

Fluctuation-response relation for steady states

Marco Paniconi

Department of Physics and Astronomy, University of Pittsburgh, Pittsburgh, Pennsylvania 15260

(Received 31 July 1997; revised manuscript received 20 October 1997)

The fluctuation-response relation for Langevin dynamics in the small noise limit, recently introduced, is generalized for the purpose of computing the fluctuation spectrum of a nonequilibrium system. The fluctuation-response relation provides an efficient and operational means to compute the fluctuations around a nonequilibrium steady state. As an example, we consider a model of a magnetic system driven away from (local) equilibrium by an oscillating magnetic field. The generalized fluctuation-response relation is utilized to compute the fluctuation spectrum of the driven system, which is shown to display some interesting behavior near the transition region (where the system undergoes a transition from a nonzero to zero *time-averaged* state). [S1063-651X(98)10303-3]

PACS number(s): 02.50.Ey, 05.20.-y, 05.40.+j

I. INTRODUCTION

The fluctuation-response relation for systems in equilibrium [1] is the well-known statement that relates spontaneous thermodynamic fluctuations to thermodynamic responses (susceptibility). The generalization of this relation to the frequency and wave vector domain is the equilibrium fluctuation dissipation theorem (FDT) [2,3]. The relation gives us a means to obtain, e.g., the spectrum of an observable at a particular frequency, by adding the appropriate conjugate force to the system Hamiltonian.

The computation of the fluctuation spectrum for nonequilibrium steady states is, in contrast, a difficult task. Since ‘‘Hamiltonians’’ for nonequilibrium steady states, even if they exist, are not known, there is no guiding principle that tells us how to add appropriate perturbations to the system. It would be desirable, and interesting in its own right, to have a method to compute the fluctuation spectrum operationally via a linear response. From an experimental standpoint, this would make the determination of the fluctuation spectrum easily accessible.

In this paper, in the context of an arbitrary Langevin dynamics, we will discuss a generalized fluctuation response that provides an efficient and operational means to compute the fluctuation spectrum of a nonequilibrium steady state. Here, steady state implies any state whose long-time statistics is meaningful. The fluctuation-response relation around a nonequilibrium steady state was introduced in [4] to compute the fluctuations of time-averaged observables. In this paper we extend the formalism to the frequency domain, and use it to compute the full fluctuation spectrum [$\langle |M(\omega) - \langle M(\omega) \rangle|^2 \rangle$, for some observable $M(t)$] of a periodically driven system.

The system is a simple model of a magnetic system driven away from local equilibrium by a (large) oscillating magnetic field. It was shown [5] to undergo a transition from a state with a nonzero (NZ) time-averaged magnetization to a zero (Z) time-averaged magnetic state. The fluctuation spectrum displays rather interesting and peculiar behavior near the transition region that will be illustrated and discussed below. The model system considered here is experimentally realizable. Therefore, the elucidation of a generalized fluctuation-response relation, and the results that follow,

should be of direct interest to experimentalists.

General relations between fluctuations and response functions for Markov processes have been studied in the past [6,7]. However, without the condition of detailed balance, the correct coupling of the forces to the system to elicit the correct response requires knowledge of the steady state measure, which makes the approach not feasible in practice. The approach we discuss in this paper (introduced in [4]) is not only operational, but practical. In contrast to the usual formulations of fluctuation response relations, we introduce a generalized fluctuation-response relation from the starting point of capturing (via a linear response function) the fluctuations of *time-averaged* observables. The proper perturbing force required to extract the fluctuation is explicitly realized as an external force in the dynamical model (Langevin equation).

The paper is organized as follows. In the next section, we briefly introduce some necessary theoretical background. In Sec. III, we discuss the generalized fluctuation-response relation. The model system and the results are presented in Sec. IV, with a concluding discussion in Sec. V.

II. THEORY

Consider the class of stochastic processes described by Langevin equations of the form

$$\dot{M}_i(t) = b_i(M, t) + \epsilon \sigma_{ij}(M) \eta_j(t), \quad (2.1)$$

where $i = 1, 2, \dots, N$ are the N components of the stochastic vector $M(t)$ field, $b(M, t)$ a time-dependent (vector-valued) function of $M(t)$, $\sigma(M)$ a (matrix-valued) function, $\eta(t)$ is the zero mean Gaussian white noise with covariance $\langle \eta_i(t) \eta_j(s) \rangle = \delta(t-s) \delta_{ij}$, and the parameter ϵ is the overall strength of the noise. If the noise corresponds to fluctuations from internal degrees of freedom, it typically scales (according to the central limit theorem) as $\epsilon^2 \approx 1/V$, where V is the system size (or the total number of degrees of freedom). Hence for macroscopic systems the noise strength serves as a natural small parameter.

The random process (2.1) has the following large deviation (LD) [8–10] property for the trajectories $M(t)$ in the small noise limit $\epsilon \rightarrow 0$,

$$P(M(t)) \sim \exp\left(-\frac{1}{\epsilon^2} S(M(t))\right), \quad (2.2)$$

where $P(M(t))$ is the probability of the trajectory $M(t)$, and the ‘‘action functional’’ is given by

$$S(M(t)) = \frac{1}{2} \int \sum_{ij} a_{ij} [\dot{M}_i(t) - b_i(M(t))] \times [\dot{M}_j(t) - b_j(M(t))] dt, \quad (2.3)$$

with $a_{ij} = (\sum_k \sigma_{ik} \sigma_{jk})^{-1}$. Equation (2.2) is the generalization [11] of the path probability functional for linear irreversible processes close to global equilibrium, introduced by Hashitsume [12], and also by Onsager and Machlup [13].

