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The status of the quantum dissipation–fluctuation relation and the Langevin equation

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Abstract

I examine the arguments which have been given for quantum fluctuation–dissipation theorems. I distinguish between a weak form of the theorem, which is true under rather general conditions, and a strong form which requires a Langevin equation for its statement. I argue that the latter has not been reliably derived in general.

1. Introduction

A quantum generalization of the Nyquist dissipation–fluctuation relation was discussed by a number of authors many years ago. I shall refer explicitly to the papers of Callen and Welton [1] and of Senitzky [2], and to the books by Landau and Lifschitz [3], Feynman and Hibbs [4], Gardiner and Zoller [5], Kogan [6], Balescu [7] and Kreutzer [8]. I will distinguish between the weaker version (not including a Langevin equation) of the relation first discussed by Callen and Welton and the stronger version first formulated by Senitzky, and examine the range of validity in each case. The latter author seeks to establish a quantum Langevin equation containing a dissipation term and a noise term, connected by the fluctuation–dissipation relation. The text books [3, 6–8] follow [1]. The monograph [5] includes a version of [2]. I also briefly review the formalism of [4].

Another approach, which should contain much of the same information, is based on the master equation for the density operator (see [5]). I discuss this approach in section 4.

A *simple quantum system* is envisaged in interaction with a *bath* (the 'loss mechanism') which has many degrees of freedom, closely spaced energy levels and is initially in thermal equilibrium at temperature T. The bath dissipates energy from the simple system and at the same time feeds noise into it. The generalized Nyquist relation connects the noise with the dissipation.

There is a special case in which all the equations of motion for the bath degrees of freedom are linear (that is, the loss mechanism consists of oscillators which are linearly coupled to the simple system). In this case, the theorem is certainly well understood [5]. This special case covers many important applications, such as when the bath consists of photons or phonons

(if the interaction with the system is limited to emission and absorption). But a bath consisting of fermionic or spin degrees of freedom would not fall within the special case.

The epithet 'quantum' implies that terms of order $\hbar$ are retained in the expectation value of two noise operators. For consistency, this implies that the noise term is indeed a non-commuting operator. Since the Langevin equation gives the behaviour of the simple system in terms of the noise, the simple system must also be quantum. It has been stressed in [10] that the expectation values of the noise operators in their two different orderings have different physical interpretations; so it is impossible to ignore the fact that they do not commute.

The quantum Langevin equation has been quoted in connection with experiments [11, 12] (see also [6, 13]) in which a Josephson junction is shunted by a resistor. The Josephson phase difference δ is modelled as the simple system, and the resistor is modelled as the bath. The resistor R tends to dissipate the Josephson junction voltage $U = \frac{\hbar}{2e}\dot{\delta}$ because of its conductance $1/R$. The noise current which couples to U must be bilinear in the electron creation and annihilation operators. Therefore the equations of motion for these electron operators are not linear in the complete set of degrees of freedom (U together with the electron operators); and so the use of the Langevin equation is questionable.

2. The method of Callen and Weston

In this section I review a weak form of the fluctuation–dissipation theorem, which is proved (originally in [1]) under rather general conditions, provided only that departures from equilibrium are small.

The complete system has quantum variables q_i, p_i with $i = 1, \ldots, N$ with N large. If it is driven by an external classical driving force $F(t)$, the Hamiltonian is

$$H(q_i, p_i) - F(t)Q(q_i, p_i), \tag{1}$$

where Q is some particular (real) combination of the dynamical variables. (In one example, F is an applied voltage and $\dot{Q}$ the resulting current.) The whole system is, in the absence of $F(t)$, in thermal equilibrium at temperature T. The eigenvalues of H are E_n, and are assumed to be closely spaced (so sums over n can be approximated by integrals). Thermal expectation values are given by the distribution function

$$\rho(H) = \frac{\exp(-H/kT)}{\operatorname{tr}\exp(-H/kT)}. \tag{2}$$

Following Landau and Lifshitz [3], we expect, provided that F is small enough, a linear response of the form

$$\langle \dot{Q}_F(t)\rangle \equiv \operatorname{tr}(\rho \dot{Q}_F) = \int_0^\infty \mathrm{d}t' \chi(t - t')F(t') \tag{3}$$

(the suffix F on Q_F indicates that this is the response to the external force F; I shall use Q with no suffix to denote a fluctuation in the absence of F). Equation (3) defines a 'linear response function' or 'generalized susceptibility' χ (the inverse of the impedance). Note that it is the expectation value of Q_F which appears in (3), so the whole equation refers to classical quantities.

