\sigma;t]P[\sigma,t]\ . \tag{4.7}$$

There is one important aspect of our development to be discussed. Under a renormalization-group analysis we expect (if the method is to be useful) a certain amount of self-similarity between the original and coarse-grained problems. In the case at hand, this requires that $P[\sigma,t]$ [given by (2.7)] map into

$$\bar{P}[\mu,t]=e^{tD_\mu(K_F')}P_I[\mu,K_I']\ . \tag{4.8}$$

However, there is no simple general connection between $\bar{P}[\mu,t]$ and $P[\mu,t]$ as given by (4.1). We can, however, define a quantity relating them:

$$P[\mu;t]=R[\mu,t]\bar{P}[\mu,t]\ . \tag{4.9}$$

It will turn out that we can construct $R[\mu,t]$ in perturbation theory. We can easily see that

$$R[\mu,0]=1\ . \tag{4.10}$$

Let us now outline the general procedure to be followed in our analysis.

(i) Expand $D_\sigma(K)$, $H[\sigma,K]$ in a series where the lowest-order terms correspond to a system of uncoupled cells. One reasonable decomposition is discussed in detail in Ref. 16.

(ii) With the use of this expansion, construct order by order in perturbation theory, $P[\mu,K']$, $D_\mu(K')$, and $T[\mu\,|\,\sigma;K]$ which enter into the equilibrium theory. Then, given K_I and K_F, one has the quantities $P[\mu,K_I']$, $P[\mu,K_F']$, $D_\mu(K_F')$, $T[\mu\,|\,\sigma;K_I]$, and $T[\mu\,|\,\sigma;K_F]$.

(iii) Given $\tilde{D}_\sigma(K_F)$, $D_\mu(K_F')$, and $T[\mu\,|\,\sigma;K_I]$ one can construct, order by order in perturbation theory, $\tilde{T}[\mu\,|\,\sigma;t]$ using (4.5). One then combines this result with (4.6) to construct a rotation $M[\mu\,|\,\mu',t]$ such that $T[\mu\,|\,\sigma;t]$ satisfies (4.3). Once one has $M[\mu\,|\,\mu';t]$, then $T[\mu\,|\,\sigma;t]$ is determined and one, in turn, has $P[\mu,t]$.

(iv) Given $D_\mu(K_F')$ and $P[\mu,K_I']$ one can construct $\bar{P}[\mu,t]$ from (4.8) in perturbation theory. Knowing $P[\mu,t]$ and $\bar{P}[\mu,t]$ allows one to determine $R[\mu,t]$ via (4.9).

(v) One can then determine any collective variable $A[\mu,t]$ from (4.7) order by order in perturbation theory.

(vi) Rewrite (4.7) in the form

$$A[\mu,t]R[\mu,t]\bar{P}[\mu,t]=\sum_\sigma A[\sigma]T[\mu\,|\,\sigma;t]P[\sigma,t]\ . \tag{4.11}$$

Then insert our perturbation theory expansions for $A[\mu,t]$ and $R[\mu,t]$ on the left-hand side and sum over μ. After using (4.2) we find that we have a recursion relation relating the nonequilibrium average of $A[\sigma]$, with respect to $P[\sigma,t]$, to the nonequilibrium average of $A[\mu,t]R[\mu,t]$ with respect to $\bar{P}[\mu,t]$. Let us illustrate this procedure via the zeroth-order calculation.

B. Zeroth-order analysis

The preceding formal development may seem a bit cumbersome, but we can now show, at least to lowest order in perturbation theory, that it leads to a recursion relation that makes good physical sense. Let us follow the steps outlined in the preceding section.

(i) The perturbation expansion for $\tilde{D}_\sigma$ and $H[\sigma]$ has been thoroughly discussed in Ref. 16.

