Quantum Nyquist formula and the applicability ranges of the Callen-Welton formula

V. L. Ginzburg and L. P. Pitaevskiĭ

P. N. Lebedev Physics Institute, Academy of Sciences of the USSR; S. I. Vavilov Institute of Physics Problems, Academy of Sciences of the USSR

We discuss Yu. L. Klimontovich's objections to the generally accepted derivations of the fluctuation-dissipation theorem and his proposed additional restrictions on the applicability of this theorem. We demonstrate that Yu. L. Klimontovich's arguments contradict the basic principles of statistical physics and hence cannot be correct.

1. Let us recall the problem at hand.

In an electrical circuit described by the equations

$$L\frac{dI}{dt} + RI + \frac{q}{C} = \mathscr{E}, \qquad \frac{dq}{dt} = I, \tag{1}$$

a fluctuating e.m.f. $\mathscr{E}$ induces currents I, with

$$\mathscr{E}_\omega = Z(\omega) I_\omega, \quad Z(\omega) = R - i\left(\omega L - \frac{1}{\omega C}\right);$$

and L, C, and R are taken to be constants in the above equation and hereafter. In thermal equilibrium at temperature T, the spectral e.m.f. density is determined by the expression

$$(\mathscr{E}^2)_\omega = Rf(\omega, T) = 2R\left[\frac{\hbar\omega}{2} + \frac{\hbar\omega}{\exp(\hbar\omega/kT) - 1}\right]$$

$$= R\hbar\omega \operatorname{cth}\frac{\hbar\omega}{2kT}, \tag{2}$$

and consequently

$$(I^2)_\omega = \frac{Rf(\omega, T)}{|Z(\omega)|^2}, \quad \langle I^2\rangle = \int_{-\infty}^{+\infty} \frac{Rf(\omega, T)}{|Z(\omega)|^2}\frac{d\omega}{2\pi}. \tag{3}$$

The notation here corresponds to that of Yu. L. Klimontovich,[1] except that he usually replaces $f(\omega, T)$ by $2kT_\omega$ (in Ref. 2, $k = 1$; in Ref. 3, the coefficient $1/2\pi$ is omitted in integrals (3) and hence appears in formulae analogous to (2)).

In the classical limit, when $\hbar\omega \ll kT$, formula (2) takes the form

$$(\mathscr{E}^2)_\omega = 2RkT \tag{4}$$

and is called the Nyquist formula (or the classical Nyquist formula); whereas (2) is known as the quantum generalization of the Nyquist formula or the quantum Nyquist formula.

2. In a circuit described by (1) the classical Nyquist formula is undoubtedly valid (see Ref. 4 for more details). As for the quantum Nyquist formula (2), obtained by Nyquist already in 1928 (albeit without the $\hbar\omega/2$ term),[5] Yu. L. Klimontovich argues that it is incorrect and should be replaced by the following:

$$(\mathscr{E}^2)_\omega = R\hbar\omega_0 \operatorname{cth}\frac{\hbar\omega_0}{2kT}, \quad \omega_0 = (LC)^{-1/2}. \tag{5}$$

In the classical limit (more precisely when $\hbar\omega_0 \ll kT$) Klimontovich's formula obviously reduced to the Nyquist formula (4). But in the quantum regime the difference between formula (5) and the quantum Nyquist formula (2) can be arbitrarily large. Indeed, expression (5) does not depend on

the varying frequency ω, whereas in the $\hbar\omega \gg kT$ regime expression (2) falls off exponentially as the frequency ω increases.[*] Obviously, reaching the quantum regime requires lowering the temperature T and (or) going to higher frequencies ω. We believe that the quantum regime is quite achievable even under conditions when the quasistationary equation (1) is valid. In fact, however, no experimental data are available to test the validity of formula (2). Hence the question of whether this formula is valid or not cannot yet be considered irrelevant.

Let us note at the outset that we believe the quantum Nyquist formula (2) to be absolutely correct, certainly as long as the assumptions leading to it hold true—above all, the microscopic (phenomenological) equation (1) must describe the circuit in question (see also Refs. 2–6).

