

Structure pulses in a simple nonequilibrium system

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(Received 6 March 1981)

We have studied the time-dependent structure factor for a one-dimensional kinetic Ising (KI) model quenched from an initial to a final temperature. Our results deviate from those predicted by a comparable time-dependent Ginzburg-Landau model in which one has simple exponential relaxation from the initial to the final value of the structure factor. We find in our KI model that there is a pulse in the structure factor which moves from large to small wave numbers as time evolves. We discuss the physical origin of this effect.

I. INTRODUCTION

The study of strongly nonequilibrium situations is becoming increasingly important in statistical physics. In this paper we study a simple strongly nonequilibrium problem. Consider a one-dimensional ferromagnetic Ising chain with spins interacting via a nearest-neighbor coupling only. Suppose this system is initially in equilibrium at temperature T_i . At some time $t_0 = 0$ we quench the system so that the time evolution of the Ising spins is governed by a kinetic Ising (KI) dynamics which drives the system to some final temperature T_f . There are two main points we make in this paper:

(i) We can solve this problem exactly. That is, we can calculate the nonequilibrium time evolution of quantities like the static structure factor over the entire time regime. It seems useful to investigate any such soluble nonequilibrium models.

(ii) We have found that even in this simple case there is an interesting physical effect that we did not anticipate. This effect, which will probably also occur in higher-dimensional systems, corresponds to the generation of a pulse which propagates in time from large to small wave numbers in the static structure factor. The existence of such a pulse seems to depend only upon the existence of a temperature-independent sum rule on the static structure factor and a clear separation of time scales between short and long wavelengths.

In Sec. II we define the nonequilibrium model of interest which we then solve exactly in Sec. III. We develop in Sec. IV the corresponding time-dependent Ginzburg-Landau (TDGL) description of the same problem for comparison. We discuss the properties of our solution of the KI model in Sec. V compared with the TDGL description. We end the paper in Sec. VI with a discussion of the implications of our work with regard to higher dimensions and other types of systems.

II. PROBLEM STUDIED

Let us consider a one-dimensional chain of ferromagnetically coupled Ising spins governed by a nearest-neighbor Hamiltonian (multiplied by $-1/k_B T$ where T is the temperature)

$$H_K[\sigma] = K \sum_i \sigma_i \sigma_{i+1} . \tag{2.1}$$

Here σ_i is the Ising spin at lattice site i and $K = J/k_B T$ where J is the exchange coupling. The equilibrium statics for this system are governed by the Boltzmann probability distribution

$$P_K[\sigma] = e^{H_K[\sigma]} / Z_K , \tag{2.2}$$

where the partition function is given by

$$Z_K = \sum_{\sigma} e^{H_K[\sigma]} . \tag{2.3}$$

In this simple case we can work out explicitly any equilibrium quantity. For example, the static structure factor for this system,

$$\tilde{C}(q) = \frac{1}{N} \sum_{i,j} e^{iqa(i-j)} \langle \sigma_i \sigma_j \rangle , \tag{2.4}$$

where a is the lattice spacing, N the total number of spins, and $\langle \rangle$ indicates an equilibrium average, can be evaluated and is found to be

$$\tilde{C}(q) = \frac{1 - u^2}{1 + u^2 - 2u \cos qa} , \tag{2.5}$$

where $u = \tanh K$.

In this paper we are interested in the dynamics of this system as generated by a stochastic time evolution process. In particular, we consider the kinetic Ising model due to Glauber.¹ In this model the nonequilibrium probability distribution $P[\sigma, t]$ evolves according to a master equation

$$\frac{\partial P[\sigma, t]}{\partial t} = D_{\sigma}^K P[\sigma, t] , \tag{2.6}$$

where D_σ^K is a spin-flip operator (SFO)² of the form, in matrix notation,

$$D^K[\sigma|\sigma'] = -\frac{\alpha}{2} \sum_i \Lambda_{\sigma,\sigma'}^{[i]} \left[1 - \frac{\gamma}{2} \sigma'_i (\sigma'_{i+1} + \sigma'_{i-1}) \right] \sigma_i \sigma'_i, \quad (2.7)$$

where

$$\Lambda_{\sigma,\sigma'}^{[i]} = \prod_{k(\neq i)} \delta_{\sigma_k, \sigma'_k} \quad (2.8)$$

and

$$\gamma = \tanh 2K. \quad (2.9)$$

Various properties of this operator have been discussed elsewhere.² Here we point out the important property that

$$D_\sigma^K P_K[\sigma] = 0. \quad (2.10)$$

That is, the equilibrium probability distribution is invariant under time evolution:

$$e^{iD_\sigma^K} P_K[\sigma] = P_K[\sigma]. \quad (2.11)$$

Furthermore this system is ergodic³

$$\lim_{t \rightarrow \infty} e^{iD_\sigma^K} P_{K_0}[\sigma] \rightarrow P_K[\sigma]. \quad (2.12)$$