For the case where

$$F(t) = \operatorname{Re}[F_0 \exp(\mathrm{i}\omega t)], \tag{4}$$

we have (in terms of complex Fourier transformed functions, denoted by $\tilde{}$)

$$\mathrm{i}\omega\langle \tilde{Q}_F(\omega)\rangle = \tilde{\chi}(\omega)F_0, \tag{5}$$

where

$$\tilde{\chi}(-\omega) = -\tilde{\chi}^*(\omega). \tag{6}$$

The power provided by F and dissipated into the system is

$$W = \langle \partial H/\partial t \rangle = -\langle Q_F \rangle \dot{F}(t) \tag{7}$$

and its mean value (over time) is

$$\overline{W} = \tfrac{1}{2}\,\mathrm{Re}\{\tilde{\chi}(\omega)\}|F_0|^2. \tag{8}$$

But we can also calculate $\overline{W}$ by applying lowest order perturbation theory to the perturbing Hamiltonian $-QF$. The result can be expressed in terms of the expectation value

$$S(\omega, T) \equiv \frac{1}{2\pi}\int \mathrm{d}t\, \exp(-\mathrm{i}\omega t)\, \mathrm{tr}\{\rho Q(0) Q(t)\}. \tag{9}$$

Comparison of this result with (8) (as shown in [1] or [3]), yields the theorem

$$S(\omega, T) = \frac{2}{\pi}\left[\frac{\hbar\omega}{\exp(\hbar\omega/kT) - 1}\right] \mathrm{Im}\{\tilde{\chi}(\omega)\}. \tag{10}$$

If we choose instead in (9) the symmetrized product of operators, we get

$$S_{\mathrm{sym}} \equiv \frac{1}{2}[S(\omega, T) + S(-\omega, T)] = \frac{1}{\pi} N(\omega, T)\ \mathrm{Re}\{\tilde{\chi}(\omega)\}, \tag{11}$$

where

$$N(\omega) = \hbar\omega\left[\frac{1}{\exp(\hbar\omega/kT) - 1} + \frac{1}{2}\right] \tag{12}$$

is the Bose distribution function.

I call (10) or (11) the weak fluctuation–dissipation theorem. It is very general and simple, but it has the a limitation, which I shall now explain. If Q were a classical quantity, one could have, more generally than (3),

$$\dot{Q}_F = \int_0^\infty \mathrm{d}t'\, \chi(t - t') F(t'). \tag{13}$$

Then it would be natural to define a fluctuation f in the force related to the fluctuation Q by

$$\dot{Q}(t) = \int_0^\infty \mathrm{d}t'\, \chi(t - t') f(t'). \tag{14}$$

It is then possible to deduce from (10) and (14) a formula for

$$S_f \equiv \frac{1}{2\pi}\int \mathrm{d}t\, \exp(-\mathrm{i}\omega t)\, \mathrm{tr}\{f(0) f(t)\}. \tag{15}$$

But in the quantum case, using only (3), one cannot take these steps, and so cannot go beyond the fluctuation–dissipation relation (10).

Some authors (for example Callen and Welton [1], Landau and Lifshitz [3] and Kogan [6]) tacitly assume (14) even in the quantum case. Landau and Lifshitz write 'It is convenient to write the formula (14) *as if* Q were a classical quantity' (my italics). These authors also call f a 'fictitious random force'. But, in my opinion, f is not fictitious; it is a real dynamical force exerted on the degree of freedom Q by the other degrees of freedom in q_i, p_i. In order to exhibit this, and to justify (14) in the quantum case (if that is possible), one needs a Langevin equation, and this is the subject of the next section.

