Fluctuation-dissipation dispersion relation and quality factor for slow processes

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(Received 9 May 2003; published 28 January 2004)

A generalization of the Callen-Welton formula for systems with slowly varying parameters is given. Using the momentum method and the time multiscale technique, it is shown that not only the dissipation but also the dispersive contributions determine the spectral function of the fluctuations in these systems. The general formalism is illustrated for an oscillating electrical circuit, and the influence of the dispersion contributions on the quality factor of the system is discussed.

DOI: 10.1103/PhysRevE.69.017104 PACS number(s): 02.50.Ey, 05.40.−a, 05.10.Gg, 72.70.+m

Any oscillating system is characterized by two main parameters: the proper frequency and the quality factor (Q factor). The latter is directly linked with the sensitivity of the system. The higher the Q factor, the more sensitive the system is. The Q factor is inversely proportional to the width of the spectral line of the parameter fluctuations. In thermodynamic equilibrium, the fluctuations are determined by the system temperature Θ and the dissipation. The first fluctuation-dissipation relation between the diffusion coefficient and the dissipative friction coefficient was derived independently by Einstein and Smoluchowski in their theory of Brownian motion [1,2]. Later, this relation was established by Nyquist [3] for electric circuits and was experimentally confirmed by Johnson [4]. The Nyquist-Johnson relation was extended by Callen and Welton [5] to a general class of dissipative thermodynamic equilibrium systems (see also Ref. [6]). In the classical case the spectral function of the fluctuations has the following form:

$$(x^2)_\omega = \frac{2\Theta}{\omega} \mathrm{Im}\, \alpha(\omega), \tag{1}$$

where $\alpha(\omega)$ is the response function, and Θ is the temperature in energy units. The linear response theory and the fluctuation-dissipation theorem (FDT) for arbitrary dynamic systems was developed by Kubo [7], Mori [8], and Zwanzig [9]. In the Kubo method the response of the density matrix to the external field is calculated, whereas the Mori-Zwanzig technique introduces a projection operator to the space of variables that describe the macroscopic states of the system. This technique was further developed by Lee [10] with the assumption that the space of variables, describing macroscopic states of the system is formed not only by the set of dynamic operators but also by their time derivatives to any order. The slow processes and long time correlations in connection with ergodicity, anomalous diffusion, and Fick's law has been studied in Ref. [11]. The most comprehensive review of the state of the art concerning dynamical correlation has been presented in a recent publication by Balucani, Lee, and Tognetti [12].

Klimontovich showed [13] that the standard FDT leads to several difficulties if applied to concrete systems. Klimontovich stated that the FDT always has system-specific forms. Indeed, in general case, the system parameters may depend both on time and space. Inhomogeneities in space and time on scales greater than the fluctuation scales will certainly also contribute to fluctuations. Recently, in the context of plasma physics, and using the Langevin approach and the time-space multiscale technique, it has been shown that the amplitude and the width of the spectral lines of the electrostatic field fluctuations and the electron form factor are determined not only by the imaginary part of the dielectric susceptibility but also by the derivatives of its real part [14]. As a result of the inhomogeneity, these properties become asymmetric with respect to the inversion of the sign of the frequency. In the kinetic regime, the form factor is more sensitive to space gradients than the spectral function of the electrostatic field fluctuations. This asymmetry of lines can be used as a diagnostic tool to measure local gradients in the plasma.

In this Brief Report we generalize the fluctuation-dissipation theorem for slowly varying processes. Using the momentum method and the time multiscale technique, a generalized Callen-Welton formula is derived. The width and the amplitude of the spectral lines of the fluctuations are determined not only by the dissipation but also by the derivatives of the dispersion. These two effects have a comparable influence for systems with a high Q factor. The non-Joule dispersion contribution is characterized by a new non-local effect originating from an additional phase shift between the force and the response of the system. This phase shift results from the parametric control to the system. As an application we consider a LC circuit. It is shown that the spectral function of the current depends not only on the real part of the impedance (dissipation) but also on the derivatives of its imaginary part (dispersion). It is also shown that at finite time intervals one can drastically increase the Q factor by simultaneous increasing the inductance and decreasing the capacity.