Much of the work on this system has been concerned with fluctuations in equilibrium. In that case one studies equilibrium time correlation functions of the form

$$C_{ij}(t) = \langle \sigma_j e^{iD_\sigma^K} \sigma_i \rangle \quad (2.13)$$

and the average is over the equilibrium probability distribution $P_K[\sigma]$ and $\tilde{D}^K[\sigma|\sigma'] \equiv D^K[\sigma'|\sigma]$. One of the nice features of the Glauber form for D_σ^K given by Eq. (2.7) is that we can solve for the Fourier transform of $C_{ij}(t)$ exactly:

$$C(q,t) = \tilde{C}(q) e^{-\Gamma(q)t}, \quad (2.14)$$

where

$$\Gamma(q) = \alpha(1 - \gamma \cos qa). \quad (2.15)$$

In this paper we address a different physical situation. Suppose for times $t < 0$ we have a system in equilibrium at temperature T_I and coupling K_I and described statistically by the stationary probability distribution $P_{K_I}[\sigma] \equiv P_I[\sigma]$. At time $t = 0$ we rapidly quench the system so that the subsequent dynamics are governed by the SFO $D_\sigma^{K_F}$. For times $t \geq 0$ we assume that the probability distribution governing the system is given by

$$P[\sigma,t] = e^{iD_\sigma^{K_F}} P_I[\sigma]. \quad (2.16)$$

We are then interested in the subsequent time evolution of the system. We know that eventually

$$\lim_{t \rightarrow \infty} P[\sigma,t] = P_{K_F}[\sigma] \equiv P_F[\sigma] \quad (2.17)$$

and we are interested in the time evolution between the initial and final states.

In higher-dimensional systems there has been interest in the evolution of the magnetization defined as

$$M(t) = \sum_\sigma \sigma_i P[\sigma,t] \quad (2.18)$$

as a function of time. In the one-dimensional case, in the absence of a magnetic field, this is zero unless $T_I = 0$, in which case we obtain

$$m(t) = e^{-\Gamma^F(0)t}, \quad (2.19)$$

where

$$\Gamma^F(q) = \alpha(1 - \gamma_F \cos qa) \quad (2.20)$$

and

$$\gamma_F = \tanh 2K_F. \quad (2.21)$$

For the rest of this paper we will concentrate on the time evolution of the structure factor

$$\tilde{C}(q,t) = \frac{1}{N} \sum_{ij} e^{iqa(i-j)} \tilde{C}_{ij}(t), \quad (2.22)$$

$$\tilde{C}_{ij}(t) = \sum_\sigma \sigma_i \sigma_j P[\sigma,t]. \quad (2.23)$$

III. DETERMINATION OF $\tilde{C}(q,t)$

As a first step in determining $\tilde{C}(q,t)$ let us introduce the auxiliary quantity

$$D_{ij}(t) = \tilde{C}_{ij}(t) - \tilde{C}_{ij}^F \quad (3.1)$$

which decays to zero for long times. After a few rearrangements we can write

$$D_{ij}(t) = \sum_\sigma (P_I[\sigma] - P_F[\sigma]) e^{iD_\sigma^{K_F}} \sigma_i \sigma_j. \quad (3.2)$$

If we use the identity

$$\begin{aligned} \tilde{D}_\sigma^{K_F} \sigma_i \sigma_j = -\alpha \left[2\sigma_i \sigma_j - \frac{\gamma_F}{2} [\sigma_j (\sigma_{i+1} + \sigma_{i-1}) \right. \\ \left. + \sigma_i (\sigma_{j+1} + \sigma_{j-1}) \right] \\ \left. + \alpha \delta_{ij} [2 - \gamma_F \sigma_i (\sigma_{i+1} + \sigma_{i-1})] \right] \quad (3.3) \end{aligned}$$

and Fourier-Laplace transform $D_{ij}(t)$,

$$D(q, z) = -i \int_0^{+\infty} dt e^{+izt} \frac{1}{N} \sum_{i,j} e^{iqa(t-j)} D_{ij}(t) \quad , \quad (3.4)$$

we find that

$$\begin{aligned} [z + 2i\Gamma^F(q)] D(q, z) \\ = \tilde{C}^I(q) - \tilde{C}^F(q) - i\alpha\gamma_F [D_{i,i+1}(z) + D_{i,i-1}(z)] \quad . \end{aligned} \quad (3.5)$$