The generalized potential $I(y)$ (rate function or entropy functional) that quantifies the probability of a spontaneous fluctuation y in the steady state is obtained, according to the contraction principle [8,9], by minimizing the action $S(M(t))$ over all paths $M(t)$ [$t \in (-\infty, \infty)$], under the constraint of a fluctuation y at some time $t=0$,

$$I = \inf_{M(t=0)=y} S(M(t)). \quad (2.4)$$

In this paper, we study the fluctuation of the amplitude spectrum. Experimentally, the amplitude spectrum $M(\omega)$ of an observable $M(t)$ is obtained through its Fourier transformation:

$$M(\omega) = \frac{1}{T_{\text{obs}}} \int_0^{T_{\text{obs}}} dt M(t) \exp(-i\omega t), \quad (2.5)$$

where T_{obs} is the observation time. Since our observation time cannot be infinitely long, $M(\omega)$ is still a fluctuating quantity. We wish to study this fluctuation. The usual power spectrum is $P(\omega) \equiv \langle |M(\omega)|^2 \rangle$, where the average is over initial conditions. We are interested in the fluctuation, i.e., the second moment quantity

$$Q_M(\omega) = \langle |M(\omega) - \langle M(\omega) \rangle|^2 \rangle = \langle |M(\omega)|^2 \rangle - |\langle M(\omega) \rangle|^2, \quad (2.6)$$

where $\langle \rangle$ implies the ensemble average over independent samples. If $M(t)$ is strictly periodic, then $\langle M(\omega) \rangle$ vanishes except for integer multiples of the basic frequency, so that this fluctuation is the empirically obtained power spectrum. Obtaining $Q_M(\omega)$ for long time asymptotic behaviors experimentally is not easy, because the fluctuations are small. As is noted in [14], it is very difficult to obtain accurate second moments. Hence, the method we are proposing here could be practically meaningful (as a means to obtain the Gaussian approximation of the rate functions in large deviation theory).

In order to study the quantity (2.6) we proceed as follows. The LD principle (2.2) will be used to characterize the fluctuations of time-averaged quantities. We introduce a Lagrange multiplier to minimize the action functional $S(M(t))$ under the time-average constraint. The Lagrange multiplier will play the role of a generalized conjugate force,

as in the usual equilibrium case. In Sec. III B we discuss how to realize this force operationally as a perturbation on the system dynamics.

Consider the time average of an observable $f(M(t))$,

$$\bar{f} = \frac{1}{T_{\text{obs}}} \int_0^{T_{\text{obs}}} dt f(M(t)). \quad (2.7)$$

The rate function for the quantity \bar{f} is given by, for sufficiently large T_{obs} ,

$$I(\bar{f}) = \lim_{T_{\text{obs}} \rightarrow \infty} \frac{1}{T_{\text{obs}}} \inf \left(S(M(t)) + \lambda \int_0^{T_{\text{obs}}} dt f(M(t)) \right). \quad (2.8)$$

The rate function determines the asymptotic ($\epsilon \rightarrow 0$, $T_{\text{obs}} \rightarrow \infty$) behavior of the probability of the fluctuation \bar{f} ,

$$P(\bar{f}) \sim \exp\left(-\frac{T_{\text{obs}}}{\epsilon^2} I(\bar{f})\right). \quad (2.9)$$

The quantity λ in Eq. (2.8) is the Lagrange multiplier that enforces the constraint \bar{f} . λ may be interpreted as a conjugate force in the sense that

$$\lambda(\bar{f}) = -\frac{\partial I(\bar{f})}{\partial \bar{f}}, \quad (2.10)$$

and

$$\left. \frac{d\lambda}{d\bar{f}} \right|_{\bar{f}=\bar{f}_0} = -\left. \frac{\partial^2 I(\bar{f})}{\partial^2 \bar{f}} \right|_{\bar{f}=\bar{f}_0} = -\chi^{-1}, \quad (2.11)$$

where \bar{f}_0 is the most probable value of \bar{f} . The quantity χ is the susceptibility that characterizes, at the quadratic level, the fluctuation about the most probable state.

The computation of the generalized entropy I for a fluctuation \bar{f} involves minimizing the action $S(M(t))$ over all paths $M(t)$ under the constraint $\overline{f(M(t))} = \bar{f}$. The *optimal* path (or path of least action) for a given λ satisfies, as can be seen from Eq. (2.8), the Euler-Lagrange equation

$$\frac{d}{dt} \partial_{\dot{M}} L = \partial_M L, \quad (2.12)$$

where

$$L = \frac{1}{2} \sum_{ij} a_{ij} [\dot{M}_i(t) - b_i(M(t))] [\dot{M}_j(t) - b_j(M(t))] + \lambda f(M(t)). \quad (2.13)$$

III. GENERALIZED FLUCTUATION-RESPONSE RELATION

A. Preliminary comments

The generalization of the equilibrium fluctuation-response relation to frequency (and spatial) perturbations is the usual equilibrium FDT [2,3]. The theorem tells us that

$$k_B T = \omega S(k, \omega) / [2 \operatorname{Im} \operatorname{Re}(k, \omega)], \quad (3.1)$$

where $\operatorname{Re}(k, \omega)$ is the response function, with the component $\omega \operatorname{Im} R(k, \omega)$ proportional to the dissipation generated in the system. The structure factor $S(k, \omega)$ is equal to $\langle |M(k, \omega) - \langle M(k, \omega) \rangle|^2 \rangle$ [i.e., the space-time Fourier transform of $\langle M(x, t)M(x', t') \rangle - \langle M(x, t) \rangle \langle M(x', t') \rangle$] for space and time translationally invariant systems, such as the equilibrium state.