Let us consider an arbitrary system whose evolution is described by the following equation:

$$\left(\frac{\partial}{\partial t} + \underline{\underline{L}}(t) \right) \cdot \underline{\underline{G}}(t,t') = 0, \quad t > t', \tag{2}$$

where $\underline{\underline{L}}(t)$ is generally a non-self-conjugate, linear operator in the Hilbert space. This operator varies slowly in time. The term ''slowly'' means that the control parameter undergoes only a small change during the period of the system

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motion. $\underline{\underline{G}}(t,t')$ may be the Heisenberg operator. Then $\underline{\underline{L}}(t)\cdot\underline{\underline{G}}(t,t')$ will be the commutator with the Hamiltonian. In other cases $\underline{\underline{G}}(t,t')$ could be a density matrix, and $\underline{\underline{L}}(t)$ would appear as the Liouville operator. Finally, for $\underline{\underline{G}}(t,t')$ we can take the two-time correlator $\underline{\underline{G}}(t,t')=\langle\delta f_{nm}(t)\delta f^{*}_{n_1m_1}(t')\rangle$ of the deviation from the referent state $f_n(t)$ of the density matrix in the energy representation $\delta f_{nm}(t)$ [15,16]. In such a case $\underline{\underline{L}}(t)$ takes into account the self-consistent field and collisions. The time dependence in $\underline{\underline{L}}(t)$ manifests itself in the referent state and in the terms containing the external force. The slow scale is much larger than the characteristic fluctuation time. We can therefore introduce a small parameter μ, which allows us to describe fluctuations on the basis of a multiple time scale analysis. Obviously, fluctuations vary on both ''fast'' and ''slow'' time scales. The solution of the linear equation (2) can be expressed through Green's function or the propagator $\underline{\underline{U}}(t,t')$ of Eq. (2) as

$$\underline{\underline{G}}(t,t')=\underline{\underline{U}}(t,t')\cdot\underline{\underline{G}}(0), \tag{3}$$

where in the case of the kinetic fluctuations, the one-time moment $\underline{\underline{G}}(0)$ is given by

$$\underline{\underline{G}}(0)=\langle\delta f_{nm}(t')\delta f^{*}_{n_1m_1}(t')\rangle = \delta_{nn_1}\delta_{mm_1}\frac{f_n(\mu t')+f_m(\mu t')}{2}. \tag{4}$$

If the operator $\underline{\underline{L}}$ does not depend on time, the dependence on time of Green's function appears only through the interval $t-t'$. However, when we consider an operator $\underline{\underline{L}}(\mu t)$ slowly varying in time, and when we take nonlocal effects into account, the time dependence of $\underline{\underline{U}}(t,t')$ is more subtle [14,17].

$$\underline{\underline{U}}(t,t')=\underline{\underline{U}}(t-t',\mu t'). \tag{5}$$

Here we want to stress that the nonlocal effects appear due to the slow time dependences $\mu t'$. At first order, the expansion of Eq. (5) with respect to μ leads to

$$\underline{\underline{U}}(t,t')=\left(1-\mu\tau\frac{\partial}{\partial\mu t}\right)\underline{\underline{U}}(\tau,\mu t),\quad \tau=t-t'. \tag{6}$$

Let us introduce the resolvent operator $\check{\underline{\underline{R}}}(z)$ which can be defined formally as the Laplace transform of the propagator $\underline{\underline{U}}(\tau)$:

$$\check{\underline{\underline{R}}}(z)=\int_0^\infty\underline{\underline{U}}(\tau)\exp(iz\tau)d\tau,\quad z=\omega+i0 \tag{7}$$

The Laplace transform of Eqs. (3) and (6) gives

$$\underline{\underline{G}}^{+}(z)=\left(1+i\frac{\partial^2}{\partial t\partial\omega}\right)\check{\underline{\underline{R}}}(z)\cdot\underline{\underline{G}}(0). \tag{8}$$