However

$$D_{i,i+1}(z) = D_{i,i-1}(z) = \int_{-\pi}^{\pi} \frac{dq}{2\pi} e^{-iq\alpha} D(q, z) \quad , \quad (3.6)$$

so we can easily solve for $D_{i,i+1}(z)$ to obtain

$$D_{i,i+1}(z) = \frac{1}{2i\alpha\gamma_F} \frac{I_1(z)}{I_0(z)} \quad , \quad (3.7)$$

where

$$I_1(z) = \int_{-\pi}^{\pi} \frac{dq}{2\pi} [z + 2i\Gamma^F(q)]^{-1} [\tilde{C}^I(q) - \tilde{C}^F(q)] \quad (3.8)$$

$$\frac{I_1(z)}{I_0(z)} = \frac{2i\alpha(1-\gamma_F^2)^{1/2}}{Q(z)} \left\{ \frac{1}{z + 2i\alpha(1-\gamma_F/\gamma_I)} \left[1 - \frac{\gamma_F}{\gamma_I} \left(\frac{1-\gamma_I^2}{1-\gamma_F^2} \right)^{1/2} Q(z) \right] - \frac{1}{z} [1 - Q(z)] \right\} \quad , \quad (3.12)$$

where

$$Q(z) = \left(\frac{1-\gamma_F^2}{1-\gamma_F^2 - (z/2\alpha)^2 - iz/\alpha} \right)^{1/2} \quad . \quad (3.13)$$

In the limit as $z \rightarrow 0$ one obtains the result

$$\frac{I_1(0)}{I_0(0)} = \frac{2u_F(u_I - u_F)}{(1 - u_I u_F)(1 - u_F^2)} \quad . \quad (3.14)$$

$$\tilde{C}(q, t) = \tilde{C}^F(q) + \frac{2\beta}{\pi} \int_{2\Gamma^F(0)}^{2\Gamma^F(\pi)} dx e^{-xt} \frac{[x - 2\Gamma^F(0)][2\Gamma^F(\pi)]^{1/2}}{x(2\beta - x)[2\Gamma^F(q) - x]} \quad , \quad (3.16)$$

where the integral is a principal-value integral and $\beta = \alpha(1 - \gamma_F/\gamma_I)$.

IV. TIME-DEPENDENT GINZBURG-LANDAU DESCRIPTION OF THE SAME PROBLEM

Before looking at Eq. (3.15) it is worthwhile to look at the results for the same problem analyzed using the time-dependent Ginzburg-Landau model (TDGL).⁴ In this case the fixed length spin variables are replaced by continuum fields $\phi(\bar{x})$ and the

and

$$I_0(z) = \int_{-\pi}^{\pi} \frac{dq}{2\pi} \frac{1}{z + 2i\Gamma^F(q)} \quad . \quad (3.9)$$

Inserting this result back into the equation for $D(q, z)$ we obtain

$$D(q, z) = [z + 2i\Gamma^F(q)]^{-1} \left[\tilde{C}^I(q) - \tilde{C}^F(q) - \frac{I_1(z)}{I_0(z)} \right] \quad . \quad (3.10)$$

In this form we see that the exact sum rule

$$\int_{-\pi}^{\pi} \frac{dq}{2\pi} D(q, z) = D_{ii}(z) = 0 \quad , \quad (3.11)$$

which follows from Eq. (3.2) evaluated for $i = j$, is satisfied trivially by our solution. It is then a matter of straightforward integration to evaluate the ratio $I_1(z)/I_0(z)$ explicitly:

We then have the solution for $\tilde{C}(q, t)$ given by

$$\tilde{C}(q, t) = \tilde{C}^F(q) + i \int_{-\infty}^{+\infty} \frac{dz}{2\pi} e^{-izt} D(q, z) \quad (3.15)$$

together with Eqs. (3.10), (3.12), and (3.13). This can be simplified using complex variable theory. We find

equilibrium statistics are governed by the probability distribution

$$P[\phi] = e^{-F[\phi]}/Z_G \quad , \quad (4.1)$$

where F is the Ginzburg-Landau free energy

$$F[\phi] = \frac{1}{2} \int d^d x \left[c[\nabla\phi^{(x)}]^2 + r_0\phi^2(x) + \frac{u}{2}\phi^4(x) \right] \quad (4.2)$$