Note that in the limit $\omega \rightarrow 0$, $S(k, \omega)$ measures the fluctuation of the long-time average,

$$M(k, 0) = \lim_{T_{\text{obs}} \rightarrow \infty} \frac{1}{T_{\text{obs}}} \int_0^{T_{\text{obs}}} dt M(k, t). \quad (3.2)$$

However, the FDT relation is not defined in this limit. For $\omega = 0$, the response probes only the fluctuations of *single-time* observables (by single-time observable we mean an (ensemble or space averaged) observable evaluated at a given instant of time). This is the equilibrium fluctuation-response relation

$$k_B T = S(k, t=0) / \operatorname{Re}(k, 0), \quad (3.3)$$

where $S(k, t=0) = \int d\omega S(k, \omega)$ for time-translationally-invariant systems. Thus the appropriate response to probe the fluctuations of *time-averaged* observables is not obtained by the usual coupling in the (equilibrium) Hamiltonian that is used to obtain $S(k, \omega)$ for $\omega \neq 0$. However, this is a consequence of an obvious fact that the fluctuations of time-averaged quantities are distinct from the fluctuations of single-time (ensemble averaged) quantities [4]. The discrepancy between the two averaging methods is simply because, while the ensemble average is strictly over independent samples, time averages of a single sample crucially depend on the time correlation. We can illustrate this in the context of the rate function as follows.

Consider the fluctuation of the quantity

$$\bar{x} = \frac{1}{T_{\text{obs}}} \int_0^{T_{\text{obs}}} dt x(t) \quad (3.4)$$

in the steady state, where $x(t)$ may represent the spatial average (over sample size V) at time t of some observable. Asymptotically, the fluctuation \bar{x} decays according to the LD principle [14],

$$P(\bar{x}) \sim \exp\left(-\frac{VT_{\text{obs}}}{2\chi} (\bar{x})^2\right). \quad (3.5)$$

We have for the susceptibility χ ,

$$\chi = \frac{V}{T_{\text{obs}}} \int_0^{T_{\text{obs}}} \int_0^{T_{\text{obs}}} dt ds \langle x(t)x(s) \rangle \quad (3.6)$$

$$= 2V \int_0^{T_{\text{obs}}} dt \langle x(t)x(0) \rangle \quad (3.7)$$

for a time-translationally-invariant steady state. For a simple exponential decay $x(t) = x(0)\exp(-t/\tau)$ (away from critical points) we have that

$$\chi = 2\tau V \langle x^2(0) \rangle = 2\tau \chi_{\text{th}}. \quad (3.8)$$

For notational simplicity we assume $\langle x \rangle = 0$. The quantity $\chi_{\text{th}} = V \langle x^2 \rangle$ is the usual thermodynamic susceptibility for ensemble- (space-) averaged observables. Thus the fluctuations (susceptibility) of a long-time averaged quantity per $2 \times$ correlation time unit is equal to the susceptibility of the (single-time) ensemble averaged quantity. For systems without time-translational symmetry, which are the cases where time averaging may be a better method to characterize the system behavior phenomenologically (such as the model considered in this work), the relation $\chi = 2\tau \chi_{\text{th}}$ is, strictly speaking, not valid. However, one still expects that $\chi \approx \tau \chi_{\text{th}}$. Such a relation is natural since the configurations of the system generated along the time axis become independent after a time separation τ .

Note that close to a critical point, both τ and χ_{th} diverge. Hence, near a phase transition the divergence of the susceptibility for space-time-averaged quantities has a stronger divergence than that of ensemble-averaged quantities.

B. Fluctuation-response relation

In a previous paper [4], we discussed the fluctuation-response relation for time-averaged observables. Here we point out the extension of the fluctuation-response relation to compute, operationally, Q_M in Eq. (2.6). As mentioned above, if the system under consideration is strictly periodic, then $Q_M(\omega)$ becomes identical to the empirically obtained power spectrum, except for the integer multiples of the fundamental frequency of the system. We note here that for time-dependent steady states (i.e., steady states that are not time-translationally invariant), the quantity Q_M is the Fourier transform of the time-averaged time-displaced correlation function $\overline{C(\tau)}$, where

$$\overline{C(\tau)} = \frac{1}{T_{\text{obs}}} \int_0^{T_{\text{obs}}} dt \langle [M(t+\tau)M(t) - \langle M(t+\tau) \rangle \langle M(t) \rangle] \rangle. \quad (3.9)$$

To establish the fluctuation-response relation, we proceed as follows. For the general model (2.1), the Euler-Lagrange equations (2.12) can be written as follows:

$$a_{kj} \frac{d}{dt} (\dot{M}_j - b_j) = -a_{ij} (\dot{M}_i - b_i) \frac{\partial b_j}{\partial M_k} + \lambda \partial_{M_k} f(M), \quad (3.10)$$

where $a_{ij} = (\sum_k \sigma_{ik} \sigma_{jk})^{-1}$. One can rewrite the equations as two first-order equations

$$\dot{M}_i = b_i(M, t) + \lambda a_{ij}^{-1} g_j, \quad (3.11)$$

with the force $g(t)$ obeying the equation

$$\dot{g}_i = -g_j \frac{\partial b_i}{\partial M_j} + \partial_{M_i} f. \quad (3.12)$$

