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Spectral density from nonlinear Fokker-Planck equations: The high-frequency limit

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Using a method introduced by Zwanzig, we study the power spectrum of a system described by a simple nonlinear Fokker-Planck equation. The high-frequency region is analyzed, and the asymptotic behavior is established.

The study of power spectra for nonlinear system has received some attention in the last few years, especially in connection with the broadband spectra characteristics of nonperiodic flow regimes. The high-frequency part of those spectra can often be fitted by power laws, but some controversy has arisen about the exponent of the leading term in the high-frequency limit.[1,2]

We have recently reported some results about the behavior of the spectral density in several limiting cases.[3] In those works, we have obtained expressions valid for a broad range of frequencies and which fit very well the experimental data.

The purpose of this report is to show that the high-frequency behavior of the spectral density for nonlinear systems can be studied in an exact manner. As a consequence, we can establish that the high-frequency spectra of systems described by first-order Langevin equations have an ω^{-2} behavior independently of the nonlinearity. This result is in agreement with those of Caroli, Caroli, and Roulet[1] and it seems to be at variance with the numerical solution reported by Kawakubo.

Although the theory can be established in a general and formal way, for the sake of simplicity we are going to consider the following particular model. Let a system be described by the variable x satisfying the first-order Langevin equation

$$\frac{dx}{dt} = -U'(x) + F(t) \quad , \tag{1}$$

where $U'(x)$ is a nonlinear function of x and $F(t)$ is the noise term assumed to be Gaussian and δ correlated. The probability density $f(x,t)$ obeys the Fokker-Planck equation

$$\frac{\partial f(x,t)}{\partial t} = Df(x,t) \quad , \tag{2}$$

where

$$D \equiv \frac{\partial}{\partial x}U'(x) + \alpha\frac{\partial^2}{\partial x^2} \tag{3}$$

is the Fokker-Planck operator and α the diffusion constant.

Let us define the time correlation function

$$C(\tau) = \langle x(\tau)x_t'\rangle_t = \int dx\, x e^{\tau D}x_t' f(t) \quad , \tag{4}$$

where $x_t' = x - \langle x\rangle_t$ and the angular bracket with subindex t means ensemble average at time t. It is our aim to study the evolution of this quantity as a function of τ. We will follow a method due to Zwanzig.[4] Let us introduce an operator $P(t)$ as

$$P(t)G = \frac{x_t' f(t)}{\langle (x_t')^2\rangle_t}\int dx\, xG \quad . \tag{5}$$

One easily proves that

$$P^2(t) = P(t) \quad . \tag{6}$$

On the other hand, it follows from Eq. (4) that

$$\frac{dC(\tau)}{d\tau} = \int dx\, xDe^{\tau D}x_t' f(t) \quad . \tag{7}$$

The quantity $e^{\tau D}x_t' f(t)$ can be separated into two parts by means of the operator $P(t)$, i.e.,

$$\begin{aligned} e^{\tau D}x_t' f(t) &= P(t)e^{\tau D}x_t' f(t) + [1-P(t)]e^{\tau D}x_t' f(t) \\ &= \frac{x_t' f(t)}{\langle (x_t')^2\rangle_t}C(\tau) + [1-P(t)]e^{\tau D}x_t' f(t) \quad . \end{aligned} \tag{8}$$

Although $P(t)$ is a time-dependent operator, the variable t plays the role of a parameter as long as the τ evolution is concerned. Then the standard procedure allows us to obtain

$$[1-P(t)]e^{\tau D}x_t' f(t) = [1-P(t)]e^{\tau D[1-P(t)]}x_t' f(t) + \int_0^\tau ds\,[1-P(t)]e^{sD[1-P(t)]}DP(t)e^{(\tau-s)D}x_t' f(t) \quad . \tag{9}$$

Inserting (9) into (8) we get

$$e^{\tau D}x_t' f(t) = \frac{x_t' f(t)}{\langle (x_t')^2\rangle_t}C(\tau) + \int_0^\tau ds\,[1-P(t)]e^{sD[1-P(t)]}D\frac{x_t' f(t)}{\langle (x_t')^2\rangle_t}C(\tau-s) + [1-P(t)]e^{\tau D[1-P(t)]}x_t' f(t) \quad . \tag{10}$$

