Fluctuation -Dissipation-Dispersion Relation for Slow Processes and Quality Factor for Oscillation Systems

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***Abstract*—We have generalized the Fluctuation-Dissipation Theorem to the 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 dissipation but also by the derivatives of the dispersion. 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. 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.**

***Index Terms*—non-equilibrium fluctuations, FDT, Q-factor**

I. Introduction

Any oscillating system is characterized by two main parameters: the proper frequency and the quality factor. The latter is inversely proportional to the width of the spectral line of the parameter fluctuations. In thermodynamic equilibrium, 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 [6]). In the classical case the spectral function of the fluctuations has the form:

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

where $\alpha(\omega)$ - is the response function, and Θ - is the temperature in energy units. The linear response theory and the fluctuation-dissipation theorem 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 macroscopic states of the system. Generally, the system parameters may depend on both 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 [10]. 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 communication 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 quality 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 increase drastically the quality factor by the simultaneous increasing the inductance and decreasing the capacity.

II. Results

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

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

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 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 $\underline{\underline{G}}(t,t')=\left\langle\delta f_{nm}(t)\delta f^{*}_{n_1m_1}(t')\right\rangle$ of the deviation from the referent state $f_n(t)$ of the density matrix in the energy representation $\delta f_{nm}(t)$ [11], [12]. 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 the 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

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

If the operator $\underline{\underline{L}}$ does not depend on time, the dependence on time of the 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 non-local effects into account, the time dependence of $\underline{\underline{U}}(t,t')$ is more subtle [13], [14].

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

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

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

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

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

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

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

For sake of convenience we omit μ from that equation and throughout this communication, 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

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

The spectral density of the fluctuations of the internal parameters of the system in local equilibrium can be defined as usual [12], [15].

$$(\delta A\delta B)_\omega=\underline{\underline{A}}\cdot\underline{\underline{G}}(\omega)\cdot\underline{\underline{B}}$$

$$=\hbar[\mathrm{Im}\,\alpha_{AB}(\omega)+\frac{\partial^2}{\partial t\partial\omega}\,\mathrm{Re}\,\alpha_{AB}(\omega)]\coth(\hbar\omega/2\Theta), \tag{10}$$

where

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

is the response function for diagonal resolvent [12].

In the classical limit $\hbar\longrightarrow 0$ the generalized Callen-Welton formula (10) takes the form

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

In deriving Eqs. (10,12) we assumed the system to be in a local equilibrium state, so that the characteristic time for parameters variation exceeds the relaxation time of the distribution function. When expanding the 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 quality factor of the system is of the order of 1 (it can 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 quality 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 quality factor. An example of such system with a high quality factor could be plasma fluctuations near the Langmuir frequency when the quality factor is inversely proportional to the small plasma parameter [10]. When this small parameter is comparable with μ, the second term in Eqs. (10,12) may have an effect comparable to the first term. This will be shown in the next 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. (10,12), appear in the geometrical optics approximation [16] and play an important role in defining the adiabatic invariant in a dispersive medium [17].

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 parameters 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 quality factor of LC-circuit.

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

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

where q is the electric charge, J is the current, and $\check{E}$ is the Langevin source. It can be treated as the e.m.f. 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

$$G_J(t,t') = U(t,t')G_J(0), \qquad (14)$$

where $U(t,t')$- is the propagator of the set of equations (13), and where the initial condition $G_J(0)$ for the local equilibrium state is

$$G_J(0) = \frac{(L/C)^{1/2}}{2\pi\Theta}\int J^2 \exp\left(-\frac{LJ^2+q^2/C}{2\Theta}\right) dqdJ$$
$$= \frac{\Theta(\mu t')}{L(\mu t')}. \qquad (15)$$

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

$$(J^2)_\omega = 2\,\mathrm{Re}(1 + i\frac{d^2}{dtd\omega})\check{\mathrm{R}}(z)\frac{\Theta}{L}$$
$$= \frac{2[\mathrm{Re}\,Z(\omega) + \frac{d^2}{dtd\omega}\,\mathrm{Im}\,Z(\omega)]\Theta}{\mathrm{Im}^2\,Z(\omega) + [\mathrm{Re}\,Z(\omega) + \frac{d^2}{dtd\omega}\,\mathrm{Im}\,Z(\omega)]^2}, \qquad (16)$$