For sake of convenience we omit μ from that equation and throughout this Brief Report, keeping in mind that the time derivatives are taken with respect to the slowly varying variables. Thus in first approximation the expression for the spectral function of the fluctuations is

$$\underline{\underline{G}}(\omega)=2\mathrm{Re}\left(1+i\frac{\partial^2}{\partial t\partial\omega}\right)\check{\underline{\underline{R}}}(z)\cdot\underline{\underline{G}}(0). \tag{9}$$

The spectral density of the fluctuations of the internal parameters of the system in local equilibrium can be defined as usual [16,18].

$$(\delta A\,\delta B)_\omega=\underline{\underline{A}}\cdot\underline{\underline{G}}(\omega)\cdot\underline{\underline{B}} =\hbar\left[\mathrm{Im}\alpha_{AB}(\omega)+\frac{\partial^2}{\partial t\partial\omega}\mathrm{Re}\alpha_{AB}(\omega)\right]\coth(\hbar\omega/2\Theta), \tag{10}$$

where

$$\alpha_{AB}(\omega)=i\hbar\sum_{nm}\check{R}_{nmnm}(z)A_{mn}B_{nm}(f_m-f_n) \tag{11}$$

is the response function for diagonal resolvent [16].

In the classical limit $\hbar\to0$ the generalized Callen-Welton formula (10) takes the form

$$(\delta A\,\delta B)_\omega=\left[\mathrm{Im}\alpha_{AB}(\omega)+\frac{\partial^2}{\partial t\partial\omega}\mathrm{Re}\alpha_{AB}(\omega)\right]\frac{2\Theta}{\omega}. \tag{12}$$

In deriving Eqs. (10) and (12) we assumed the system to be in a local equilibrium state, so that the characteristic time for the variation of parameters exceeds the relaxation time of the distribution function. When expanding Green's function in Eq. (6) in terms of the small parameter μ, there appears an additional term at first order. It is important to note that the imaginary part of the response function is now replaced by the real part. If the Q factor of the system is of the order of 1 (it could be a broad-band system or a process near the zero frequency), the real and imaginary parts of the response function are of the same order and the correction is negligibly small. But in the case of systems with a high Q factor, for which the real part of the response function is greater than the imaginary part, the second small parameter appears to be inversely proportional to the Q factor. An example of such system with a high Q factor could be plasma fluctuations near the Langmuir frequency when the Q factor is inversely proportional to the small plasma parameter [14]. When this small parameter is comparable with μ, the second term in Eqs. (10) and (12) may have an effect comparable to the first term. This will be shown in the following example. At the second order in the expansion in μ, the corrections appear only in the imaginary part of the response function, and they can reasonably be neglected. It is therefore sufficient to retain the first order corrections to solve the problem. The same derivatives of the dispersion, as in Eqs. (10) and (12), appear in the geometrical optics approximation [19] and play an important role in defining the adiabatic invariant in a dispersive medium [20].

As an example we consider the electrical oscillation circuit which can be used to model many oscillation processes in nature. We assume that all the circuit elements (resistance R, inductance L, and capacity C) have the same temperature Θ, which can change adiabatically. Therefore the system pa-

rameters R, L, and C will vary slowly in time. Moreover the change of these parameters may also be mechanical, due to the action of external forces, by ''hand.'' It is this case that we will consider when evaluating the Q factor of an LC circuit.

The thermal motion of the charged particles in the circuit give rise to electric oscillations which can be considered to be equivalent to Brownian motion. The corresponding Langevin equation is

$$\frac{dq}{dt}=J, \quad L(\mu t)\frac{dJ}{dt}+R(\mu t)J+\frac{q}{C(\mu t)}=\check{E}, \tag{13}$$

where q is the electric charge, J is the current, and $\check{E}$ is the Langevin source. It can be treated as the emf equivalent to the action of the thermal motion of the charged particles in the circuit. Coming back to the momentum method, we can represent the two-time correlator of the electric current $G_J(t,t')$ as $G_J(t,t')=U(t,t')G_J(0)$, where $U(t,t')$ is the propagator of the set of Eqs. (13), and where the initial condition $G_J(0)$ for the local equilibrium state is

$$G_J(0)=\frac{(L/C)^{1/2}}{2\pi\Theta}\int J^2\exp\left(-\frac{LJ^2+q^2/C}{2\Theta}\right)dqdJ=\frac{\Theta(\mu t')}{L(\mu t')}. \tag{14}$$