(we define the model in d dimensions) and Z_G is the

partition function which is the functional integral

$$Z_G = \int D(\phi) e^{-F[\phi]} . \quad (4.3)$$

The temperature dependence is absorbed in the constants c , r_0 , and u . The dynamics in this model are generated by a generalized Fokker-Planck operator

$$D_\phi = \int d^d x \frac{\delta}{\delta \phi(x)} \Gamma_0 \left[\frac{\delta}{\delta \phi(x)} + \frac{\delta F}{\delta \phi(x)} \right] , \quad (4.4)$$

where Γ_0 is assumed to be temperature independent. The nonequilibrium structure factor of interest in this case is given by

$$\begin{aligned} & \tilde{C}_{\text{TDGL}}(q, t) \\ &= \frac{1}{V} \int d^d x d^d x' e^{i \vec{q} \cdot (\vec{x} - \vec{x}')} \tilde{C}_{\text{TDGL}}(\vec{x} - \vec{x}', t) , \end{aligned} \quad (4.5)$$

where

$$\tilde{C}_{\text{TDGL}}(\vec{x} - \vec{x}'; t) = \int D(\phi) \phi(x) \phi(x') e^{D_\phi^T P_{T_I}[\phi]} . \quad (4.6)$$

It is straightforward to show, to zeroth order in the quartic coupling u , that

$$\begin{aligned} \tilde{C}_{\text{TDGL}}(q, t) &= \tilde{C}_{\text{GL}}^F(q) \\ &+ e^{-2\Gamma_G^F(q)t} [\tilde{C}_{\text{GL}}^I(q) - \tilde{C}_{\text{GL}}^F(q)] , \end{aligned} \quad (4.7)$$

where

$$\tilde{C}_{\text{GL}}^F(q) = \frac{1}{c^F q^2 + r_0^F} , \quad (4.8)$$

$$\tilde{C}_{\text{GL}}^I(q) = \frac{1}{c^I q^2 + r_0^I} , \quad (4.9)$$

$$\Gamma_G^F = \Gamma_0(c^F q^2 + r_0^F) . \quad (4.10)$$

The result for the TDGL model given by (4.7) is very simple and intuitively obvious. Each Fourier component “relaxes” from its initial to its final values with a simple exponential time dependence.

For a large quartic coupling u and negative r_0 in (4.2) we expect that the TDGL and kinetic Ising models should be rather similar.⁴ It is also natural, because of our experiences in dynamic critical phenomena, to associate the TDGL model with the kinetic Ising model. Presumably they are in the same universality class. Typically, in dealing with the TDGL model, we must resort to perturbation theory in the quartic coupling u . As a first approximation then, we expect that a “relaxational” form like (4.7), given by

$$\tilde{C}_R(q, t) = \tilde{C}^F(q) + e^{-2\Gamma^F(q)t} [\tilde{C}^I(q) - \tilde{C}^F(q)] , \quad (4.11)$$

might be a good approximation to $\tilde{C}(q, t)$ given by Eq. (3.15).

V. BEHAVIOR OF $\tilde{C}(q, t)$

Let us consider first the short-time behavior of $\tilde{C}(q, t)$. We easily obtain

$$\tilde{C}(q, t) = \tilde{C}^I(q) - \alpha t S(q) + O(t^2) , \quad (5.1)$$

where

$$S(q) = \frac{2(\gamma_I - \gamma_F)(\cos qa - u_I)}{(1 - \gamma_I^2)^{1/2}(1 - \gamma_I \cos qa)} . \quad (5.2)$$

Notice that for a wave number q_2 , defined by

$$\cos q_2 a = u_I , \quad (5.3)$$

the linear term in time in (5.1) vanishes. If we treat the case $\gamma_F > \gamma_I$ then for $q > q_2$, $S(q) > 0$ and $\tilde{C}(q, t)$ initially decreases. If, however, $q < q_2$, $S(q) < 0$, and $\tilde{C}(q, t)$ initially increases. Note also, however, that there is some wave number q_1 where $\tilde{C}_I(q_1) = \tilde{C}_F(q_1)$ and which is given by

$$\cos q_1 a = \tanh(K_I + K_F) . \quad (5.4)$$

If, for example, $K_I = 0.5$ and $K_F = 1$, then $q_2 a = 1.09$ and $q_1 a = 0.439$. For $q < q_1$, $\tilde{C}^I(q) < \tilde{C}_F(q)$, and for $q > q_1$, $\tilde{C}_I(q) > \tilde{C}_F(q)$. We see then for $q_1 < q < q_2$ $\tilde{C}(q, t)$ initially increases even though $\tilde{C}_I^F(q) < \tilde{C}_I^I(q)$. Therefore there must be a time when $\tilde{C}(q, t)$ stops growing and begins its final decay to $\tilde{C}_F(q)$.

