PHYSICAL REVIEW A VOLUME 35, NUMBER 12 JUNE 15, 1987

Center-manifold renormalization in dynamic critical phenomena for dissipative spin systems

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(Received 8 December 1986)

We consider a purely dissipative spin system operating far from thermodynamic equilibrium. We prove that a coarse graining for short-wavelength modes is obtained near criticality by performing a center-manifold reduction of fast-relaxing modes. The spin systems considered are realizations of a time-dependent Ginzburg-Landau model. Agreement with renormalization-group derivations is obtained. Neutron scattering cross sections for a magnetic material in the dynamic critical case are calculated making use of the center-manifold reduction. Experimental measurements of static spin autocorrelations are used to obtain the distribution of fast modes about the center manifold. Making use of this information, predictions are made on neutron scattering for magnetic materials coupled to a heat bath near a dynamic critical point. The existence of a center manifold determines scaling relations between the strength of the statistical forcing field and the spin-correlation length. Thus, the relevance of a time-dependent experiment under far-from-equilibrium conditions becomes apparent inasmuch as such an experiment can lead to the elucidation of the nature and strength of the statistical noise.

I. INTRODUCTION

The stability and permanence of far-from-equilibrium organizations in dissipative systems may be ensured when a center manifold (CM) can be associated with the emerging structures.[1–4] This manifold constitutes the locally attractive and locally invariant portion of phase space emerging beyond a dynamic instability. The CM reduction accounts for the contraction in phase space due to a statistical subordination of fast-relaxing modes to order parameters which occurs in dynamic critical phenomena.[4–6] The basic tenet of this approach is that the probability density is distributed in a narrow strip along the CM. The width of this strip depends on the position on the CM, that is, on the CM coordinates and it can be taken as constant only to a first approximation.[2–4] The distribution of fast modes about the CM will be determined in this paper and the results will be used to get information on neutron scattering cross sections for dissipative spin systems near a dynamic critical point.

The "critical slowing down" property for spin systems implies that long-wavelength modes also have long-relaxation-time scales.[5–7] We shall take advantage of this fact in order to obtain a coarse-graining CM reduction of the short-wavelength modes. The CM-reduced Fokker-Planck (FP) equation determines the dominant role of long-relaxation-time modes. That is, the CM elimination of fast-relaxing modes can be adequately viewed as a decrease in spatial resolution to eliminate short-wavelength modes as in a dynamic Kadanoff transformation.[5,8]

In spin systems, the probability distribution P may be factorized into an equilibrium stationary distribution times a perturbation from equilibrium. The distribution P obeys a Liouville master equation. The transition probability rates satisfy a detailed balance which ensures the ergodicity of the system.[8] Our approach is analogous in that it introduces a factorization of P determined by the renormalization-group (RG) transformation R_s. We represent P as a product of a time-dependent factor for the slow modes, Q_1, and a time-independent factor Q_2, conditionally dependent on the CM coordinates. This factorization must ensure a continuous flow of probability about the CM. Instead of obtaining the Gaussian widths for the probability density in analytic form, we shall present the results of a numerical integration of the Fokker-Planck equation making use of adequate scaling for the Gaussian widths in order to display the relative size of each term in the CM-reduced equation. Thus, the integration reveals the scaling relations between the static spin correlation length and the other relevant small parameters of the system: the Gaussian widths and the intensity of the fluctuations due to the coupling of the system to the heat bath. These scaling relations determine the range for the statistical noise. Therefore, a neutron scattering experiment[9] performed under far-from-equilibrium conditions for a dissipative spin system would be most useful since the distribution about the CM can be derived from scattering cross sections and that information can be used to obtain the range for the statistical noise forcing field. This point will be developed in Sec. IV.

The CM reduction has a counterpart in static phenomena. This counterpart is given by the smooth cutoff procedure to eliminate long-range interactions in coordinate space.[6] But while this procedure is a purely mathematical artifact, the CM reduction finds a physical justification in the statistical enslavement of the fast-relaxing degrees of freedom by the order parameters.