We consider the simple case of a *scalar* field M and drift $b(M, t)$, and additive noise with $a = 1$, as in our example system discussed in Sec. IV. Thus we have

$$\dot{M} = b(M, t) + \lambda g, \quad (3.13)$$

$$\dot{g} = -g \partial_M b(M, t) + \partial_M f. \quad (3.14)$$

Now let us consider the fluctuation of the following quantity for large, but finite, observation time T_{obs} ,

$$M(\omega) = \frac{1}{T_{\text{obs}}} \int_0^{T_{\text{obs}}} dt \exp(i\omega t) M(t). \quad (3.15)$$

We define the real and imaginary components of $M(\omega)$ as

$$M_R(\omega) = \frac{1}{T_{\text{obs}}} \int_0^{T_{\text{obs}}} dt \cos(\omega t) M(t), \quad (3.16)$$

$$M_I(\omega) = \frac{1}{T_{\text{obs}}} \int_0^{T_{\text{obs}}} dt \sin(\omega t) M(t). \quad (3.17)$$

In order to realize the fluctuations of the real and imaginary components operationally, we denote for $f = \cos(\omega t)M(t)$ [$\sin(\omega t)M(t)$], the corresponding perturbing forces as $\lambda_1 g_1(t)$ [$\lambda_2 g_2(t)$].

The fluctuation-response relation is realized once we regard the force $\lambda g(t)$ as the external force we experimentally impose to the system to realize the fluctuation (deviation). The linear response about the steady state [denoted as $M_0(t)$, where $\dot{M}_0(t) = b(M_0(t), t)$] is the response of the system in the limit $\lambda \rightarrow 0$. In this limit, one may linearize the equations to obtain for the forces

$$\dot{g}_1(t) = -b'(M_0(t), t)g_1(t) + \cos(\omega t), \quad (3.18)$$

$$\dot{g}_2(t) = -b'(M_0(t), t)g_2(t) + \sin(\omega t), \quad (3.19)$$

where $b' = \partial b / \partial M_0$. From the definition of λ as the ‘‘conjugate’’ force in Eqs. (2.10) and (2.11), we have that the susceptibilities $\langle [M_R(\omega) - \langle M_R(\omega) \rangle]^2 \rangle$, $\langle [M_I(\omega) - \langle M_I(\omega) \rangle]^2 \rangle$, are given by the linear responses

$$\langle [M_R(\omega) - \langle M_R(\omega) \rangle]^2 \rangle = \chi_2 = - \lim_{\lambda_1 \rightarrow 0} \left(\frac{\Delta M_R(\omega)}{\lambda_1} \right)_{\lambda_2=0}, \quad (3.20)$$

$$\langle [M_I(\omega) - \langle M_I(\omega) \rangle]^2 \rangle = \chi_1 = - \lim_{\lambda_2 \rightarrow 0} \left(\frac{\Delta M_I(\omega)}{\lambda_2} \right)_{\lambda_1=0}. \quad (3.21)$$

The subscript on the quantity χ is to remind us that the response is computed (operationally) by perturbing the system with forces $g_1(t)$ [$g_2(t)$ absent, i.e., $\lambda_2=0$] or $g_2(t)$ ($\lambda_1=0$).

Since the equations governing the response are linear, we may use the superposition principle and consider the system response to one (complex) force $g(t) = g_1 + i g_2$,

$$\dot{g}(t) = -b'(M_0(t), t)g(t) + \cos(\omega t) + i \sin(\omega t), \quad (3.22)$$

$$\Delta \dot{M}(t) = b'(M_0(t), t)\Delta M + \lambda g(t), \quad (3.23)$$

where the complex response is $\Delta M(t) = \Delta M_1(t) + i \Delta M_2(t)$. The fluctuation response can then be simply written as

$$Q_M(\omega) = \langle |M(\omega) - \langle M(\omega) \rangle|^2 \rangle = \tilde{R}(\omega), \quad (3.24)$$

where

$$\tilde{R}(\omega) = - \lim_{\lambda \rightarrow 0} \frac{\Delta M_{1R}(\omega) + \Delta M_{2I}(\omega)}{\lambda}. \quad (3.25)$$

$\Delta M_{1R}(\omega)$ [$\Delta M_{2I}(\omega)$] are the $\cos(\omega t)$ [$\sin(\omega t)$] transform [i.e., Eqs. (3.16), (3.17)] of $\Delta M_1(t)$ [$\Delta M_2(t)$], respectively. Note that we have scaled out the factor of the noise strength and averaging time in Eq. (3.24). Otherwise the relation should read [from the LD formula (2.9)]

$$Q_M(\omega) = \frac{\epsilon^2}{T_{\text{obs}}} \tilde{R}(\omega) \sim \frac{1}{VT_{\text{obs}}} \tilde{R}(\omega), \quad (3.26)$$

where for macroscopic systems $\epsilon^2 \sim 1/V$ (V is the system size).