Formula (2) may be derived by three different methods: the first may be termed "thermodynamical",[3,5,6] the second employs the fluctuation-dissipation theorem and, specifically, the Callen-Welton formula[7] (see also Refs. 3, 4, 6, and 8); finally, the third method is based on microscopic arguments and sheds light on the physical nature of the problem. Yu. L. Klimontovich criticizes the above methods,[1] and specifically the first and the second. We shall also consider these two methods (we omit the microscopic analysis, covered in V. I. Tatarskiĭ's paper[4]). It is appropriate to note that Yu. L. Klimontovich's argument goes far beyond the particular problem of the quantum Nyquist formula. Indeed, it is claimed in Ref. 1 that in the quantum regime the Callen-Welton formula is only valid under very strong restrictions—equivalent, roughly speaking, to weak dissipation. At the same time, it is usually held that the Callen-Welton formula is valid in the presence of strong dissipation as well, and particularly at any value of resistance R in a circuit described by (1). It is specifically because of this that the Callen-Welton formula leads to the quantum Nyquist formula (2).[2–4,6] Consequently, Yu. L. Klimontovich's assertion, if correct, would significantly alter statistical physics, in particular severely restricting the applicability of the Callen-Welton formula. Accordingly, the editorial board of *Uspekhi Fizicheskikh Nauk* deemed it advisable to publish Yu. L. Klimontovich's paper[1] in conjunction with our paper, in which we conclude not only that the quantum Nyquist formula (2) is valid, but that so is the usual interpretation of the more general and important Callen-Welton formula.

3. Let us turn to the "thermodynamic" derivation of the quantum Nyquist formula (2). The word "thermodynamic" is in quotation marks because the derivation is only partly

thermodynamic. More precisely, thermodynamic equilibrium assures that for every circuit described by (1) the following expression holds

$$(\mathscr{E}^2)_\omega = Rf\,(\omega,\ T),\qquad(6)$$

where $f(\omega,T)$ is some universal function of ω and T, i.e. a function independent of the parameters L, C, and R. In order to derive (6), Refs. 3, 6, and 9 consider two open-ended circuit "branches" 1 and 2 with impedances Z_1 and Z_2 and resistances $R_1 = \mathrm{Re}\{Z_1\}$ and $R_2 = \mathrm{Re}\{Z_2\}$. Connecting the two branches in series produces a single closed circuit with parameters $Z = Z_1 + Z_2$ and $R = R_1 + R_2$. In thermodynamic equilibrium fluctuating e.m.f. $\mathscr{E}_1$ and $\mathscr{E}_2$ occurring in branches 1 and 2, lead to liberation of heat with spectral power

$$P = R\,(I^2)_\omega = R\,\frac{(\mathscr{E}^2)_\omega}{|\,Z(\omega)\,|^2} = P_1 + P_2 + P_{12} + P_{21},$$

where

$$P_{12} = \frac{R_2(\mathscr{E}_1^2)_\omega}{|\,Z(\omega)\,|^2},\qquad P_{21} = \frac{R_1(\mathscr{E}_2^2)_\omega}{|\,Z(\omega)\,|^2}$$

are heats liberated respectively in branch 2 due to e.m.f. fluctuations $\mathscr{E}_1$ (in branch 1) and in branch 1 due to e.m.f. fluctuations $\mathscr{E}_2$. In thermal equilibrium $P_{12} = P_{21}$ and hence

$$\frac{(\mathscr{E}_1^2)_\omega}{R_1} = \frac{(\mathscr{E}_2^2)_\omega}{R_2}.\qquad(7)$$

This result is obtained more rigorously in Ref. 9 and is cited without opposition in Ref. 1 (see formula (2.3)). Since the branch parameters are arbitrary, i.e., (7) is true for any parameters of branches 1 and 2 and cannot depend on these parameters. Consequently, in equilibrium any circuit described by (1) exhibits $(\mathscr{E}^2)_\omega/R = f(\omega,T)$, where $f(\omega,T)$ is a universal function possibly dependent on ω and T. Expression (6) is thus derived.

The average electric energy in the circuit is

$$\bar U = \frac{\overline{q^2}}{2C} = \frac{1}{2C}\int_{-\infty}^{+\infty}\frac{(J^2)_\omega}{\omega^2}\frac{d\omega}{2\pi} = \frac{1}{C}\int_0^\infty\frac{(\mathscr{E}^2)_\omega\,d\omega/2\pi}{\omega^2\,|\,Z(\omega)\,|^2}$$

$$= \int_0^\infty\frac{GRf\,(\omega,\ T)\,d\omega/2\pi}{R^2C^2\omega^2 + (LC\omega^2 - 1)^2},\qquad(8)$$

where expression (6) is employed in an obvious fashion; analogously, we may proceed from the expression for the average magnetic energy $\bar K = L\overline{I^2}/2$ to reach the same conclusion.