Looking at the long-time behavior we find (for $q > 0$)

$$\begin{aligned} \tilde{C}(q, t) &= \tilde{C}^F(q) + \frac{1}{4\sqrt{\pi}} \frac{e^{-2\Gamma^F(0)t}}{(\alpha \gamma_F t)^{3/2}} \\ &\times \frac{\gamma_F - \gamma_I}{(1 - \gamma_F)(1 - \gamma_I)} \frac{1}{(1 - \cos qa)} . \end{aligned} \quad (5.5)$$

The zero at $\gamma_F = \gamma_I$ corresponds to no quench, while the poles at γ_F or $\gamma_I = 1$ correspond to “freezing in” at $T = 0$. Again we can see a difference from the relaxation result given by Eq. (4.11). Note first that the asymptotic decay goes as $e^{-2\Gamma_0^I t}/t^{3/2}$ instead of the considerably more rapid behavior $e^{-2\Gamma^F t}$. Next we observe that the relaxation result for $q < q_1$ predicts that $\tilde{C}(q, t) - \tilde{C}^F < 0$ as $t \rightarrow \infty$ and we approach $\tilde{C}^F(q)$ from below. Equation (5.4) tells us however that $\tilde{C}(q, t) - \tilde{C}^F > 0$ as $t \rightarrow \infty$. That is, we approach $\tilde{C}^F(q)$ from above.

The $q = 0$ limit of $\tilde{C}(q, t)$ for long times is a special case not given by (5.5). We find in the long-time

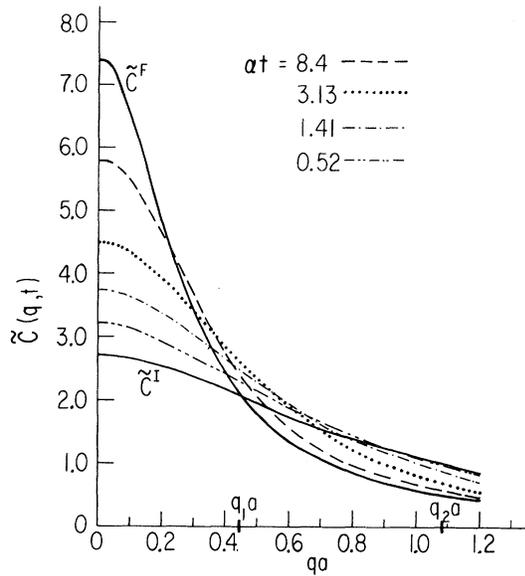


FIG. 1. $\tilde{C}(q, t)$ as a function of q for $K_I=0.5$, $K_F=1.0$. The solid lines are $\tilde{C}^I(q)$ and $\tilde{C}^F(q)$. Intermediate times $\alpha t = 0.52, 1.41, 3.13, 8.4$ are shown in dashed lines and/or dots.

limit

$$\tilde{C}(0, t) \sim \tilde{C}^F(0) + \frac{1}{\sqrt{\pi}} e^{-2\gamma^F(0)t} \left[\frac{\gamma_I - \gamma_F}{(\alpha\gamma^F t)^{1/2} (1 - \gamma_F)(1 - \gamma_I)} \right] \quad (5.6)$$

and $\tilde{C}(0, t)$ approaches $\tilde{C}^F(0)$ from below.

In Figs. 1–3 we present results for intermediate

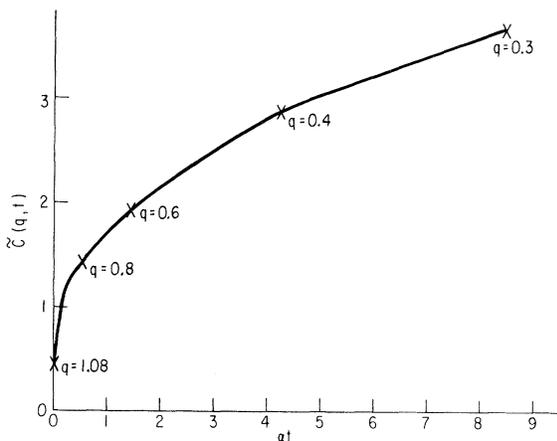


FIG. 2. Peak values of $\tilde{C}(q, t)$ are plotted as a function of the time at which they occur for a given q . Some specific values of q are marked with an x to show that large- q modes reach a maximum much earlier than small- q modes. These data are for $K_I=0.5$ and $K_F=1.0$.

