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On the Quantum Nyquist Formula

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Abstract—Yu.L. Klimontovich's assertion on the incorrectness of the quantum Nyquist formula is discussed. It is shown that, in quantum physics, Rytov's fluctuation formula, the Casimir force theory as treated by E.M. Lifshitz, and the quantum Nyquist formula are all incorrect, as they are united by a common basis.

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In his recent book *Strokes to Portraits of Scientists: Disputed Topics in Statistical Physics* [1], Klimontovich addressed some open problems in modern physics. As early as 1987 [2], he asserted the incorrectness of the quantum Nyquist formula, which was derived in 1928 [3] and has been reproduced in handbooks and monographs [4, 5]. This is a delicate question. The fact is that relaxation constants, such as the electric resistance R, appear in the theory as a result of approximate calculations. Thus, it was stated that the quantum Nyquist formula cannot involve a phenomenological constant that satisfactorily describes kinetic phenomena under different conditions. Klimontovich's assertion drew fierce criticism [6] but, unfortunately, the discussion was stopped without clarifying the subject [7]. Completed in 2002, Klimontovich's memoirs suggest that he did not change his point of view over the many years that passed.

In 1998, it was shown in [8] that, according to the Gibbs distribution, simultaneous quantum averages at thermodynamic equilibrium are determined only by elastic interactions in the system. The terms of the Feynman series that correspond to inelastic processes (in particular, to induced emission) cancel out in the calculations. This means that, even in approximate calculations, the relaxation parameters determined by the Boltzmann equation (the resistance R, the complex permittivity of the medium, etc.) cannot participate in the formation of simultaneous quantum averages at thermodynamic equilibrium. Therefore, the fluctuation-dissipation theorem (FDT) integrated over the frequency cannot depend on such dissipative characteristics. Any "proof" of the opposite statement is erroneous. This argument justifies the limited applicability of the quantum Nyquist formula, which supports Klimontovich's assertion.

At present, there are other, more visual arguments indicating that not only the Nyquist formula but also Rytov's optical fluctuation formula [4, 9, 10], the Casimir force theory as treated by Lifshitz [4, 10, 11], etc., are also incorrect. These arguments are presented below.

As the simplest model, consider an electrical oscillator circuit governed by the standard equation

$$L\frac{d^2q(t)}{dt^2} + R\frac{dq(t)}{dt} + \frac{1}{C}q(t) = E(t), \tag{1}$$

where $q(t)$ is the charge on a capacitor of capacitance C, L is the inductance, R is the resistance, and $E(t)$ is the electromotive force (emf). When $R = E(t) = 0$, the solution to this equation is

$$q(t) = \gamma(\alpha e^{-i\omega_0 t} + \alpha^* e^{i\omega_0 t}), \quad \omega_0 = \frac{1}{\sqrt{LC}},$$

where γ and α are constants. To study thermodynamic quantum fluctuations, we need a quantum description of the system, which is obtained at $R = E(t) = 0$ by replacing the classical variables with the operators

$$\alpha \longrightarrow \hat{\alpha}, \quad \alpha^* \longrightarrow \hat{\alpha}^+,$$

$$\gamma = \sqrt{\frac{\hbar\omega_0 C}{2}}, \quad \hat{\alpha}\hat{\alpha}^+ - \hat{\alpha}^+\hat{\alpha} = [\hat{\alpha}, \hat{\alpha}^+] = 1,$$

$$q(t) \longrightarrow \hat{q}(t) = \gamma(\hat{\alpha}e^{-i\omega_0 t} + \hat{\alpha}^+ e^{i\omega_0 t})$$

(see [12]). The Hamiltonian of the system is

$$\hat{H}_0 = \frac{\hbar\omega_0}{2}(\hat{\alpha}\hat{\alpha}^+ + \hat{\alpha}^+\hat{\alpha}).$$