Since the function $f(\omega,T)$ is universal, it may be determined by considering any circuit. It is most convenient to treat a weakly damped circuit, where $R/L \ll (LC)^{-1/2} = \omega_0$. As a result, the function $f(\omega_0,T)$ may be taken outside the integral in (8), and the integral then reduces to 1/4 (see Refs. 3 and 6), whence $\bar U = f(\omega_0,T)/4$. On the other hand, we know, that in an arbitrarily weakly damped circuit (oscillator) with intrinsic frequency ω the average values

$$\bar U = \bar K = \frac{\hbar\omega}{4}\coth\frac{\hbar\omega}{2kT},\qquad(8')$$

where we drop the subscript zero in ω_0 since the intrinsic frequency is arbitrary. Consequently, $f(\omega,T) = \hbar\omega\coth(\hbar\omega/2kT)$ and we obtain the quantum Nyquist formula. Evidently, the second part of the derivation—where

expression (8') is employed—is not thermodynamic but rather uses quantum statistics.

Yu. L. Klimontovich's arguments against the above conclusion reduce to the following (see Ref. 1, paragraph 2): the function $f(\omega_0,T) = \hbar\omega_0\coth(\hbar\omega_0/2kT)$ "also satisfies the equality" (7), "since the frequency ω_0 corresponds to the entire circuit with total impendance $Z(\omega)$". However, we see no grounds for such a conclusion, since precisely from (7) it follows that the function $f(\omega,T)$ is independent of all circuit parameters, including the intrinsic frequency ω_0 of a two-branch circuit (here we speak of an intrinsic frequency given $R_1 = R_2 = 0$). Allowing the quantities $(\mathscr{E}_{1,2}^2)_\omega$ to depend on the frequency ω_0 is also completely unacceptable on physical grounds. Indeed, how can the electrical noise of resistances R_1 and R_2 of branches 1 and 2 depend on the intrinsic frequency ω_0 of the entire circuit, which is determined by the self-inductances and capacitances of both branches? By the way, let us note that the branch impendances Z_1 and Z_2 for given R_1 and R_2 do not uniquely determine the self-inductances and capacitances $L_{1,2}$ and $C_{1,2}$ (see, for instance, Ref. 3, Ch. 13). Furthermore, in the $\hbar\omega \gg kT$ regime, how can the noise fail to decrease as the frequency ω increases in view of (5)?[*] Finally, let us note that the cited derivation of the universality of $f(\omega,T)$ is quite analogous to the derivation of Kirchhoff's law stating that in thermal equilibrium the relation between the emissivity of a body and its absorptivity is universal (see Ref. 8, §63, and Refs. 9 and 10). We do not know whether the corresponding derivation of Kirchhoff's law was challenged in the 19th century, but no such objections appear in contemporary literature and Kirchhoff's law itself is certainly valid. We believe that the same can be said about expression (6) with its universal function $f(\omega,T)$.

In all, despite our sincere efforts, we have discovered no "hidden reefs" to "sink" the "thermodynamic" derivation of the quantum Nyquist formula (2). This derivation is fully described above, and the reader himself may judge its persuasiveness. It remains to be said that the validity of the "thermodynamic" derivation is further supported by the fact that the same result (i.e., the quantum Nyquist formula (2)) is obtained by the other two previously mentioned methods. Consequently all these methods are mutually consistent and reinforce each other. In particular, as was noted in Ref. 3, to a certain extend the "thermodynamical" derivation may be viewed as a proof of the Callen-Welton formula, including the case of strong dissipation, of course. The Callen-Welton formula is so important, however, that its derivation and applicability warrant a separate discussion.

4. Let us consider a certain physical quantity x that characterizes some body (system), with its quantum-mechanical average value x being zero in the absence of an external perturbing interaction. If an interaction described by a perturbing force f is turned on, then $\bar x_\omega = \alpha(\omega)f$, where we use the Fourier components of $\bar x$ and f and $\alpha(\omega) = \alpha'(\omega) + i\alpha''(\omega)$ is some generalized susceptibility (see Ref. 8, 123 for more detail). In thermodynamic equilibrium at a temperature T the fluctuations of quantity x are due to the imaginary part α'' of susceptibility α—this is the fluctuation-dissipation theorem or the Callen-Welton formula:

$$(x^2)_\omega = \hbar\alpha''(\omega)\coth\frac{\hbar\omega}{2kT} = 2\hbar\alpha''\left[\frac{1}{2} + \frac{1}{\exp(\hbar\omega/kT) - 1}\right].\quad(9)$$

A derivation of this relation is presented in Ref. 8, § 124, among others. Taking an electrical circuit as an example, we choose the current I to represent the quantity x, with $I_\omega = \mathscr{E}_\omega / Z(\omega) = i\omega f_\omega / Z(\omega)$ where $Z(\omega)$ is the aforesaid impedance of the circuit. Evidently in this case the generalized susceptibility $\alpha(\omega) = i\omega/Z(\omega)$, and $\alpha'' = \mathrm{Im}\{\alpha\} = \omega R/|Z|^2$, $R = \mathrm{Re}\{Z\}$. Hence from the Callen-Welton formula (9) we immediately obtain the quantum Nyquist formula (2) (see Ref. 2, § 78 for more detail).