(ii) One can then easily solve the zeroth-order eigenvalue equation defined by (3.4) to find that the zeroth-order mapping function $T^0[\mu\,|\,\sigma;K]$ can be written as a product of contributions from each cell,

$$T^0[\mu\,|\,\sigma;K]=\prod_{i=1}^{N'}T_i^0[\mu\,|\,\sigma;K]\ , \tag{4.12a}$$

where, for cell i,

$$T_i^0[\mu \mid \sigma;K]=\tfrac{1}{2}[1+\mu_i\psi_i^{(1)}(\sigma,K)] , \quad (4.12b)$$

where $\psi_i^{(1)}(\sigma,K)$ is the slowest varying odd eigenfunction associated with the zeroth-order SFO, $\tilde{D}^0_\sigma(K)$, and is given by

$$\psi_i^{(1)}(\sigma,K)=N_1(K)\sigma_i^s , \quad (4.13)$$

where σ_i^s is the sum of the four spins in cell i. The normalization constant $N_1(K)=1/[4\nu_1(K)]$ and ν_1 is given by (3.7) in terms of averages in a single cell. The zeroth-order renormalized SFO is

$$D^0[\mu \mid \mu']=\frac{-\lambda^{(1)}}{2}\sum_i \Lambda^{[i]}_{\mu,\mu'}\mu_i\mu_i' , \quad (4.14)$$

and $\lambda^{(1)}$ is the eigenvalue associated with $\psi_i^{(1)}(\sigma)$. $T^0[\mu \mid \sigma]$ given by (4.12) is easily shown to satisfy (3.2) and (3.5) and the renormalized-probability distribution is found to be, at this order,

$$P_0[\mu,K]=(\tfrac{1}{2})^{N'} . \quad (4.15)$$

(iii) We can then easily show, using (4.5), that

$$T^0[\mu \mid \sigma;t]=T^0[\mu \mid \sigma;K_I] . \quad (4.16)$$

The lack of time dependence results because $\psi_i^{(1)}(\sigma,K_I)$ and $\psi_i^{(1)}(\sigma,K_F)$ are linearly related. Otherwise $\tilde{T}^0[\mu \mid \sigma,t]$ has a nontrivial time dependence. One immediately sees that $\tilde{T}^0$ does not satisfy the normalization condition (4.3):

$$\sum_\sigma \tilde{T}_i^0[\mu \mid \sigma,t]\tilde{T}_i^0[\mu' \mid \sigma,t]P_0^i[\sigma,t] = \tfrac{1}{2}[1+\mu_i\mu_i' B(t)] , \quad (4.17)$$

where $P_0(t)$ is the nonequilibrium probability distribution governing the ith cell

$$P_0[\sigma,t]=e^{tD^0_\sigma(K_F)}P_0[\sigma,K_I] , \quad (4.18)$$

where D^0_σ is the zeroth-order SFO, and

$$B(t)=\sum_\sigma P_0[\sigma,t]N_1^2(K_I)(\sigma_i^s)^2 . \quad (4.19)$$

A rotation of the form

$$M[\mu \mid \mu',t]=\prod_{i=1}^{N'}\tfrac{1}{2}[1+q(t)\mu_i\mu_i'] \quad (4.20)$$

can be used to rotate $\tilde{T}^0$ into a T^0 which satisfies (4.2) and (4.3). The appropriate choice of $q(t)$ which completes the rotation is

$$q(t)=[B(t)]^{-1/2} . \quad (4.21)$$

The final result for T^0 after multiplying T by M is,

$$T^0[\mu \mid \sigma;t]=\prod_{i=1}^{N'} T_i^0[\mu \mid \sigma;t] , \quad (4.22a)$$

$$T_i^0[\mu \mid \sigma;t]=\tfrac{1}{2}[1+\mu_i\psi_i^{(1)}(\sigma,t)] , \quad (4.22b)$$

where

$$\psi_i^{(1)}(\sigma,t)=N_1(t)\sigma_i^s . \quad (4.23)$$

We see that $T_0[\mu \mid \sigma;t]$ is of the same form as in equilibrium except the normalization $N_1(K)$ in $\psi_i^{(1)}(\sigma,K)$ is replaced by its time-dependent generalization

$$N_1(t)=\tfrac{1}{2}[1+2r(t)+s(t)]^{-1/2} ,$$

where $r(t)$ and $s(t)$ are the time-dependent nearest- and next-nearest-neighbor correlation functions for a single cell. We have

$$r(t)=\sum_\sigma \sigma_{i,a}\sigma_{i,a\pm1}P_0[\sigma,t] , \qquad s(t)=\sum_\sigma \sigma_{i,a}\sigma_{i,a\pm2}P_0[\sigma,t] . \quad (4.24)$$

Since $r(0)=r(K_I)$, $r(\infty)=r(K_F)$, etc., we see explicitly that $T^0[\mu \mid \sigma;0]=T^0[\mu \mid \sigma;K_I]$ and $T^0[\mu \mid \sigma;t\to\infty]=T^0[\mu \mid \sigma;K_F]$.