We are interested in the correlation function $\langle \hat{q}(t)\hat{q}(t')\rangle$, where the average is taken in both the quantum and statistical sense according to the Gibbs distribution. The advanced and retarded Green's functions are defined as

$$G_{r,a}(t-t') = \pm\frac{i}{\hbar}\langle[\hat{q}(t), \hat{q}(t')]\rangle\vartheta(\pm t \mp t'), \qquad (2)$$

where $\vartheta(t)$ is the Heaviside step function. Direct verification shows that the Fourier transforms

$$\langle\hat{q}\hat{q}\rangle_\omega = \int_{-\infty}^{\infty} e^{i\omega(t-t')}\langle\hat{q}(t)\hat{q}(t')\rangle d(t-t')$$

satisfy the identity

$$\langle\hat{q}\hat{q}\rangle_\omega = -i\hbar\left(1+\frac{1}{e^{\frac{\hbar\omega}{T}}-1}\right)[G_r(\omega)-G_a(\omega)],$$
$$G_a(\omega) = G_r^*(\omega). \qquad (3)$$

Identity (3) is a mathematical statement of the FDT [4, 13]. The form of (3) is invariant under any interaction of the subsystem under study with its surroundings if the whole system is described by some Hamiltonian. In our view, FDT is an extremely unsuitable name, because identity (3) holds for Hamiltonian systems, which do not involve dissipative processes. It will be shown below that, when expressed in terms of generalized functions, the unconditionally exact formula (3) is unstable with respect to approximations of its right-hand side. In fact, this point was indicated by Klimontovich [1, 2], unfortunately, without accepting the exact interpretation of formula (3) itself.

With allowance for the vacuum term, the quantum Nyquist formula is given by

$$\langle\varepsilon^2\rangle_\omega = \hbar\omega\left(1+\frac{1}{e^{\frac{\hbar\omega}{T}}-1}\right)2R, \quad -\infty<\omega<\infty \qquad (4)$$

(see [3]). Here, $\langle\varepsilon^2\rangle_\omega$ denotes thermodynamic fluctuations of the emf in the circuit. Formula (4) cannot be interpreted exactly, since there is no quantum emf operator and the left-hand side of (4) is not rigorously defined. However, given the impedance

$$z(\omega) = R - i\left(\omega L - \frac{1}{\omega C}\right),$$

it is assumed that formula (4) can be used to derive the spectrum of charge fluctuations on the capacitor:

$$\langle\hat{q}\hat{q}\rangle_\omega = \frac{\langle\varepsilon^2\rangle_\omega}{\omega^2|z(\omega)|^2}$$
$$= \hbar\omega\left(1+\frac{1}{e^{\frac{\hbar\omega}{T}}-1}\right)\frac{2R}{\left(\omega^2 L - \frac{1}{C}\right)^2+\omega^2R^2}. \qquad (5)$$

It is this formula that we discuss below. Specifically, we show that it is not true in quantum theory.

Returning to the quantum description of the electric circuit, we take into account the presence of an active resistance in the circuit by assuming that the charge $\hat{q}$ interacts with an external (with respect to the circuit) reservoir, which is also described in a quantum manner. Let the interaction between the circuit and the reservoir be specified by an interaction Hamiltonian $\hat{H}'$. Then the total Hamiltonian of the system in the Schrödinger representation is

$$\hat{H} = \hat{H}_0 + \sum_i \varepsilon_i\hat{\beta}_i^+\hat{\beta}_i + \hat{H}' - \hat{q}E(t). \qquad (6)$$

Assume that the reservoir represents a Bose gas and

$$\hat{H}' = -g\int\hat{\psi}^+(x)\hat{P}\hat{q}\hat{\psi}(x)dx.$$

Here,

$$\hat{\psi}(x) = \sum_i \psi_i(x)\hat{\beta}_i,$$

$$\hat{\psi}^+(x) = \sum_i \psi_i^*(x)\hat{\beta}_i^+, \quad \hat{q} = \gamma(\hat{\alpha}+\hat{\alpha}^+),$$

where $\hat{\beta}_i$ and $\hat{\beta}_i^+$ are annihilation and creation operators for particles in the state ψ_i with energy ε_i such that