II. COARSE GRAINING CENTER-MANIFOLD REDUCTION

Consider a set of block spins $\{y_i(x,t)\}$, where the subindex i labels the spin component and x is the spatial coordinate. We shall use the Fourier representation and consider the components $y_{ip}=y_{ip}(t)$.

Each y_{ip} is regarded as a random variable. Thus, the object of interest is the probability density functional $P(\{y_{ip}\},t)$. We shall now demonstrate that the distribution of the y_{ip}'s about the CM provides the necessary information to calculate dynamic spin autocorrelations. These quantities are directly measurable in slow neutron scattering experiments. The magnetic material should be coupled to a heat reservoir constituting a dissipative system operating far from thermodynamic equilibrium.

We shall consider an initial spatial resolution to order L^{-1}. A coarse graining Kadanoff transformation K_s corresponds to a cutoff in the wavelength range and spatial resolution to order s/L. That is, the short-wavelength modes in the range $L/s \le q \le L$ must be eliminated and a reduced equation for the y_{ik}'s with $0 \le k < L/s$ must be obtained. Throughout the paper, the ranges for the indexes k and q are as indicated above, the i's and j's range from 1 to n and the p's from 0 to L.

We associate a CM to a transformation K_s in the following way:

$$\hat{y}_{jq}=\sum_{n'=2}^{\infty} b_{jqn'}\left[\prod_{\substack{i,k\\ \Sigma l_{ik}=n'}} y_{ik}^{l_{ik}}\right] . \tag{1}$$

This CM is denoted CM(s). The long-wavelength modes y_{ik}'s are therefore regarded as the CM coordinates. They are the order parameters when we downgrade the spatial resolution from order L^{-1} to order s/L. Following the methods of the standard CM reduction, we factorize $P=P(\{y_{ip}\},t)$ in the following way:

$$P=Q_1(\{y_{ik}\},t)Q_2(\{y_{jq}\}\mid\{y_{ik}\}) . \tag{2}$$

The explicit form of Q_2 was derived elsewhere:[2–4]

$$Q_2=\prod_{j,q}(g_{jq}/\pi)^{1/2}\exp\{-g_{jq}[y_{jq}-\hat{y}_{jq}(\{y_{ik}\})]^2\} . \tag{3}$$

The Gaussian widths w_{jq} are given by

$$w_{jq}=g_{jq}^{-1/2}=g_q^{-1/2} . \tag{4}$$

These quantities are functions of the CM coordinates and they are determined making use of the condition that they should allow for a continuous flow of probability about the CM.[2–4]

The CM-reduced FP equation will be directly obtained by numerical integration of the FP equation for P with adequate scaling relations to display the relative size of each term, introducing the factorization $P=Q_1Q_2$. The analytical derivation of $g_q=g_q(\{y_{ik}\})$ is a formidable task. Instead we shall obtain an approximate solution in terms of static spin autocorrelations and also display the second moments $\theta_q=\langle(y_{jq}-\langle y_{jq}\rangle)^2\rangle$ which result from the numerical integration. The general form of the g_q's is $g_q=G(q)^{-1}+O(\{\,|y_{ik}|^2\})$. The constant term represents the balance between the fast drift towards the CM and the diffusion effect provided by the statistical noise.[1–4] This term is equal to the reciprocal of the static spin autocorrelation, $G(q)$, and it is directly accessible from neutron scattering data for static critical phenomena.[9]

At this point, it is worth outlining a smooth cutoff procedure introduced in static critical phenomena to eliminate unwanted long-range interactions in coordinate space. These interactions are reminiscent of the Friedel oscillations due to a sharp Fermi surface which occurs in the physics of metals.[6]