In the more general case where $\psi_i^{(1)}(\sigma,K_I)$ and $\psi_i^{(1)}(\sigma,K_F)$ are not simply related, the calculation goes through in essentially the same fashion, and one finds

$$T_i^0[\mu \mid \sigma,t]=\tfrac{1}{2}(1+q(t)\phi_i(\sigma,t)\mu_i] , \quad (4.26)$$

where

$$q(t)=[B(t)]^{-1/2} , \quad (4.27)$$

$$B(t)=\sum_\sigma P_i^0[\sigma,t][\phi_i(\sigma,t)]^2 , \quad (4.28)$$

$$\phi_i(\sigma,t)=\sum_\sigma e^{-(\lambda_F^{(n)}-\lambda_F^{(1)})t}\psi_i^{(n)}(\sigma,K_F) \times\sum_{\sigma'} P_i^0[\sigma',K_F]\psi_i^{(1)}(\sigma',K_I) \times\psi_i^{(n)}(\sigma',K_F) , \quad (4.29)$$

and the $\lambda_F^{(n)}$ and $\psi_i^{(n)}(\sigma,K_F)$ satisfy the eigenvalue equation

$$\tilde{D}^0_\sigma\psi_i^{(n)}(\sigma,K_F)=-\lambda_F^{(n)}\psi_i^{(n)}(\sigma,K_F) . \quad (4.30)$$

(iv) It is trivial in this case to find

$$P_0[\mu,t]=\bar{P}_0[\mu,t]=(\tfrac{1}{2})^{N'} \quad (4.31)$$

and identify

$$R_0[\mu,t]=1 . \tag{4.32}$$

(v) We can now, for example, construct the coarse-grained equivalent of $\sigma_i\sigma_j$ using (4.7):

$$\Pi_{i,a;j,a'}[\mu,t]P[\mu,t]=\sum_{\sigma}\sigma_{i,a}\sigma_{j,a'}T[\mu\mid\sigma;t]P[\sigma,t]. \tag{4.33}$$

We find to lowest order in perturbation theory,

$$\Pi^0_{i,a;j,a'}[\mu,t]=[\delta_{a,a'}+r(t)(\delta_{a',a+1}+\delta_{a',a-1})+s(t)\delta_{a',a+2}]\delta_{i,j}+(1-\delta_{i,j})\nu_1^2(t)\mu_i\mu_j , \tag{4.34}$$

where $r(t)$ and $s(t)$ are given by (4.24) and (4.25) and

$$4\nu_1^2(t)=1+2r(t)+s(t) . \tag{4.35}$$

(vi) Using our zeroth-order results for Π and R in (4.11) we can then sum over all μ's and Fourier transform as in (2.8) to obtain the recursion relation satisfied by the structure factor

$$\begin{aligned}\tilde{C}(q,t)=&1+2r(t)g_1(q)\\&+s(t)g_2(q)-\nu_1^2(t)f(q)\\&+\nu_1^2(t)f(q)\tilde{C}(2q,t') ,\end{aligned} \tag{4.36}$$

where $g_1(q)$, $g_2(q)$, and $f(q)$ are given by Eqs. (3.8)–(3.10), respectively, and $t'=\Delta t$ where Δ is the time rescaling[22] factor $[\Delta=\alpha'(K_F)/\alpha(K_F)]$ given by Eq. (3.50) in Ref. 16. We note here that $\Delta\to 1$ as $K_F\to 0$ and $\Delta\to 1/[4\nu_1^2(K_F)]$ as K_F approaches its critical value.

We note that a key step in the derivation of (4.36), which is our central result, is that in multiplying $\Pi^0[\mu]R^0[\mu]$ times $\bar{P}[\mu,t]$ and summing over all μ, we can interpret $\sum_\sigma\mu_i\mu_j\bar{P}[\mu,t]$ as being equivalent to $\sum_\sigma\sigma_i\sigma_jP[\sigma,t]$ except we must use the renormalized parameters K_I', K_F', and α' and take into account that the σ lattice has a lattice constant c while the μ lattice has a lattice constant $2c$.