$$[\hat{\beta}_i, \hat{\beta}_j^+] = \delta_{ij};$$

g is an interaction constant; and $\hat{P}$ is a Hermitian operator. When $E(t)$ is low, Hamiltonian (6) yields Kubo's formula [14]

$$\langle\check{q}(t)\rangle = \int_{-\infty}^{\infty} G_r(t-t')E(t')dt',$$

where $\check{q}(t)$ is a charge operator in the Heisenberg representation. The function $G_r(t-t')$ is given by (2) with the quantum average taken over the eigenfunctions of total Hamiltonian (6) with $E(t) = 0$. We need the equations of motion for the Heisenberg operators $\check{\alpha}(t)$ and $\check{\beta}_i(t)$. Proceeding in the standard manner gives

$$i\hbar\frac{d\check{\alpha}(t)}{dt} = [\check{\alpha}, \check{H}]$$
$$= \hbar\omega_0\check{\alpha}(t) - g\gamma\sum_{ij}P_{ij}\check{\beta}_j^+(t)\check{\beta}_i(t) - \gamma E(t),$$
$$i\hbar\frac{d\check{\beta}_j(t)}{dt} = [\check{\beta}_i, \check{H}] \qquad (7)$$
$$= \varepsilon_j\check{\beta}_j(t) - g\gamma\sum_i P_{ji}(\check{\alpha}(t)+\check{\alpha}^+(t))\check{\beta}_i(t),$$

where

$$P_{ij} = P_{ji}^* = \int \psi_i^* \hat{P} \psi_j dx.$$

Taking the Hermitian conjugate, we derive equations for $\breve{\alpha}^+(t)$ and $\breve{\beta}_i^+(t)$. The equation of motion for the product $\breve{\beta}_i^+(t)\breve{\beta}_j(t)$ in (7) is

$$i\hbar \frac{d\breve{\beta}_i^+(t)\breve{\beta}_j(t)}{dt} = -\hbar\omega_{ij}\breve{\beta}_i^+(t)\breve{\beta}_j(t)$$
$$+ g\sum_{j'} P_{j'i}\breve{\beta}_{j'}^+(t)\breve{\beta}_j(t)\breve{q}(t)$$
$$- g\sum_{i'} P_{ji'}\breve{\beta}_i^+(t)\breve{\beta}_{i'}(t)\breve{q}(t), \quad \hbar\omega_{ij} = \varepsilon_i - \varepsilon_j.$$

Applying the Fourier transform to these equations, we easily find

$$\begin{aligned} &-i\hbar(\omega^2 - \omega_0^2)\langle \breve{q}(\omega)\rangle \\ &= 2i\omega_0 g^2\gamma^2 \left\langle \sum_{ijj'} P_{ij}(P_{ij'}^* \breve{q}\breve{\beta}_{j'}^+\breve{\beta}_j - P_{jj'}\breve{q}\breve{\beta}_i^+\breve{\beta}_{j'}) \right\rangle \\ &\times (\hbar\omega + \hbar\omega_{ij})^{-1} + 2i\omega_0\gamma^2 E(\omega). \end{aligned} \tag{8}$$

Assuming that the interaction is weak, the correlation functions in Eq. (8) are split as follows:

$$\langle \breve{q}\breve{\beta}_j^+\breve{\beta}_{j'}\rangle = \delta_{jj'}N_j\langle \breve{q}(\omega)\rangle,$$

where $N_j = \langle \breve{\beta}_{i'}^+\breve{\beta}_j\rangle$ denotes the average occupation numbers of the states ψ_j. The resulting equation is explicitly solved to obtain

$$\langle \breve{q}(\omega)\rangle = -\frac{E(\omega)}{L\left(\omega^2 - \omega_0^2 - \dfrac{2\omega_0}{\hbar}\pi_r(\omega)\right)}, \tag{9}$$

where

$$\pi_r(\omega) = g^2\gamma^2 \sum_{ij} |P_{ij}|^2 \frac{N_j - N_i}{\hbar\omega - \hbar\omega_{ij} + i0}. \tag{10}$$