We note by H the spin Hamiltonian. The transformation $K_sH=H'$ is defined as follows:

$$e^{-H'(y')}=\int\left[\prod_{i,p} dy_{ip}\right]e^{-H(y)}Q(y,y') , \tag{5}$$

where

$$Q(y,y')=N\exp\left[-\frac{w}{2}\sum_{i,p}(y'_{ip}-x_py_{ip})^2\right] \tag{6}$$

and N is the normalization constant. The variable w can be fixed arbitrarily large and x_p is a smooth function subject to the restrictions

$$x_p=\begin{cases}1 & \text{for } p\le L/s ,\\ 0 & \text{for } p\ge L/s+\Delta,\ \ \Delta \ll L/s .\end{cases} \tag{7}$$

We can pose the problem of finding the dynamic counterpart of this procedure. This will involve taking advantage of the subordination of fast variables in the integration of the FP equation for P factorized as indicated in Eqs. (1)–(4), over the fast-relaxing modes. This procedure is analogous to the one described above except that now each mode has a Gaussian width $g_p^{-1/2}$ instead of the constant $(w/2)^{-1/2}$ and the variables x_py_{ip} are replaced by $\hat{y}_{ip}$ for $p\ge L/s$. The smoothing is accomplished by the functional dependence of modes determined by Eq. (1). We should emphasize that while the static smoothing is a mathematical device, its dynamic counterpart is rooted in the CM statistical subordination of fast modes, that is, on physical grounds.

III. CENTER MANIFOLD FOR A DISSIPATIVE SPIN SYSTEM

The onset of a CM determines scaling relations among the small parameters in the system.[4(b)] This fact will be used in order to properly display the size of the terms which occur in the integration of the FP equation for P along the CM. In the case of spin systems near criticality, a convenient set of such small parameters is the following.

(a) The inverse of the spin correlation length.

(b) The Gaussian widths.

(c) The intensity of the random source terms.

Specifically, we consider a generic time-dependent Ginzburg-Landau spin model in which each of the block spins is in contact with a thermal reservoir. The heat conduction occurs sufficiently fast so that the condition of each reservoir is independent of the spin configuration. This is a valid assumption since the spin correlation length ξ diverges as we reach criticality; therefore, we have $\rho/\xi\to 0$, where ρ is the correlation length for the thermal statistical source. That is, we can regard the heat bath as a set of independent noise sources corresponding to additive noise and independent of each other.

In the Fourier representation, the model is determined by the equations[6]

$$\frac{\partial y_{ip}}{\partial t}=-MD_{i-p}H+f_{ip} , \quad (8)$$

$$D_{ip}=\frac{\partial}{\partial y_{ip}} , \quad (9)$$

$$H=H_0+H_1 , \quad (10)$$

$$H_0=\tfrac{1}{2}\sum_{i,p}[a(T-T_c)+p^2]\,|y_{ip}|^2 , \quad (11)$$

$$H_1=\tfrac{1}{2}uW^{-d}\sum_{i,j,p,p',p''} y_{i,-p}y_{j,p'}y_{j,p''}y_{i,p-p'-p''} , \quad W=\text{size parameter} . \quad (12)$$

$$\langle f_{ip}(t)f_{ip'}(t')\rangle=2M\delta_{ij}\delta_{-pp'}\delta(t-t') . \quad (13)$$

The parameter space is the vector space $[(M,a(T-T_c),u)]$, where a and u are the Ginzburg-Landau parameters.

To a first approximation,[2–4] the g_{jq}'s can be regarded as constants representing the balance between the fast drift, given by the inverse of the relaxation time, T_q, and the strength of the intrinsic fluctuations given by the effective diffusion coefficient M. That is,

$$g_q=\frac{M[a(T-T_c)+q^2]}{M}=a(T-T_c)+q^2=G(q)^{-1} , \quad (14)$$

where the relaxation time is given by

$$T_p=[a(T-T_c)+p^2]^{-1}M^{-1} . \quad (15)$$

The static spin correlation $G(q)$ is defined: $G(q)=\langle\,|y_{jq}|^2\rangle$.