The last term in Eq. (10) identically vanishes as

$$P(t)x_t' f(t) = x_t' f(t) \quad . \tag{11}$$

Therefore, using (7), (10), and (11) we finally get

$$\frac{d}{d\tau}C(\tau)=\frac{\langle (D_x^\dagger)x_t'\rangle_t}{\langle (x_t')^2\rangle_t}C(\tau)+\frac{1}{\langle (x_t')^2\rangle_t}\int_0^\tau ds C(\tau-s)\int dx(D_x^\dagger)[1-P(t)]e^{sD[1-P(t)]}Dx_t'f(t) \;, \tag{12}$$

where we have introduced the adjoint Fokker-Planck operator

$$D^\dagger=-U'(x)\frac{\partial}{\partial x}+\alpha\frac{\partial^2}{\partial x^2} \;. \tag{13}$$

We want to notice that Eq. (12) is exact. In particular, no hypothesis about the initial condition of the system has been assumed. The projection operator $P(t)$ has only been introduced as a convenient tool in order to show that $C(\tau)$ obeys a linear equation. Furthermore, no hypothesis about the projected quantities appearing in (12) is needed.

A particularly simple case corresponds to the equilibrium time correlation function $C^{eq}(\tau)=\langle x(\tau)x\rangle_{eq}$. In this case, the coefficients in Eq. (12) are expressed as averages taken with the equilibrium distribution function. Namely, we get

$$\frac{dC^{eq}(\tau)}{d\tau}=-\Omega^2C^{eq}(\tau)+\int_0^\tau ds\,\Phi(s)C^{eq}(\tau-s) \;, \tag{14}$$

$$\Omega^2=\frac{\langle (D_x^\dagger)x\rangle_{eq}}{\langle x^2\rangle_{eq}} \;, \tag{15}$$

$$\Phi(s)=\int dx(D_x^\dagger)[1-P]e^{sD[1-P]}Dxf_{eq} \;, \tag{16}$$

with P given by Eq. (5) but replacing $f(t)$ by f_{eq}. We are also considering that $\langle x\rangle_{eq}=0$. To obtain an expression for $C^{eq}(\tau)$ valid for all τ, one has to evaluate the function $\Phi(s)$. In practice, this requires to resort to some kind of procedure to approximate the memory kernel which may contain long-time memory effects. This will not be needed here.

The spectral density is defined as

$$S(\omega)=\mathrm{Re}\int_0^\infty d\tau\, e^{-i\omega\tau}C^{eq}(\tau) \;. \tag{17}$$

Laplace transform of Eq. (14) yields

$$S(\omega)=\frac{C^{eq}(0)[\Omega^2+\tilde{\Phi}_r(\omega)]}{[\Omega^2+\tilde{\Phi}_r(\omega)]^2+[\omega+\tilde{\Phi}_i(\omega)]^2} \;, \tag{18}$$

where $\tilde{\Phi}_r$ and $\tilde{\Phi}_i$ are, respectively, the real and imaginary parts of $\tilde{\Phi}(i\omega)$, the transform of $\Phi(s)$.

The high-frequency part of the spectrum can then be easily analyzed from Eqs. (16) and (18). We just need to know the first few terms of the asymptotic representation of $\tilde{\Phi}(i\omega)$ for ω going to infinity. By expanding the exponential one easily finds

$$\tilde{\Phi}_r(\omega)=-\frac{\phi^{(1)}}{\omega^2}+O\left(\frac{1}{\omega^4}\right) \tag{19}$$

and

$$\tilde{\Phi}_i(\omega)=-\frac{\phi^{(0)}}{\omega}+O\left(\frac{1}{\omega^3}\right) \;, \tag{20}$$

where $\phi^{(0)}$ and $\phi^{(1)}$ are given by

$$\phi^{(0)}=\alpha\left(\langle U''(x)\rangle_{eq}-\frac{1}{\langle x^2\rangle_{eq}}\right) \;, \tag{21}$$

$$\phi^{(1)}=-\alpha\langle [U''(x)]^2\rangle_{eq}+\frac{2\alpha^2}{\langle x^2\rangle_{eq}}\langle U''(x)\rangle_{eq}-\frac{\alpha^2}{\langle x^2\rangle_{eq}} \;. \tag{22}$$

From the above results it is clear that the spectral density behaves as ω^{-2} in the high-frequency limit. This result is valid for any expression of the force term $U'(x)$. In addition, explicit expressions for the coefficients of the first few terms of the expansion are obtained. They are given in terms of equilibrium averages.

The same method can also be applied to higher-order Langevin equations. In particular, for those of second order a ω^{-4} asymptotic behavior is obtained, in agreement with the result found by Caroli *et al.*[1]

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