Here, $i0$ in the denominator arises since we chose a retarded solution. A comparison of (9) with the solution

$$q(\omega) = -\frac{E(\omega)}{L\left(\omega^2 - \omega_0^2 + i\dfrac{R}{L}\omega\right)} \tag{11}$$

to Eq. (1) shows that these formulas are identical if

$$\pi_r(\omega) = -i\frac{\hbar\omega}{2\omega_0 L}R. \tag{12}$$

Combining (11) with Kubo's formula yields

$$G_r(\omega) = -\frac{1/L}{\omega^2 - \omega_0^2 - \dfrac{2\omega_0}{\hbar}\pi_r(\omega)}. \tag{13}$$

Substituting this result into an unconditionally exact formula (3), which represents the FDT, and taking into account (12), we derive the quantum Nyquist formula (5). Can this procedure be regarded as a proof of the Nyquist formula? It turns out that the answer is no, even if R is assumed to be a function of frequency rather than a constant. To show this, we evaluate

$$\langle (\hat{q})^2\rangle = \int_{-\infty}^{\infty} \langle \hat{q}\hat{q}\rangle_\omega \frac{d\omega}{2\pi}. \tag{14}$$

First, we calculate $G_{r,a}(\omega)$ up to second-order perturbative terms and then apply the FDT. Actually, the calculation result is exact in the approximation $\sim g^2$ and no additional approximations are required. Equation (8) is solved by iteration. In the zero approximation, the correlation functions on the right-hand side are exactly split, and we have

$$\langle \breve{q}(\omega)\rangle = -\frac{E(\omega)}{L(\omega^2 - \omega_0^2)}.$$

In the g^2 approximation,

$$\begin{aligned} G_r(\omega) = &-\frac{1}{L(\omega^2 - \omega_0^2)}\Bigg[1 + \frac{1}{\omega^2 - \omega_0^2}\frac{2\omega_0 g^2\gamma^2}{\hbar^2} \\ &\times \sum_{ij} |P_{ij}|^2 \frac{N_j - N_i}{\omega - \omega_{ij}}\Bigg] \end{aligned} \tag{15}$$

with the change $\omega \longrightarrow \omega + i0$ used to preserve the causality principle. This expression is substituted into (3), which is then integrated over the frequency according to (13). In view of (15), as expected, $G_r(\omega)$ and $G_a(\omega) = G_r^*(\omega)$ are represented by a unified analytical function of complex argument ω with poles on the real axis. Therefore, the integration of the difference of functions in (3) can be replaced by integration along a contour around the real axis with all the poles of $1/(1 - \exp(-\hbar\omega/T))$ lying outside. Then

$$\langle (\hat{q})^2\rangle_\omega = -\hbar\sum_{\text{res}} \frac{1}{1 - e^{-\frac{\hbar\omega}{T}}} G(\omega),$$

where the sum is taken over all the residues inside the contour. For simplicity, we consider the two-level approximation with indices 1 and 2 denoting the ground and excited states of the medium. If $T \gg \hbar\omega_{21}$, we find that

$$\langle(\hat{q})^2\rangle = CT\left(1 + \frac{g^2 C}{T}|P_{21}|^2 N\right), \quad (16)$$