Applying the procedure above, we obtain the following expression for the spectral function of the current in the circuit:

$$(J^2)_\omega=2\,\mathrm{Re}\left(1+i\frac{d^2}{dtd\omega}\right)\check{\mathrm{R}}(z)\frac{\Theta}{L}=\frac{2\left[\mathrm{Re}\,Z(\omega)+\dfrac{d^2}{dtd\omega}\mathrm{Im}\,Z(\omega)\right]\Theta}{\mathrm{Im}^2Z(\omega)+\left[\mathrm{Re}\,Z(\omega)+\dfrac{d^2}{dtd\omega}\mathrm{Im}\,Z(\omega)\right]^2}, \tag{15}$$

where $Z(\omega)=R-i(L\omega-1/C\omega)$ is the complex impedance.

In deriving Eq. (15) we assumed that the time variations of the parameters in the resolvent take place at scales much greater than the oscillation period, and the local equilibrium initial state (14) is achieved when R is greater than dL/dt. The second restriction can be relaxed by introducing the nonequilibrium initial correlator of the current $G_J^{neq}(0)$. In this case the Eq. (15) takes the following form:

$$(J^2)_\omega=\frac{2\left[\mathrm{Re}\,Z(\omega)+\dfrac{d^2}{dtd\omega}\mathrm{Im}\,Z(\omega)\right]\tilde{\Theta}}{\mathrm{Im}^2Z(\omega)+\left[\mathrm{Re}\,Z(\omega)+\dfrac{d^2}{dtd\omega}\mathrm{Im}\,Z(\omega)\right]^2}, \tag{16}$$

where $\tilde{\Theta}=LG_J^{neq}(0)$. We will see that the initial correlator is not important when calculating the spectral line width and the Q factor of the electrical oscillation circuit.

Using the Langevin equations (13) the expressions for the spectral function of the current takes the form

$$(J^2)_\omega=\frac{(\check{E}^2)_\omega}{\mathrm{Im}^2Z(\omega)+\left[\mathrm{Re}\,Z(\omega)+\dfrac{d^2}{dtd\omega}\mathrm{Im}\,Z(\omega)\right]^2}. \tag{17}$$

The comparison of Eqs. (15) and (17) gives for the spectral density of the emf

$$(\check{E}^2)_\omega=2\left[\mathrm{Re}\,Z(\omega)+\frac{d^2}{dtd\omega}\mathrm{Im}\,Z(\omega)\right]\tilde{\Theta}=2\left[R-\frac{dL}{dt}+\frac{1}{\omega^2C^2}\frac{dC}{dt}\right]\tilde{\Theta}, \tag{18}$$

which is a generalized Nyquist formula. One can see that in the general case the spectral density of the emf for slow processes depends on the frequency and is not always white noise.

Now let us come back to a point discussed in the beginning, namely to the Q factor of the oscillating system. As the time derivative can have different signs, the dispersion corrections in Eq. (15) may both decrease or increase the linewidth and therefore also the oscillating system Q factor. The independent variation of the reactive parameters L and C gives rise a shift of the circuit proper frequency. To avoid this frequency shift we should change the reactive parameters L and C as

$$\frac{dC}{dt}=-\frac{C}{L}\frac{dL}{dt}, \tag{19}$$

which follows from the condition of the stability of the circuit frequency: $\omega_0=(LC)^{-1/2}=\mathrm{const}$. In this case Eq. (15) takes the form

$$(J^2)_\omega=\frac{2\tilde{\Theta}\left[R-\dfrac{dL}{dt}\left(1+\dfrac{1}{\omega^2LC}\right)\right]}{(L\omega-1/C\omega)^2+\left[R-\dfrac{dL}{dt}\left(1+\dfrac{1}{\omega^2LC}\right)\right]^2}. \tag{20}$$