The fluctuation-response relation requires one to apply a force $g(t)$ that, in general, is a function of the steady state $M_0(t)$. The (experimental) determination of $g(t)$ was discussed and demonstrated in [4]. First, we must determine b' by observing the natural relaxation of the system to the steady state. Next, we must solve Eq. (3.14) [linearized about $M_0(t)$] for $g(t)$. Here we note that since Eq. (3.14) is unstable (because of the negative sign in the linear term), the best method to compute $g(t)$ is to solve the (stable) time-reversed equation

$$\dot{g}'(t) = b'(M_0(-t), -t)g' - \partial_{M_0(-t)} f(M_0(-t), -t), \quad (3.27)$$

where $g' = g(-t)$, and then time reverse the steady state solution back to obtain $g(t)$.

The above prescription allows one to compute the generalized fluctuational entropy function $I(M_R(\omega), M_I(\omega))$ at the quadratic level,

$$I(M_R, M_I) = M_R^2(\omega)/2\chi_I + M_I^2(\omega)/2\chi_R + M_R(\omega)M_I(\omega)/\chi. \quad (3.28)$$

The susceptibilities, $\chi_{I,R}, \chi$, are determined as $\chi_{I,R} = (-\bar{\chi}^2 + \chi_1\chi_2)/\chi_{2,1}$, and $\chi = (\bar{\chi}^2 - \chi_1\chi_2)/\bar{\chi}$. The quantity $\bar{\chi}$ is the response function

$$\bar{\chi} = - \lim_{\lambda \rightarrow 0} \frac{\Delta M_{2R}(\omega)}{\lambda} = - \lim_{\lambda \rightarrow 0} \frac{\Delta M_{1I}(\omega)}{\lambda}. \quad (3.29)$$

The relation between the two sets of susceptibilities [and Eq. (3.29)] follows from the Legendre transform and integrability conditions of the rate function I .

The generalized fluctuation-response relation (3.24) is constructed from the starting point of capturing the fluctuations of time-averaged quantities ($\omega=0$), and then generalizing to nonzero ω , whereas the usual equilibrium FDT begins with the single-time simultaneous correlations ($t=0$, $f d\omega$), and then generalizes to the cases with time delay (consequently, to nonzero ω). For steady states that are time-

translationally invariant, the single-time fluctuation can be obtained from our response theory, by using the relation

$$\langle [M(t=0) - \langle M \rangle]^2 \rangle = \int d\omega \tilde{R}(\omega). \quad (3.30)$$

This means that the forcing term in the linear equation for the perturbing force $g(t)$ becomes $\int d\omega [\cos(\omega t) + i \sin(\omega t)] = \delta(t)$. Thus, for single-time fluctuations, the force $g(t)$ is obtained via the equation

$$\dot{g}(t) = -b'(M_0(t))g(t) + \delta(t=0), \quad (3.31)$$

which, as discussed in [4], must be solved from $t = -\infty$ up to $t = 0$, with $g(t) = 0$ for $t > 0$.

IV. EXAMPLE SYSTEM AND RESULTS

A. Model system

As an illustration of the generalized fluctuation-response relation, we consider, as an example, a simple model of a magnetic spin system under the influence of a time-dependent magnetic field [5]. The system was modeled phenomenologically using a time-dependent Ginzburg-Landau equation for the dynamics of the spatially coarse-grained magnetization. We study the model at the mean-field level, but with a small noise (more realistically, the total magnetization of a small magnetic particle under constant temperature condition). The model takes the following form:

$$\dot{M}(t) = -\gamma_0[-r_0 M(t) + u_0 M^3(t) - h_0 \cos(\omega_0 t)] + \epsilon \eta(t), \quad (4.1)$$

where the field $M(t)$ denotes the (space-averaged) magnetization, $h(t) = h_0 \cos(\omega_0 t)$ is the external magnetic field, u_0 is a positive constant, γ_0 is the kinetic coefficient, and r_0 is the temperature parameter [proportional to $(T_c - T)$ with T_c being the unrenormalized critical temperature, if T is close to T_c ; constant if T is sufficiently away from T_c]. In the following we rescale the field M and time to express the dynamics in terms of the minimal set of parameters, $r = r_0 \gamma_0 / \omega_0$, $h = h_0 (u_0 \gamma_0^3 / \omega_0^3)^{1/2}$, $\epsilon \rightarrow \epsilon (u_0 \gamma_0 / \omega_0^3)^{1/2}$:

$$\dot{M} = rM - M^3 + h \cos(t) + \epsilon \eta(t). \quad (4.2)$$

In the zero noise limit, the steady states of the system are periodic in frequency ω_0 . The system undergoes a phase transition at a critical field $h_c(r)$ from a zero time-averaged magnetization phase (Z phase) to a nonzero time-averaged magnetization phase (NZ phase). The transition between the Z and the NZ phases is a *continuous* transition. For $r < 0$ (i.e., $T > T_c$) there is only the Z phase.