where N is the sum of the occupation numbers of both states. Importantly, this formula is independent of ω_{21}. In a different manner, it was derived in [12]. Since $|P_{ij}|^2 \sim \hbar$, which can be verified for the quantum oscillator model assuming that $\hat{P} = -i\hbar\partial/\partial x$, we conclude that formula (16) is a classical physics result plus a quantum addition that is linear in $\hbar$. Formula (16) shows that the quantum addition is completely determined by expression (15) with poles on the real line. Therefore, no relaxation constants take part in the formation of (16). It follows that the active resistance of the circuit and the imaginary part of the permittivity do not pertain to the formation of quantum corrections. This argument is sufficient to assert the incorrectness of the quantum Nyquist formula, according to which $\langle(\check{q})^2\rangle$ depends on R, while the series expansion of $\langle(\hat{q})^2\rangle - CT$ in powers of the Planck constant begins with the term $\propto\hbar^2$. According to the classical Nyquist formula, $\langle(\check{q})^2\rangle$ is independent of R. In the same fashion, we can prove the incorrectness of other formulas related conceptually to the quantum Nyquist formula [9, 11]. Note incidentally that no argument based on perturbation theory [15] can justify the quantum Nyquist formula, at least because, in this approximation, the wave function of the system does not decay with time and no relaxation constants appear in the argument.

A further conclusion can be drawn. Specifically, substituting (13) for (15) in FDT, we obtain

$$\langle(\hat{q})^2\rangle = i\hbar\int_{-\infty}^{\infty}\frac{1}{1-e^{-\frac{\hbar\omega}{T}}} \times\left[\frac{1/L}{\omega^2-\omega_0^2-\frac{2\omega_0}{\hbar}\pi_r(\omega)} + \text{c.c.}\right]\frac{d\omega}{2\pi}. \quad (17)$$

Note that, in contrast to (15), formula (13) cannot be viewed as exact since it was derived by splitting the correlation functions in (8). Moreover, in the two-level approximation, integral (17) can be explicitly evaluated since its integrand is an algebraic function. This integral is again determined by the sum of the residues inside the above contour. However, when $\omega_{21} \ll \omega_0$, the integrand has two new imaginary poles, which are a qualitative (and unfavorable) difference of function (13) from (15). Then

$$\langle(\hat{q})^2\rangle = \frac{\hbar}{L}\sum_{\text{res}}\frac{1}{1-e^{-\frac{\hbar\omega}{T}}}\frac{\omega^2-\omega_{21}^2}{(\omega^2-\omega_{21}^2)(\omega^2-\omega_0^2)-\omega_{21}\delta},$$

$$\delta = \frac{4g^2\gamma^2\omega_0}{\hbar^2}|P_{21}|^2(N_1-N_2).$$

Performing further calculations and passing to the limit as $\omega_{21} \longrightarrow 0$, we infer from (17) that $\langle(\hat{q})^2\rangle = CT$, which is independent of $\hbar$. This result differs from the previously derived formula (16), which involves a quantum addition independent of ω_{21}. We assert that there is no correct transition between formulas (15) and (13) in quantum physics. In other words, the perturbation theory series cannot be effectively summed. It turns out that integration over the frequency has to be performed first followed by summation. This order of operations is directly dictated by the method for calculating $\langle(\hat{q})^2\rangle$ proposed in [8]. This circumstance will be manifested in any other technique, for example, in Green's temperature functions [10, 16].

Thus, in quantum physics, the FDT cannot be mathematically represented in the form of (17). This is additional evidence that indicates the incorrectness of not only the quantum Nyquist formula, which is reduced to (17), but also Rytov's fluctuation formula [9], which describes fluctuations of electromagnetic fields in absorbing media, and Lifshitz's theory [11] based on the latter formula. Moreover, the active resistance R and the permittivity with a finite imaginary component cannot be well defined in quantum theory, because, for this purpose, $G_r(\omega)$ and $G_a(\omega)$ must be represented in the form of (13). The same conclusions were drawn from a different point of view in [17], which was discussed in [12, 18].