The long-wavelength modes (p small) also have long relaxation times. This follows directly from Eqs. (14) and (15) and the relation

$$\lim_{\substack{T\to T_c\\ p\to 0}} T_p=\lim_{T\to T_c}\chi(T)M^{-1}=\infty , \quad (16)$$

where $\chi(T)$ is the susceptibility. It is this property that allows for the implementation of a coarse-graining procedure based on a CM reduction.

CM(s) can be determined from Eqs. (1) and (8)–(12).[1–4] That is, from the following polynomial relation which expresses that the y_{jq}'s are not explicitly dependent on time but are indirectly dependent since they are subordinated to the y_{ik}'s:

$$-MD_{j-q}H=\sum_{i,k}D_{ik}(\hat{y}_{jq})(-MD_{i-k}H) . \quad (17)$$

The FP equation for P is

$$\frac{\partial}{\partial t}P=M\sum_{j,p}D_{jp}[(D_{j-p}H)P+D_{j-p}P] . \quad (18)$$

We shall denote

$$\bar{F}=\int\left[\prod_{i,q}dy_{iq}\right]Q_2F \quad (19)$$

for any functional $F=F(\{y_{jp}\})$. Therefore, from Eq. (14), it follows that for large L (high initial resolution) and small s (soft coarse graining), we get

$$\bar{F}=F(\{y_{ik}\},\{\hat{y}_{jq}\}) . \quad (20)$$

Making use of Eqs. (2) and (3) and the notation given by Eq. (19), we can integrate Eq. (18) over the short-wavelength—fast-relaxing modes y_{iq}'s. This gives

$$\begin{aligned}\frac{\partial}{\partial t}Q_1=&M\sum_{i,k}\left[D_{ik}[(D_{i-k}\bar{H})Q_1]+n(D_{ik}\bar{H})\sum_q\frac{D_{ik}g_q}{2g_q}Q_1\right]-4M^2\sum_{i,j,k,q}g_q[D_{ik}(\overline{D_{j-q}H})]Q_1+M\sum_{i,k}D_{ik}D_{i-k}Q_1\\&+nM\sum_{i,k,q}\left[\frac{D_{ik}g_q}{g_q}D_{ik}Q_1\right]+nM\sum_{i,k,q}\frac{D_{ik}D_{i-k}g_q}{2g_q}Q_1-\frac{n}{4}M\sum_{i,k,q}\left[\frac{D_{i-k}g_q}{g_q}\right]^2Q_1-2M^3\sum_{i,j,k,q}g_q(D_{ik}\overline{D_{j-q}H})^2Q_1 .\end{aligned} \quad (21)$$

Instead of attempting an analytic solution of the form $g_q=g_q(\{y_{ik}\})$ to obtain the CM-reduced equation from Eq. (21), we present the results of a numerical integration of Eq. (21) (Fig. 1, curve b). The scaling adopted to get the reduced equation is $M=O(W^{-3})$, $g_q=O(W^{-2})+q^2$, $W=O(\xi)$ (since spin fluctuations have a macroscopic range near criticality). Specifically, we take $\xi=55.2$ Å following Ref. 9 (in their notation, $\xi^{-1}=\kappa=0.0181$ Å^{-1}). On the other hand, curve a in Fig. 1 gives the second moment θ_q as obtained from the approximation $g_{jq}=[G(q)]^{-1}$. In this case, the autocorrelations $G(q)$'s are obtained from neutron scattering data.[9]

Making use of this approximation and the fact that H_1 is of order W^{-3} for this problem, we get, to order W^{-3}, the reduced equation

$$\frac{\partial}{\partial t}Q_1=M\sum_{i,k}\{D_{ik}[(D_{i-k}\overline{H_0})Q_1]+D_{ik}D_{i-k}Q_1\} . \quad (22)$$

The results of numerical integration can be used to get the proper dynamic spin autocorrelations $\tilde{G}(q)=g_q^{-1}$. To first approximation, we have seen that $\tilde{G}(q)=G(q)$.