V. RESULTS

The numerical solution of the recursion relation (4.36) can be carried in essentially the same manner as for the equilibrium case. This simply amounts to repeated iteration of the recursion relations until the parameters reach the high-temperature fixed point where the process ceases. This is discussed in some detail in Sec. VI A of Ref. 23. There is, of course, a large amount of information contained in $\tilde{C}(q,t)$. It depends on the parameters K_I, K_F, q_x, q_y, and t. For simplicity let us limit ourselves here to the case where we quench from infinite temperature ($K_I=0$) and where we look along a diagonal ($q_x=q_y$) in reciprocal space. There may, however, be some interesting situations not covered by these restrictions.

In Fig. 1 we plot $\tilde{C}(q,t)$ for a fixed ($u_F=\tanh K_F=0.4$) K_F as a function of $q_x=q_y$ for various times after the quench. At all times $\tilde{C}(q,t)$ is a smooth and monotonic function of q. Note, as expected, that higher wave numbers equilibrate much faster than the smaller wave-number components that are inhibited by critical slowing down. In particular, if we quench to temperatures very near T_c, we find that

$$\tilde{C}(q,t)=\tilde{C}(q,\infty)+Ae^{-\omega_c(u,q)t} ,$$

where $\omega_c(u_c,q)\sim q^z$ with $z=1.76$ and $\omega_c(u,0)\sim(u_c-u)^{z/\nu}$ with $z/\nu=1.76$ in agreement with our notions concerning dynamic scaling.[22] We have found, however, that we must go to very long times before the system is adequately described by the exponential form above. We will return to this point below.

Careful inspection of Fig. 1 shows that there is a range of q's where $\tilde{C}(q,t)$ does not grow monotonically in time. This is better seen in Fig. 2 where we fix $q_xc=0.03\pi$ and plot $\tilde{C}(q,t)$ versus time after quench for three different values of $u_F=\tanh K_F$. We note for all three values of u_F there is a rapid initial increase in $\tilde{C}$ to a maximum followed by a

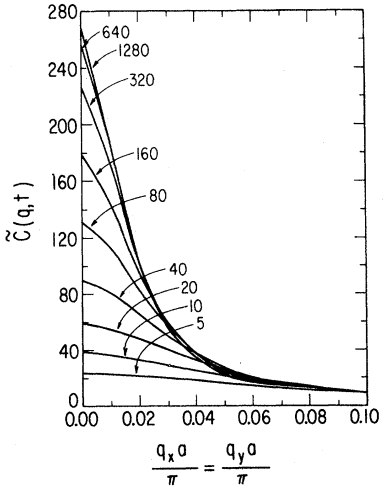

FIG. 1. Time-dependent structure factor vs wave number for $u_I=0$ and $u_F=0.4$ for various times after quench.

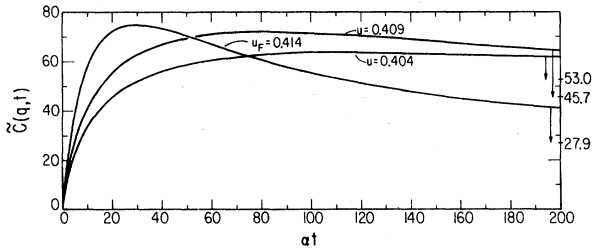

FIG. 2. Time-dependent structure factor vs time for $q_x c = q_y c = 0.03\pi$, $u_I = 0$ and several final temperatures.

very slow decay to the final asymptotic value. This peak in the structure factor, as a function of time, was also found[4] in an exact analysis of the related problem in one dimension. The physics of the situation is simple. There is a sum rule for the area under $\tilde{C}(q,t)$ for any t given by the fixed-length spin condition. However, various Fourier components evolve in time with different characteristic times. After a temperature quench from high temperatures the Fourier components near $qc = \pi$ will lose weight rapidly while those near $q = 0$ are slower to change. It therefore takes a finite time for weight to move from high to low wave numbers. We also see this effect in Fig. 3 where, for $q_x c = q_y c = 0.03\pi$, we plot $\tilde{C}(q,t)$ vs u_F for various times. The structure "pulse" is more pronounced the closer we are to the transition-temperature $u_c = \sqrt{2} - 1$. A second interesting effect can be seen in Fig. 3. For times greater than $20\,\alpha^{-1}$ the maximum in $\tilde{C}$ does not occur at u_c. In fact the maximum moves slowly to higher temperatures as time progresses. The existence of this peak in the structure factor for temperature above T_c was observed in our equilibrium