Near the resonance point $\omega=\omega_0$

$$(J^2)_\omega=\frac{\tilde{\Theta}}{L}\frac{\gamma}{(\omega-\omega_0)^2+\gamma^2}+\frac{\tilde{\Theta}}{L}\frac{\gamma}{(\omega+\omega_0)^2+\gamma^2}, \tag{21}$$

where the linewidth is given by

$$\gamma=\frac{1}{2L}\left(R-2\frac{dL}{dt}\right). \tag{22}$$

We see from Eqs. (21) and (22) that the correction is still symmetric with respect to the change of sign of ω, but the intensities and broadening are different from the stationary case. In the case of local equilibrium, the integral of the intensity over frequency remains the same as in the stationary case (Fig. 1). For $dL/dt=-(L/C)(dC/dt)=)(1/5)R$ the initial correlation differs from local equilibrium less than 1%.

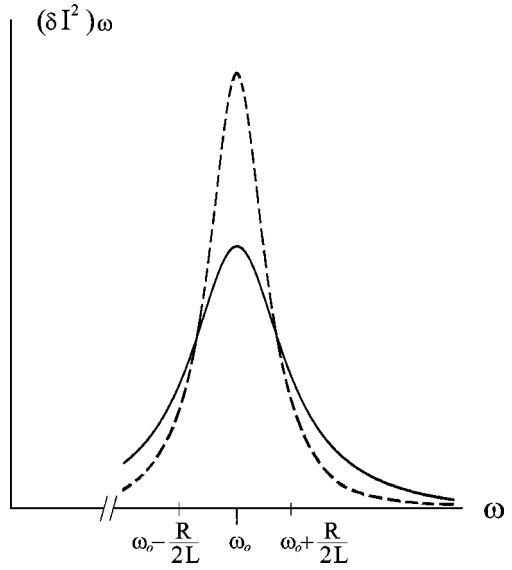

FIG. 1. Spectral function of current fluctuations as a function of frequency. The solid and dashed lines correspond to $dL/dt = dC/dt = 0$ and $dL/dt = -(L/C)(dC/dt) = (1/5)R$, respectively.

The spectral line quality factor becomes now

$$Q = \frac{\omega}{2\gamma} = \left(\frac{L}{C}\right)^{1/2} \frac{1}{R - 2\dfrac{dL}{dt}}. \tag{23}$$

Note that the initial correlation is not present in the expressions for the linewidth (22) and the Q factor (22), these expressions being fully determined by the singularities of the resolvent. Usually the Q factor increases as the inductance increases and the capacity decreases, but due to the nonstationary dispersion terms it can increase drastically. The higher the initial Q factor of the system, the stronger the effect. Thus for a circuit proper frequency of 1 kHz and a Q factor$=1000$, the second term in Eq. (22) is comparable to the first one, when the reactive parameters L and C of the system vary by several tenths per second. As we consider the linear approximation, to avoid misunderstanding we assume that $R > 2(dL/dt)$. Therefore, at finite time intervals one can increase drastically the Q factor by simultaneously increasing the inductance and decreasing the capacity. Similar situations can appear in other oscillating systems.

Using the momentum method and the time multiscale technique, we have generalized the Callen-Welton formula to systems with slowly varying parameters. The important conclusion of this analysis is to reveal that the spectral function of the fluctuations is determined not only by the dissipation but also by the derivatives of the dispersion. The non-Joule dispersion contribution is characterized by a new nonlocal effect originating from an additional phase shift between the force and the response of the system. That phase shift results from the parametric control to the system. Finally, an electrical oscillation circuit is considered as a concrete example. In that system it is shown that the dispersive contributions strongly affect the Q factor. These results are applicable to other systems and are important for the understanding of various behaviors observed in different field of physics, communication, chemistry, and biophysics.

Fruitful discussions with M. Tlidi and Yu.A. Kukharenko are gratefully acknowledged. This research was supported by the Russian Foundation for Basic Research (Grant No. 03-02-16345).

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