Yu. L. Klimontovich proceeds from the correct expressions (4.1)–(4.3)[1] to write down the Callen-Welton formula (2.6) which differs from (9) only in his choice of a tensor α_{ij} for the scalar α ((2.6) reduces to (9) for the isotropic case, when $\alpha_{ij} = \alpha\delta_{ij}$). However, he considers the formulae (4.1)–(4.3) to be approximations corresponding to the "condition of an infinitely narrow resonance for every n-m transition", whereas in fact we are dealing with fundamental principles of quantum statistical physics, rather than some "condition".

Indeed, in quantum statistical physics we consider systems described by Hermitian Hamiltonian operators confined to an arbitrarily large but finite volume. According to well-known theorems, the energy eigenfunctions of such systems are real and form a discrete spectrum. It is precisely these energy levels E_n that determine the transition frequencies $\omega_{nm} = (E_n - E_m)/\hbar$. If such transition frequencies are taken to be "resonances", then these "resonances" are by definition "infinitely narrow". In any case, the introduction of the term "resonance" in this context is misleading. The energy levels of a macroscopic body as a whole (and we are discussing precisely such levels) are spaced extremely close together, so that no real experiment can uncover the resonant properties of these transitions (unless some additional selection rules separate certain groups of levels).

To be sure, the existence of definite (sharp) energy levels of zero width is used in many other derivations. The usual partition function that determines the thermodynamic quantities of a system,

$$Z = \sum_n e^{-E_n/T} \qquad (10)$$

also presupposes the existence of such levels and is employed in statistical physics without any stipulation of "infinitely narrow resonances".

5. The categorical character of the above statements may appear excessive. The notion of the "width of a level" and the "theory of spectral linewidth" are common usage. But the true nature of the "finite linewidth" should be properly understood. It is an approximate concept or, more precisely, it is a concept used to describe approximately the properties of a system with a continuous or quasicontinuous (read "very dense") spectrum in terms of a discrete spectrum, which is helpful for a certain class of appropriately formulated problems.

Consider a simple example: the excited state of some atom. Then, neglecting completely the interaction of the atom with a transverse electromagnetic field, we have a system of discrete levels of negative energy (as usual the energies of more and more highly excited states $E_n \to 0$). Consider one such state, say $E_1(0)$. It would contribute a term $\exp(-E_1^0/T)$ to the partition function (10), and a sharp resonance $\hbar\omega_{10} = E_1^{(0)} - E_0^{(0)}$ as the system is excited by

light from its ground state, and so forth. Now consider the possible radiation of light by the atom. This implies taking into account the interaction of the atom with a transverse electromagnetic field (the longitudinal field and, specifically, the Coulomb field of the nucleus have already been taken into account when solving for the energy levels of the atom treated as a "mechanical subsystem" that does not interact with a transverse field). But the energy levels of the "mechanical subsystem" (an particularly the level $E_1^{(0)}$ are no longer energy eigenvalues of the full system: atom + transverse electromagnetic field. The corresponding wavefunction $\Psi_1^{(0)}$ is also no longer an eigenfunction of the full system—this is the reason for light radiation, i.e., a transition to a different state. An analogous process occurs in nuclear decay and so forth. Since the initial state 1 (which has energy $E_1^{(0)}$ and wavefunction $\Psi_1^{(0)}$ if we neglect interaction with a transverse field) is quasistationary, it may to some extent be characterized by a complex energy $E_1 = E_1^{(0)} - i\hbar\gamma/2$ and wavefunction

$$\Psi_1 \sim e^{-iE_1 t/\hbar} = e^{-\gamma t/2} e^{-iE_1^{(0)} t/\hbar}. \qquad (11)$$

The substitution $E_1^{(0)} \to E_1$ may be employed in expressions for the dielectric permittivity of the system, in the spectral linewidth theory, and so forth. In addition, if $\gamma \ll E_1^{(0)}$, the γ-functions that occur in certain expressions are replaced by Lorentzians:

$$\delta(\omega - \omega_{01}) \to \frac{\gamma}{2\pi} \frac{1}{(\omega - \omega_{01})^2 + (\gamma^2/4)}. \qquad (12)$$

In quantum statistics the derivation of the fluctuation-dissipation theorem considers a full (closed) system, confined to an arbitrarily large but finite volume (taking into account the transverse electromagnetic field is equivalent to placing the system inside a large "resonator" with ideally reflecting walls). In these conditions the energy levels of the system E_n are discrete, albeit very densely spaced—the larger the resonator volume, the closer together are the levels. The energy interval of the order of the level width γ of individual subsystems of the total system usually accomodates an enormous number of discrete levels E_n. Each of them makes a δ-function contribution to $\alpha''(\omega)$, it is just these levels that contribute to the partition function (10) and appear on the left in Eqs. (4.1) and (4.2) used to prove the Callen-Welton formula.