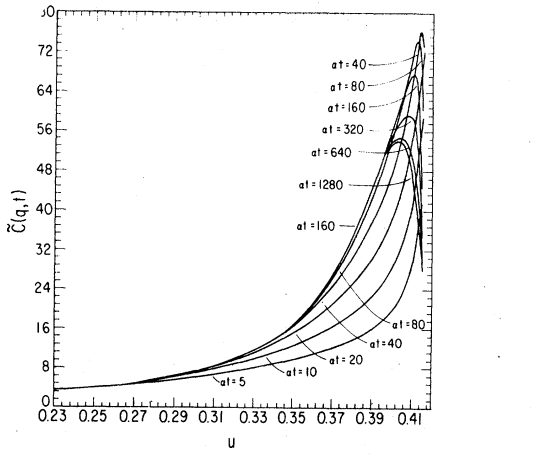

FIG. 3. Time-dependent structure factor vs the final temperature u for $q_x c = q_y c = 0.03\pi$ and a number of times.

calculations[7,16] and was in qualitative agreement with the high-temperature expansions of Fisher and Burford.[24] Note that the structure factor reaches its final value only after a time of order $1000\alpha^{-1}$. For times greater than $80\alpha^{-1}$, where there is no further change for a final coupling less than $u_F = 0.36$, there is still a large variation in the rest of the curve.

Let us return to the question of the long-time behavior of our system and, to simplify matters, let us consider the case $q_x = q_y = 0$. We said above that for sufficiently long times we have exponential time decay to the final state, but that this exponential region is itself reached only after rather long times. This is shown in Fig. 4 where we have plotted $\ln[\tilde{C}(0,\infty) - \tilde{C}(0,t)]$ vs αt. A careful analysis shows that for intermediate times $200 < \alpha t \lesssim 360\,000$, $\tilde{C}(0,t)$ is better described by a form

$$\tilde{C}(0,t) = \tilde{C}(0,\infty) + Ae^{-wt^y},$$

where $y \approx \frac{2}{3}$. For large times y crosses over to a final value of $y = 1$. A precise determination of y, w, and A is not simple since there is a bit of "noise" in the data. This takes the form of a weak oscillation in time in fitted values of y, w, and A. The nature of this artifact requires further study. If indeed there is a region for which $y \approx \frac{2}{3}$, then this is interesting since it would be an indication of a type of coarsening.

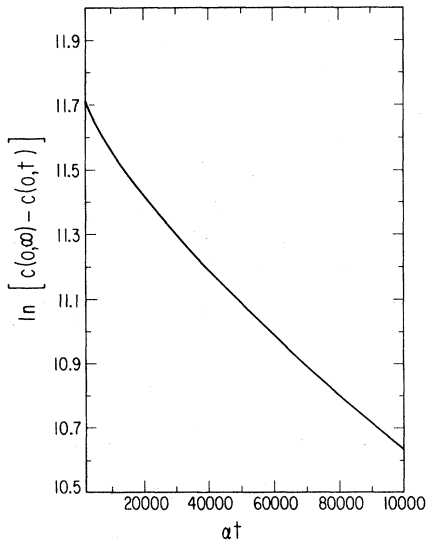

FIG. 4. $\ln\,[C(q,\infty) - C(q,t)]$ vs αt for $q = 0$, $u_I = 0$, and $u_F = 0.4138$.

VI. CONCLUSIONS

We have studied the problem of strong temperature quenches in the disordered phase using rescaling techniques. The advantages of this method are the following.

(i) It gives an accurate treatment of the initial and final equilibrium states. This leads to a rather good treatment of critical effects if the initial or final states are near the critical point.

(ii) It preserves the fixed-length spin condition [sum rule on $\tilde{C}(q,t)$] and the periodicity of the lattice.

(iii) It properly accounts for the long-time critical slowing down for quenches near the critical point.

(iv) In principle, since the method allows one to treat many length scales, it allows the possibility of building large objects from smaller ones. Thus in a problem where there is a type of coarsening, there is some hope this approach can treat it.

The description of this problem seems encouraging. However, a more crucial test involves the treatment of metastable and unstable final states.