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

In deriving Eq. (16) 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 (15) is achieved when R is greater than $\frac{dL}{dt}$. The second restriction can be relaxed by introducing the nonequilibrium initial correlator of the current $G_J^{neq}(0)$. In this case the Eq. (16) takes the form:

$$(J^2)_\omega = \frac{2[\mathrm{Re}\,Z(\omega) + \frac{d^2}{dtd\omega}\,\mathrm{Im}\,Z(\omega)]\widetilde{\Theta}}{\mathrm{Im}^2\,Z(\omega) + [\mathrm{Re}\,Z(\omega) + \frac{d^2}{dtd\omega}\,\mathrm{Im}\,Z(\omega)]^2}, \qquad (17)$$

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

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

$$(J^2)_\omega = \frac{(\check{E}^2)_\omega}{\mathrm{Im}^2\,Z(\omega) + [\mathrm{Re}\,Z(\omega) + \frac{d^2}{dtd\omega}\,\mathrm{Im}\,Z(\omega)]^2}. \qquad (18)$$

The comparison of Eqs. (16) and (18) gives for the spectral density of the e.m.f.

$$(\check{E}^2)_\omega = 2[\mathrm{Re}\,Z(\omega) + \frac{d^2}{dtd\omega}\,\mathrm{Im}\,Z(\omega)]\widetilde{\Theta}$$
$$= 2[R - \frac{dL}{dt} + \frac{1}{\omega^2C^2}\frac{dC}{dt}]\widetilde{\Theta}, \qquad (19)$$

which is a generalized Nyquist formula. One can see that in the general case the spectral density of the e.m.f. 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 quality factor of the oscillation system. As the time derivative can have different signs, the dispersion corrections in Eq. (16) may both decrease and increase the line width and therefore also the oscillation system quality factor. The independent variation of the reactive parameters L and C results in a shift of the circuit proper frequency. To avoid this frequency shift we should change the reactive parameters L and C as

$$\frac{dC}{dt} = -\frac{C}{L}\frac{dL}{dt}, \qquad (20)$$

which follows from the condition of the stability of the circuit frequency: $\omega_0 = (LC)^{-1/2} = const$. In this case Eq. (16) takes the form

$$(J^2)_\omega = \frac{2\widetilde{\Theta}[R - \frac{dL}{dt}(1 + \frac{1}{\omega^2LC})]}{(L\omega - 1/C\omega)^2 + [R - \frac{dL}{dt}(1 + \frac{1}{\omega^2LC})]^2}. \qquad (21)$$

Near the resonance point $\omega = \omega_0$

$$(J^2)_\omega = \frac{\widetilde{\Theta}}{L}\frac{\gamma}{(\omega-\omega_0)^2+\gamma^2} + \frac{\widetilde{\Theta}}{L}\frac{\gamma}{(\omega+\omega_0)^2+\gamma^2}, \qquad (22)$$

where the line width is given by

$$\gamma = \frac{1}{2L}(R - 2\frac{dL}{dt}). \qquad (23)$$

We see from Eqs. (22), (23) 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).

The quality factor becomes now

$$Q = \frac{\omega}{2\gamma} = (\frac{L}{C})^{1/2}\frac{1}{R - 2\frac{dL}{dt}}. \qquad (24)$$

Note that the initial correlation is not present in the expressions for the line width (23) and the quality factor (23), these expressions being fully determined by the singularities of the resolvent. Usually the quality factor increases as the inductance increases and the capacity decreases, but due to the nonstationary dispersion terms it can increase drastically.

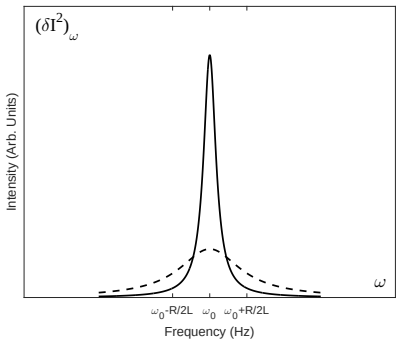

Fig. 1. Spectral function of current fluctuations as a function of frequency. The solid and dashed lines correspond to $\frac{dL}{dt} = \frac{dC}{dt} = 0$ and $\frac{dL}{dt} = -\frac{L}{C}\frac{dC}{dt} = \frac{2}{5}R$ respectively.

The higher the initial quality factor of the system, the stronger the effect. Thus for a circuit proper frequency of 1 kHz and a quality factor =1000, the second term in Eq. (23) 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 $R > 2\frac{dL}{dt}$. Therefore, at finite time intervals one can increase drastically the quality factor by simultaneously increasing the inductance and decreasing the capacity. Similar situations can appear in other oscillating systems.

III. Conclusion

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 dissipation but also by the derivatives of the dispersion. 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. 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 quality 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.

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