In Fig. 2, curves a and b correspond to different calculations making use of the Ornstein-Zernike and Hart equilibrium spin autocorrelations, respectively, reported elsewhere.[9] Curve c, instead, gives the scattering cross sections for a dissipative system, coupled to a heat bath, with the dynamic autocorrelations, $\tilde{G}(q)$'s.

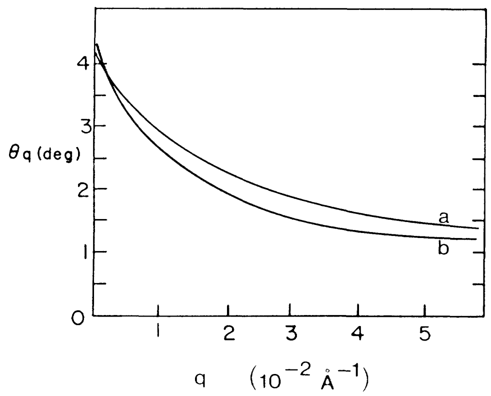

FIG. 1. Distribution of fast modes about the center manifold. Second moments θ_q's as functions of the wave number. The choice of parameters is $M=2.2W^{-3}$, $W=\xi=55.2$ Å. Curve a is obtained by making the approximation $g_{jq}=[G(q)]^{-1}$. The autocorrelations, $G(q)$'s, are determined from the scattering cross sections for equilibrium critical points (Ref. 9). Curve b is obtained by numerical integration of the CM-reduced equation (21).

The nature of this bath and the intensity of its associated random source can be determined in a time-dependent neutron scattering experiment. The dynamic spin autocorrelation in a dissipative magnetic material are directly accessible from experimental data. Making use of this information, the Gaussian widths of the distribution Q_2 can be derived. Since there are scaling relations linking the small parameters of the system at the onset of a CM, the noise intensity range can be calculated. The dynamic experiment, however, cannot be compared to its static counterpart (given in Ref. 9) yielding equilibrium spin autocorrelations. This is no since the intensity of the forcing field provided by the random source is not an independent parameter which can be varied arbitrarily. Its range is controlled by the scaling relations imposed by the existence of a CM; thus, the static case is in no sense a limit of the dynamic one taking $M\to 0$ since the latter procedure is not valid.

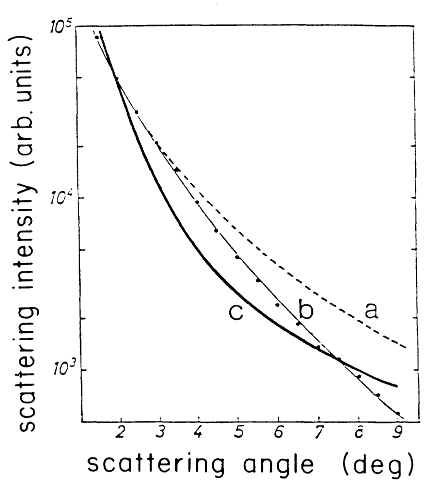

FIG. 2. Scattering intensities near an equilibrium critical point (curves a and b) and for a dissipative spin system coupled to a heat bath (curve c). The scattering angle is given in degrees. Curve a corresponds to an Ornstein-Zernike equilibrium spin correlation function with effective correlation length $\xi=(0.005\,83)^{-1}$ Å. Curve b was obtained with a Hart correlation function with $\xi=(0.0181+0.184)^{-1}$ Å. Curves a and b are from Ref. 9. Curve c was obtained making use of the numerical integration of Eq. (21) giving the dynamic correlation $\tilde{G}(q)$.

IV. CENTER-MANIFOLD RENORMALIZATION

In this section we shall consider for the sake of mathematical simplicity the case in which the dimension of the system is $d>4$. This case will serve as an illustration to show that the coarse-graining procedure based on a CM reduction and the renormalization-group approach yield the same results. The first-order approximation $g_{jq}=G(q)^{-1}$ will be assumed throughout this section.