The inconsistency of Yu. L. Klimontovich's argument is most apparent in the example of an oscillatory circuit. Certainly the resonance in an oscillatory circuit with a finite resistance has a finite width. But this does not imply that a microscopic examination of the circuit would reveal no definite energy levels, that the partition function (10) is incorrect for it and that the circuit is thereby exempt from the second law of thermodynamics. And certainly it would be inconsistent to claim that the notion of discrete energy levels applies to an oscillatory circuit in all cases except the derivation of the Callen-Welton formula. Meanwhile Yu. L. Klimontovich apparently believes that if a system does not exhibit a well-defined resonance, no connection whatever between fluctuations and susceptibility can be established for it.

Although not immediately related to this discussion, it should be stressed that knowing the "width" of a level γ does

not imply knowing the exact energy levels E_n. In general, calculating the quantity γ is insufficient for the calculation of corrections to the partition function due to interaction of atoms with a transverse field.

6. Furthermore, let us note that the modification of the Nyquist formula suggested by Yu. L. Klimontovich directly contradicts black-body radiation laws. In fact, these laws together with the aforementioned Kirchhoff's law lead to a completely unambiguous derivation of formulae for the correlation functions of random electromagnetic field sources, which are equivalent to the Callen-Welton formula.[11] Any modification of these formulae implies failure of the black-body radiation laws. As for the assertion that the usual theory leads to Plank's formula only in the case of weak damping, it is based on a misunderstanding one needs only to carry out accurately the calculations cited in Ref. 11).

Transformations of the type (4.3) occur very frequently in modern statistical physics. For instance, they are necessary to establish the analytic properties of Green's functions (see, for example, Ref. 2, Ch. 4). If we accept Yu. L. Klimontovich's argument, all these properties which form the basis for employing quantum field theory techniques in statistical physics would prove incorrect—the entire edifice of modern statistical physics would crumble. We shall produce only a single example. The transformation (4.3) is used to determine the properties of the dynamical form factor $\sigma(\omega,q)$ which describes neutron scattering in a liquid. It is precisely this transformation that leads to the relation

$$\sigma\,(-\omega,\ q)\,=\,e^{-\hbar\omega/kT}\,\sigma\,(\omega,\ q)$$

(see Ref. 2, formula (86.14)). But this relation is a direct consequence of the principle of detailed balance, the validity of which is hardly in doubt.

7. In sum, the Callen-Welton formula is an exact relation of statistical physics. On the other hand, the correlation functions and generalized susceptibilities that enter into the formula can in most cases be calculated only approximately. Thus it may turn out that their approximate nature leads to only approximate agreement with the Callen-Welton formula (see also Ref. 4). The magnitude of the deviation from these relations can serve as a measure of the applicability of the approximations. We believe that this is the proper framework for discussing the problem in terms of kinetic equations, as is done in Yu. L. Klimontovich's paper. As Yu. L.

Klimontovich himself justly observes, kinetic equations are only approximate, and hence the results obtained from kinetic equations may deviate from exact relations, which, of course, does not cast doubt on the relations themselves.

In his paper[1] Yu. L. Klimontovich addresses, in addition to the quantum Nyquist formula and the Callen-Welton formula, a number of more or less related questions. We hope the above discussion demonstrates that the criticism of the quantum Nyquist formula and the Callen-Welton formula presented in Ref. 1 in unfounded. It is then unnecessary to address the other questions discussed by Yu. L. Klimontovich.

In conclusion we would like to thank Yu. S. Barash and V. I. Tatarskiĭ for their perusal of this paper and their comments on it.

Authors' note: In our paper, "Quantum Nyquist formula and the applicability ranges of the Callen-Welton formula (comments on Yu. L. Klimontovich's paper)" (published in Uspekhi, February 1987, Vol. 30, No. 2) in passages [marked by asterisks] on page 168 and on page 169, we, of course, mean the frequency dependence only of those parts of Eqs. (2) and (5) that depend on temperature.

[11]All formulae with double numeration (i.e., (4.1)) are from Ref. 1.

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