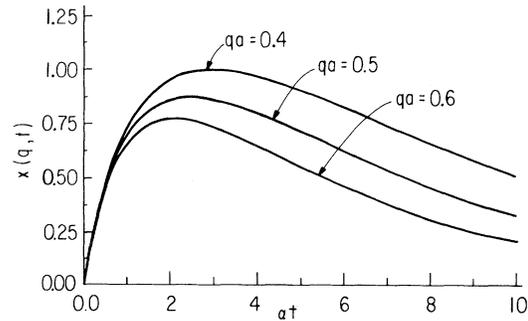


FIG. 3. The structure factor minus the relaxational component is plotted as a function of t for $qa = 0.4, 0.5, 0.6$. $x(q, t) = \tilde{C}(q, t) - \tilde{C}_R(q, t)$, $K_I=0.1$, and $K_F=1.0$.

times. In Fig. 1 we plot $\tilde{C}(q, t)$ as a function of q for various times for a quench from $K_I=0.5$ to $K_F=1$. Inspection of Fig. 1 shows an agreement with our arguments above that for intermediate wave numbers the structure factor does not simply relax from its initial to its final value. Thus we see, for example, for $qa = q_1 a \sim 0.44$ [where $\tilde{C}^I(q) = \tilde{C}^F(q)$] that initially $\tilde{C}(q, t)$ rises by a factor of $\sim 30\%$ and then decays back to its final value. We can plot the time when the maximum occurs, as shown in Fig. 2, and see that the time when the maximum occurs for a given wave number increases rapidly with decreasing value of the wave number. In Fig. 3 we have plotted the difference between our structure factor and the relaxational form (4.11). This emphasizes the role of these “structure pulses” which are not present in the relaxational approximation.

The physics behind the pulse which moves in time from large to small wave numbers is straightforward. As time evolves the short-wavelength degrees of freedom will relax to their final values more rapidly [see Eq. (2.15)] than do the long-wavelength degrees of freedom. However, we have a sum rule,

$$\int_{-\pi}^{+\pi} \frac{d(qa)}{2\pi} \tilde{C}(q, t) = 1, \quad (5.7)$$

which holds for all times. If $\tilde{C}(q, t)$ has lost weight for large q 's then where is the weight to go? Clearly it must move to progressively smaller wavenumbers.

It is clear that the nonequilibrium dynamics of the KI model and that of the TDGL model are qualitatively different for a wide range of wave numbers $0 < q < q_2$. This difference is essentially due to the fixed length spin condition in the Ising model and the existence of an associated temperature-independent sum rule.

VI. IMPLICATIONS FOR OTHER SYSTEMS AND HIGHER DIMENSIONS

It seems that these structure pulses should exist in higher dimensions and other types of dynamical systems. Physically they seem to require only that one range of Fourier components decay more rapidly than another range and that there exist a temperature independent (or weakly dependent) sum rule for the structure factor. We expect an even more pronounced effect in systems where the "order" param-

eter is conserved and where there is clearer separation of time scales as one varies the wave number.

ACKNOWLEDGMENTS

One of us (G. M.) would like to acknowledge support from an Alfred P. Sloan Foundation Fellowship. This work was also supported by the NSF Materials Research Laboratory at the University of Chicago.

¹R. J. Glauber, *J. Math. Phys.* **4**, 294 (1963). In particular Glauber discussed the nonequilibrium problem of interest here and calculated $\tilde{C}_j(t)$ as defined by Eq. (2.23). [See Eqs. (63) and (64) in Glauber's paper.] He did not analyze the Fourier transform $\tilde{C}(q,t)$.

²For further discussion of these operators see G. Mazenko, M. Nolan, and O. Valls, *Phys. Rev. B* **22**, 1263 (1980).

³M. Suzuki, *Int. J. Magn.* **1**, 123 (1971).

⁴K. Binder, *Phys. Rev. B* **8**, 3423 (1973).