ADDITIONAL REMARKS

It remains unclear what should be used instead of the quantum Nyquist formula. While correctly indicating that the quantum Nyquist formula is wrong, Klimontovich failed to answer this question. Now, given integral (14), we are interested in the form of the function $\langle\check{q}\check{q}\rangle_\omega$ or, equivalently, the function $\langle\check{q}(t)\check{q}(t')\rangle$. In this case, it is more convenient to use the Heisenberg representation. The averages of operators are invariant under the choice of a representation. At first glance, this problem seems easy to solve. It suffices to derive a differential equation for $\langle \check{q}(t)\check{q}(t') \rangle$ and solve it with the now known initial condition. System (7) yields

$$\frac{d^2\langle \check{q}(t)\check{q}(t')\rangle}{dt^2} = -\omega^2\langle \check{q}(t)\check{q}(t')\rangle + \frac{2g\omega_0\gamma^2}{\hbar}\sum_{ij} P_{ij}\langle \check{\beta}_i^+(t)\check{\beta}_j(t)\check{q}(t')\rangle,$$

$$i\hbar\frac{d\langle \check{\beta}_i^+(t)\check{\beta}_j(t)\check{q}(t')\rangle}{dt} = -\hbar\omega_{ij}\langle \check{\beta}_i^+(t)\check{\beta}_j(t)\check{q}(t')\rangle + gP_{ij}^*(N_j - N_i)\langle \check{q}(t)\check{q}(t')\rangle.$$

This system of equations arises on splitting the correlation function:

$$\langle \check{q}(t)\check{\beta}_{j'}^+(t)\check{\beta}_j(t)\check{q}(t')\rangle = \delta_{jj'}N_j\langle \check{q}(t)\check{q}(t')\rangle.$$

The solution to the system is sought for $t > t'$ and $t < t'$. A second-order equation requires two initial conditions. In fact, since there is a system of equations, in addition to $\langle \check{q}(t)\check{q}(t) \rangle$ and $\left\langle \frac{d\check{q}(t)}{dt}\check{q}(t)\right\rangle$, we have to know $\langle \check{\beta}_j^+(t)\check{\beta}_j(t)\check{q}(t) \rangle$. The last two expressions can be calculated, for example, by the method of Γ operators [8]. Their particular form is not important for our purpose. As a result, for $t > t'$, we have

$$\langle \check{q}(t)\check{q}(t')\rangle = \int_{b-i\infty}^{b+i\infty} e^{s(t-t')}\frac{\left\langle \frac{d\check{q}(t)}{dt}\check{q}(t)\right\rangle + s\langle \check{q}(t)\check{q}(t)\rangle + 2ig\omega_0\gamma\sum_{ij}|P_{ij}|^2\frac{\langle \check{\beta}_i^+(t)\check{\beta}_j(t)\check{q}(t)\rangle}{i\hbar s + \hbar\omega_{ij}}}{s^2 + \omega_0^2 - \frac{2\omega_0}{\hbar}\pi_r(is)}\frac{ds}{2\pi i}.$$

As before, this formula encounters a difficulty associated with the $\pi_r(is)$ contained in the denominator. To overcome it, we apply a semiphenomenological argument and, according to (12), replace $\pi_r(is)$ with an experimentally determined resistance R. According to the derivation, R should be regarded as a small quantity. In this approximation, the first and third terms are dropped from the numerator. Then

$$\langle \check{q}(t)\check{q}(t')\rangle = L\langle \check{q}(t)\check{q}(t)\rangle\int_{-\infty}^{\infty} e^{-i\omega(t-t')}\left(\frac{1}{z} + \frac{1}{z^*}\right)\frac{d\omega}{2\pi} = \int_{-\infty}^{\infty} e^{-i\omega(t-t')}\langle \hat{q}\hat{q}\rangle_\omega\frac{d\omega}{2\pi}. \quad (18)$$

After integration over the frequency, this semiphenomenological formula gives the correct value of $\langle \check{q}(t)\check{q}(t) \rangle$ and produces a dependence of $\langle \check{q}(t)\check{q}(t') \rangle$ on $|t - t'|$ that coincides with experiments. If the fluctuating emf in the circuit is defined by (5), it is a nonlinear function of the parameters of the electric circuit LC of the external system (via the product $R|P_{ij}|^2 \sim \hbar$ contained in $R\langle \check{q}(t)\check{q}(t) \rangle$) and loses the additivity property. The additivity of the fluctuating emf was used in [6] in the phenomenological "proofs" of the quantum Nyquist formula, which thus prove to be invalid.

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