Although we study the system at the mean-field level, we expect that in the actual spatially extended system (i.e., including spatial fluctuations) there will be a true phase transition from a NZ to a Z phase. It is in this sense that we use the term ‘‘phase transition’’ for the mean-field system (4.2). However, it should be noted that if one studies the system along the time axis, there is a phase transition for the mean-field system (4.2) in the sense that the generalized potential [4] that describes the fluctuations of time-averaged observ-

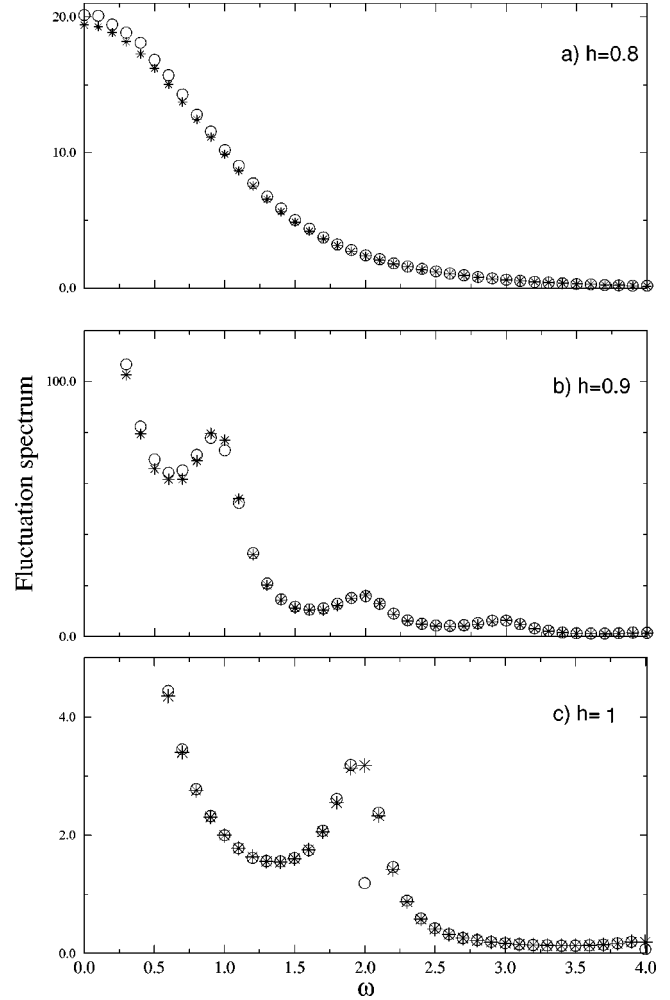


FIG. 1. The fluctuation spectrum as a function of ω for various field h values, at $r=1$, and $\omega_0=1$. The star symbols denote the linear response data $[\tilde{R}(\omega)]$, the circle symbols denote the empirical data obtained from a numerical simulation of Eq. (4.2) with $\epsilon=0.01, T_{\text{obs}}=20\pi/\omega_0$.

ables in the steady state becomes flat at the transition [i.e., the fluctuations of time-averaged quantities become large (diverge) near the transition].

B. Results

The fluctuation spectrum was computed for various field h values at a generic point $r=1$ (where $h_c \approx 0.93$), using the response method discussed above. Along with the linear response data, we also show some data obtained empirically from a numerical simulation of the stochastic equation (4.2) with $\epsilon=0.01$, and an averaging time $T_{\text{obs}}=10$ (in units of the period of the external magnetic field, $2\pi/\omega_0$). The empirical data are shown to illustrate that the zero-noise data obtained from the linear response method are reasonably robust to small noise.

The quantity $Q_M(\omega)$ for a typical parameter point in the NZ phase (away from the transition region) is shown in Fig. 1(a). One sees a Lorentzian-type shape centered around $\omega=0$, with a well-defined characteristic time scale τ (defined as the inverse half-width). τ is a measure of the time correlation, or relaxation time, of the steady state. Characteristic of a typical second-order phase transition, the quantity τ

[along with the $\omega=0$ peak, i.e., the susceptibility of the long time-averaged quantity $\bar{M}=(1/T_{\text{obs}})\int dt M(t)$], diverges as $h \rightarrow h_c \approx 0.93$. In Fig. 1(a), $\tau \approx 1$ (in units of the period of the external magnetic field $2\pi/\omega_0$). Note that, in principle, the averaging time T_{obs} for the empirical data should be larger than τ . This is to ensure that one is properly sampling an *ensemble* of time averages. In practice, the averaging time of 10 periods is sufficient, if we are not too close to the transition.

As the field h is increased closer to the transition (from the NZ phase), peaks develop in the fluctuation spectrum at the $\omega=n\omega_0$ ($n=1,2,\dots$), where ω_0 is the frequency of the external oscillating magnetic field. The case $h=0.9$ is shown in Fig. 1(b), where, as expected, the $\omega=0$ peak increases and the width of the $\omega=0$ peak decreases (there is still a well-defined peak at $\omega=0$ (not shown in the figure) with $\tau \approx 5$). The peaks at $n\omega_0$ grow to a maximum at the transition. The strongest peaks ($n=0,2$) do seem to diverge as $h \rightarrow h_c$ (the peaks at the higher harmonics are much smaller in size). Above the transition ($h > h_c$), the odd harmonics disappear quite abruptly; the peaks at the even harmonics ($n=2,4,\dots$) persist above the transition, but eventually disappear [see Fig. 1(c), for $h=1$].

The empirical data illustrate that these features near the transition are reasonably robust to the effect of nonzero noise. Above the transition, the data from the system with noise show the same trend, except that the noise tends to reduce the peaks at the even harmonics, to the extent that the narrow peaks become dips. We note here that from the scaling of the noise strength [$\epsilon^2 \sim 1/\omega_0^3$, see above Eq. (4.2)], one expects the small noise theory to become even more accurate for larger ω_0 (the regime of larger ω_0 is actually of more intrinsic interest, since for large ω_0 the system cannot locally equilibrate over the time scale of the external field, and thus is further away from local equilibrium).