As s becomes small, the distribution Q_2 behaves like a Dirac δ function peaked at the CM. That is, for soft coarse graining with sharp initial resolution (large L), we get from Eqs. (3) and (4)

$$\lim_{\substack{L/s\le q\le L\\ s\to 1\\ L\ \text{large}}} Q_2=\prod_{i,q}\delta(y_{iq}-\hat{y}_{iq})\ . \tag{23}$$

This allows us to obtain an explicit expression for the infinitesimal operator $\tilde{K}$ for the semigroup of transformations K_s induced by the family of manifolds [CM(s)]

$$\begin{aligned}\tilde{K}&=\lim_{\delta\to 0}\left[\frac{1}{\delta}(K_{1+\delta}-1)\right]\\ &=\lim_{\delta\to 0}\frac{1}{\delta}\left[\left[\prod_{\substack{L/(1+\delta)\le q\le L\\ i=1,2,\ldots,n}}\delta(y_{iq}-\hat{y}_{iq})\right]-1\right]\ .\end{aligned} \tag{24}$$

On the other hand, for large s, we find that the long-wavelength modes which have large correlations near criticality (since $q\approx L/s$ is small) are more broadly distributed about the CM than the short-wavelength modes ($q\gg L/s$).

Along the manifold $[M,a(T-T_c),0]$, we get

$$D_{i-k}\overline{H}=[a(T-T_c)+k^2]y_{ik}\ . \tag{25}$$

In order to find the renormalization-group transformation R_s, we consider the critical manifold $(M,0,0)$ and apply the rescaling transformation N_s to the set of Langevin equations equivalent to Eq. (22):

$$\frac{\partial}{\partial t}y_{ik}=-Mk^2y_{ik}+f_{ik}\ . \tag{26}$$

By replacing y_{ik} for $sy_{isk}(ts^{-z})$, we get

$$\frac{\partial}{\partial t}sy_{isk}(ts^{-z})=-Mk^2sy_{isk}(ts^{-z})+f_{ik}\ . \tag{27}$$

Let us make the substitution

$$sk = k', \quad s_t^{-z} = t', \quad s^{-1+z} f_{i(k'/s)}(t' s^z) = f'_{ik'}(t') .$$

Then we get

$$\frac{\partial}{\partial t} y_{ik'}(t') = -M'(k')^2 y_{ik'}(t') + f'_{ik'}(t') , \tag{28}$$

$$\langle f'_{ik'}(t') f'_{ik''}(t'') \rangle = 2M' \delta(t' - t'') \delta_{ij} \delta_{-k'k''} , \tag{29}$$

where $M' = Ms^{z-2}$. Therefore, $R_s(M,0,0) = (Ms^{z-2},0,0)$. This transformation has stable fixed points if and only if $z = 2$, a result already obtained from renormalization-group theory.[6]

It is worth noticing that for a spatial resolution to order s/L, the corresponding reduced equation (22) is valid in the whole parameter space; it is not restricted to the critical manifold as is the case in previous treatments.[5–8]

V. CONCLUSION

We have shown how the CM coarse-graining reduction can be implemented to predict dynamic spin autocorrelations which can be measured by neutron scattering in far-from-equilibrium systems coupled to a heat bath. In order for a CM to emerge, we have shown that the strength of the random source must be properly scaled with the size parameter of the system. [See also Ref. 4(b).] This fact determines the importance of a time-dependent neutron scattering experiment under far-from-equilibrium conditions since the range in the strength of the random source can be readily calculated from the dynamic scattering cross sections, as shown in Sec. IV. We have also shown analytically the equivalence of a CM reduction and a renormalization-group treatment in the case $d > 4$.

ACKNOWLEDGMENT

Financial support from the U.S. Office of Naval Research is gratefully acknowledged.

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