ACKNOWLEDGMENTS

I acknowledge the support of the Alfred P. Sloan Foundation, the National Science Foundation (Grant Nos. NSF DMR 80-20609 and PHY 77-27084), and the Material Research Laboratory of the NSF at the University of Chicago. I thank Dr. Jorge Hirsch and Dr. Oriol Valls for valuable conversations concerning this work, and I thank Professor Walter Kohn and the staff of the Institute for Theoretical Physics at the University of California at Santa Barbara for their hospitality during a visit in which this paper was written.

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[1]See for example the treatment of L. P. Kadanoff and P. C. Martin, Ann. Phys. (N.Y.) 24, 419 (1963).

[2]At this stage essentially all discussions have relied on stochastic systems (Navier-Stokes equations, generalized Fokker-Planck equations, or kinetic Ising models) because they allow one to couple in a convenient way to external parameters like, for example, the temperature. This is discussed by K. Binder, Phys. Rev. B 8, 3423 (1974).

[3]R. J. Glauber, J. Math. Phys. (N.Y.) 4, 294 (1963); K. Kawasaki, Phys. Rev. 145, 224 (1966); 148, 375 (1966); 150, 285 (1966); in *Phase Transitions and Critical Phenomena,* edited by C. Domb and M. S. Green (Academic, New York, 1972), Vol. 2.

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[5]For a general review of the application to problems in equilibrium see G. F. Mazenko and O. T. Valls, in *The Real Space Renormalization Group,* edited by J.M.J. van Leeuwen and T. W. Burkhardt (Springer, Berlin, 1982).

[6]We are using the short-hand notation $D_\sigma A[\sigma]=\sum_{\sigma'} D[\sigma\,|\,\sigma']A[\sigma']$.

[7]See the discussion in G. F. Mazenko, J. Hirsch, M. J. Nolan, and O. T. Valls, Phys. Rev. B 23, 1431 (1981). There has been some speculation in the literature that various results may depend rather sensitively on the particular choice of W_i in (2.2) [see for example U. Deker and F. Haake, Z. Phys. B 36, 379 (1980)]. While this can be true in one dimension where, because $T_c=0$, one can arrange things (somewhat artificially) such that one has W's in a new dynamic universality class, there is no current information to indicate that this is true in two dimensions. To the contrary H. Takano (unpublished) has found in two dimensions that the dynamic critical index is equivalent for two very different choices for W_i using a finite-size scaling method.

[8]See for example K. Binder and M. H. Kalos, in *Monte Carlo Methods in Statistical Physics,* edited by K. Binder (Springer, Berlin, 1979).

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[15]See, for example, S. Ma, *Modern Theory of Critical Phenomena* (Benjamin, New York, 1976).

[16]G. F. Mazenko and O. T. Valls, Phys. Rev. B 24, 1404

(1981).

[17]A discussion of some of the formal properties of this and related operators is given in G. F. Mazenko, M. J. Nolan, and O. T. Valls, Phys. Rev. B 22, 1263 (1980).

[18]This is worked out in detail in G. F. Mazenko, J. Hirsch, M. J. Nolan, and O. T. Valls, Phys. Rev. B 23, 1431 (1981).

[19]If K_0 is the effective coupling governing a cell and $a_0=\tanh(2K_0)$ then $r=a_0/(2-a_0^2)$, $s=a_0 r$.

[20]The justification of this thermal recursion relation is given in Ref. 18.

[21]See Ref. 5 for a discussion of the significance of the normalization condition (3.5).

[22]This choice for Δ leads to a conventional value for the dynamic critical index $z=-\ln\Delta/\ln 2=2-\eta\approx 1.76$. We know that the expression we use for Δ is very accurate in the region $0\leq u\leq u_c$ except if we are very close to u_c. There is currently considerable controversy concerning the correct value for z [see the discussion in G. F. Mazenko and O. T. Valls, Phys. Rev. B 24, 1404 (1981)]. There have been a large number of calculations and an enormous spread in values. From this point of view of the problem studied in this paper this controversy is, to a large degree, irrelevant. The reason is that the asymptotic dynamic critical region for this system is very narrow and one would have to quench very near the critical point to see a nonconventional value for z. Furthermore, when one has a reliable way of determining z, it is easy to incorporate nonconventional corrections into our development by modifying the Δ we use. As explained in Ref. 16 this will amount to a "better" choice for the relaxation rate α_0 for the relaxation rate of a set of uncoupled cells. We expect such nonconventional corrections to have very little effect on the quantities we have calculated in this paper.

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