Shneidman *et al.* [15] have studied the small noise behavior of $Q_M(\omega)$ for this system analytically, starting from a two-state rate equation with an approximate form for the transition probability. They observed peaks in the *even* harmonics in the small noise limit, for frequencies much smaller than the one used in Fig. 1. It is interesting that some of the above features have been observed in [15], since the regime they studied is quite different from that studied in this paper.

Near the transition, the system has excitable modes at the harmonics, which is essentially a reflection of the discrete time symmetry of the system, i.e., the symmetry of the system is reflected on the response. One expects that close to the phase transition, the system becomes more susceptible to perturbations that are periodic in ω_0 . The peaks observed in the spectrum are simply due to large periodic driving. These peaks are not related to the phenomenon of stochastic resonance, which is a synchronization of the noise-induced hopping with the external oscillating field (the stochastic resonance would presumably only be observable in our small noise system for sufficiently small ω_0 and $h \ll r$, i.e., well away from the transition region).

The fluctuation-response method also allows one to compute, separately, the two components of $Q_M(\omega)$:

$$Q_{M_R}(\omega) = \langle [M_R(\omega) - \langle M_R(\omega) \rangle]^2 \rangle, \quad (4.3)$$

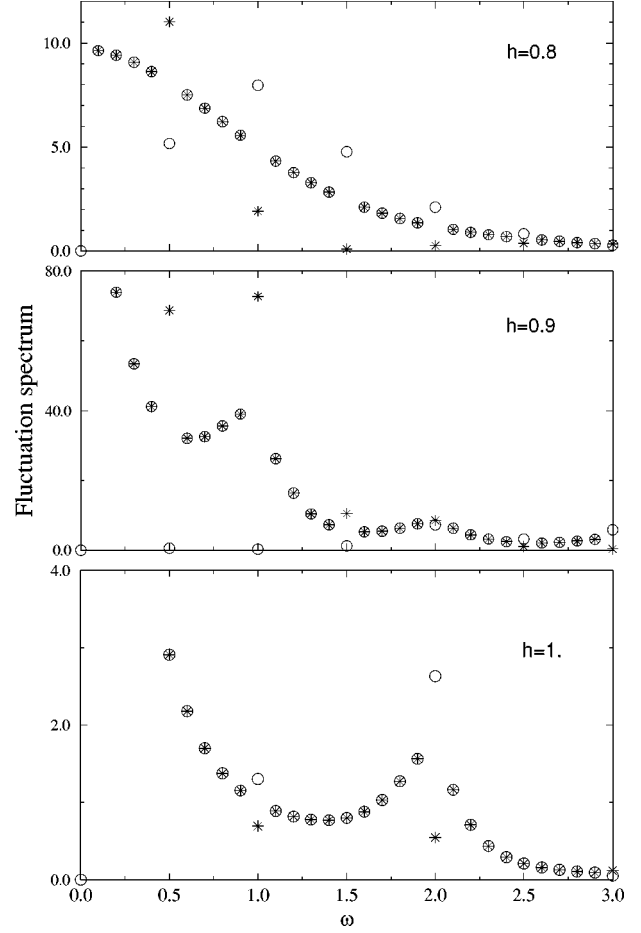


FIG. 2. The two components $Q_{M_R}(\omega)$ (star symbol) and $Q_{M_I}(\omega)$ (circle symbol) of the fluctuation spectrum, obtained with the linear response method (for $r=1, \omega_0=1$.)

and

$$Q_{M_I}(\omega) = \langle [M_I(\omega) - \langle M_I(\omega) \rangle]^2 \rangle, \quad (4.4)$$

via the linear response (3.20), (3.21). An example is shown in Fig. 2. The two components are the same [i.e., $|Q_{M_R}(\omega) - Q_{M_I}(\omega)| = 0$], except at the harmonics $n\omega_0$ [and at $(n+1/2)\omega_0$ in the NZ phase], where one component dips, and the other peaks (which component peaks or dips varies with h and n). Similar behavior is seen close to the transition, except very close to h_c , where both components show peaks at the harmonics. The empirical data at $\epsilon=0.01$ show basically the same behavior.

An interesting finding is the nonzero nature of $|Q_{M_R}(\omega) - Q_{M_I}(\omega)|$ at $\omega=(n+\frac{1}{2})\omega_0$ ($n=1,2,\dots$) in the NZ phase (it is zero in the Z phase). The difference between the two components seems to decrease smoothly to zero at the transition. Thus the quantity $|Q_{M_R}(\omega) - Q_{M_I}(\omega)|_{\omega=(n+1/2)\omega_0}$ (for $n=0$ in particular) is a good indicator of the phase transition from NZ to the Z phase. As mentioned in Sec. IV A, the typical (usual) order parameter that characterizes the phase diagram for the periodic steady states is the time-averaged magnetization $\bar{M}=M(\omega=0)$. Here we see that the phase transition [$\bar{M}=0$ (Z phase)

$\rightarrow \bar{M} \neq 0$ (NZ phase)] is reflected in the response function $|Q_{M_R}(\omega) - Q_{M_I}(\omega)|_{\omega=(1/2)\omega_0}$. The periodic symmetry with frequency ω_0 of the response function $|Q_{M_R}(\omega) - Q_{M_I}(\omega)|$ is broken in the NZ phase; there is a period doubling (i.e., the response becomes nonzero at $\frac{1}{2}\omega_0$).

V. DISCUSSION

We have discussed and illustrated the computation of the fluctuation spectrum for a nonequilibrium steady-state system via a linear-response method. The method gives an efficient and operational means to compute the fluctuation of the amplitude spectrum for nontrivial steady states. The quantity can give more insight into the dynamics of the system than the power spectrum, but it is not easy to observe without the use of the fluctuation-response relation discussed in this paper. As an illustration a periodically driven bistable system, or driven magnetic system (that should be experimentally realizable), has been considered.

The system was shown to display, in addition to the usual peak at $\omega=0$, narrow peaks at the harmonics of the external driving frequency near the transition point. The peaks at the even harmonics seem to be more dominant (namely, the second harmonic), and persist somewhat longer in the Z phase. In the NZ phase, well below the transition, the spectrum has a Lorentzian-type shape around $\omega=0$. Interesting behavior has also been observed in the fluctuation spectrum of two components, $M_R(\omega)$ and $M_I(\omega)$; in particular, a symmetry breaking (for $h < h_c$) reflected in the response function $|Q_{M_R}(\omega) - Q_{M_I}(\omega)|_{\omega=(n+1/2)\omega_0}$ has been observed.

So long as the perturbation is small (i.e., linear regime) the framework should be valid even if one is very close to a phase transition. If there is a disagreement, it is simply that the applied perturbation is too large. Of course, gentle perturbation is required near a critical point. However, it should be noted that the linear-response method is strictly confined to systems in the small noise limit $\epsilon \rightarrow 0$. Critical behavior near a phase transition invalidates the small noise limit. Thus, in an actual system (experiment), we would expect the

response method to give only qualitatively correct data very close to the phase transition.

The fluctuation-response relation has been elucidated for small noise Langevin equations. The relation is of interest for physical systems that are driven away from local equilibrium (modeled at the mesoscopic level). For nonequilibrium Langevin models, the noise strength is an unknown parameter in the theory. For our simple model system (4.1), the local equilibrium assumption (in the limit of small h_0 and ω_0) allows us to make the identification $\epsilon^2 = 2\gamma_0 k_B T/V$, where T is the equilibrium temperature, and k_B the Boltzmann constant. Away from local equilibrium, such a relation is invalid. However, the fluctuation-response relation (3.26) may be used to define the noise strength for systems outside of local equilibrium, if the experimentalist can determine the fluctuation spectrum $Q_M(\omega)$ in an independent fashion (by some scattering experiment), or perhaps one computes $Q_M(\omega)$ directly from a more microscopic model. To determine the force coupling, and hence $\tilde{R}(\omega)$, one needs to know b' (i.e., the dynamical model must be given experimentally or theoretically). This is analogous to knowing the model or effective Hamiltonian for an equilibrium system. The constant ratio $T_{\text{obs}} Q_M(\omega) / \tilde{R}(\omega)$ would then be a measure of the noise strength (or generalized temperature).

Finally, the example system considered in this paper is a one-degree-of-freedom Langevin equation. As can be seen from Eq. (3.12) in Sec. III B, the structure of the response theory is basically the same for the case of multivariable dynamics. It should be noted that a difference arises for the case of a nondiagonal noise matrix. Such cases remain to be studied further. In particular, it would be interesting to consider as a future work a two-component system, where the fluctuation spectrum around (say) a limit cycle can be studied from the linear response method discussed in this paper.

ACKNOWLEDGMENTS

The author would like to acknowledge support from National Science Foundation Grant No. NSF-DMR-93-14938.

-
- [1] H. B. Callen, *Thermodynamics* (Wiley, New York, 1960).
 - [2] H. B. Callen and T. A. Welton, *Phys. Rev.* **83**, 34 (1951).
 - [3] H. Nakano, *Int. J. Mod. Phys. B* **7**, 2397 (1993).
 - [4] M. Paniconi and Y. Oono, *Phys. Rev. E* **55**, 176 (1997).
 - [5] M. Zimmer, *Phys. Rev. E* **47**, 3950 (1993).
 - [6] R. Graham, *Z. Phys. B* **26**, 397 (1977).
 - [7] H. Risken, *The Fokker-Planck Equation* (Springer-Verlag, New York, 1984).
 - [8] S. R. S. Varadhan, *Large Deviation and Applications* (SIAM, Philadelphia, 1984).
 - [9] J.-D. Deuschel and D. W. Stroock, *Large Deviation* (Academic Press, New York, 1989).
 - [10] M. I. Freidlin and A. D. Wentzel, *Random Perturbations of Dynamical Systems* (Springer, Berlin, 1984).
 - [11] R. Graham, in *Stochastic Processes in Nonequilibrium Systems*, edited by L. Garrido, P. Seglar, and P. J. Shepherd (Springer, Berlin, 1978); *Z. Phys. B* **26**, 281 (1977).
 - [12] N. Hashitsume, *Prog. Theor. Phys.* **8**, 461 (1952).
 - [13] L. Onsager and S. Machlup, *Phys. Rev.* **91**, 1505 (1953); **91**, 1512 (1953).
 - [14] Y. Oono, *Prog. Theor. Phys. Suppl.* **99**, 165 (1989).
 - [15] V. A. Shneidman, P. Jung, and P. Hanggi, *Phys. Rev. Lett.* **72**, 2682 (1994).