3. Senitzky's derivation of a Langevin equation

In this method, one degree of freedom Q, P is singled out, representing a *simple system* and this interacts weakly with a *bath* with degrees of freedom $q_i, p_i, i = 1, \ldots, N$. It would be possible for the q_i, p_i variables to be quantum while Q, P was a classical degree of freedom; but I am concerned with the situation in which Q, P are quantum as well. For quantum effects in the simple system to be important, it presumably must be microscopic (for instance a single atom), perhaps mesoscopic (like a very small Brownian particle) or perhaps the phase of a superconducting condensate [11, 12].

For simplicity the simple system is taken to be an oscillator, and the Hamiltonian is

$$H = \frac{1}{2m}P^2 + \frac{1}{2}m\Omega^2 Q^2 + H_{\mathrm{B}}(q_i, p_i) + H_{\mathrm{int}}(Q, P; q_i, p_i) - QF(t), \quad (16)$$

with the interaction

$$H_{\mathrm{int}} = -\alpha Q K(q_i, p_i). \quad (17)$$

Here F is a classical driving force, α is a small parameter and K is some function of the bath variables. The suffix B stands for 'bath'. The choice Q rather than P in (16) is somewhat arbitrary, but it is important that this term is linear in Q, P. Some parts of the argument would go through for a general potential $V(Q)$ instead of $m\Omega^2 Q^2/2$. The Hamiltonian H is positive provided that

$$2m\Omega^2 H_{\mathrm{B}} \geqslant \alpha^2 K^2.$$

Note that I have used the same notation as in section 2, but it refers to a slightly different physical model.

The Heisenberg picture is used. The equations of motion are

$$\dot{P} = -m\Omega^2 Q + \alpha K + F, \qquad \dot{Q} = \frac{1}{m}P. \quad (18)$$

The special case in which H_{B} is quadratic in its variables and K is linear (so that the whole assembly is made up of harmonic oscillators and all the equations of motion are linear) is simple and well-studied (see for instance [5]), and there is no doubt about the validity of the fluctuation–dissipation theorem. But it is not clear that this model covers all physical examples. The argument of [2], however, claims to be more general.

It might be argued (see for example [4]) that, close to equilibrium, we can expand potentials about their equilibrium values and a quadratic approximation for H is necessarily justified. But if K is itself a quadratic function, then this approximation would decouple the simple system from the bath altogether. For example, if any of the bath variables are fermionic, then K cannot be a linear function of them.

We define operators with a superfix (0) to satisfy the equations of motion when $\alpha = 0$, and to coincide with the true operators at some initial time t_0; so for example

$$\begin{aligned} &K^{(0)}(t) = K(t; \alpha = 0), \qquad K^{(0)}(t = t_0) = K(t = t_0). \\ &\dot{P}^{(0)} = -m\Omega^2 Q^{(0)}, \quad m\dot{Q}^{(0)} = P^{(0)}; \qquad P^{(0)}(t_0) = P(t_0), \\ &Q^{(0)}(t_0) = Q(t_0). \end{aligned} \quad (19)$$

By using the Heisenberg equations of motion, Senitzky (equation (16) of [2]) obtains

$$K(t) = K^{(0)}(t) - \frac{\alpha}{\hbar^2}\int_{t_0}^{t} \mathrm{d}t' \int_{t_0}^{t'} \mathrm{d}t'' \, U(t' - t)[K(t'), [K(t''), H_{\mathrm{B}}(t'')]Q(t'')]U(t - t'), \quad (20)$$

where

$$U(t'-t) = \exp\{-\mathrm{i}(t'-t)H^{(0)}/\hbar\}. \tag{21}$$

Neglecting terms of higher order in α, we replace K by $K^{(0)}$ and H_B by $H_B^{(0)}$ on the right-hand side of (20). We may also neglect the commutators of Q with $H_B^{(0)}$ and with $K^{(0)}$ since these are relatively $\mathrm{O}(\alpha)$. Using the time translation operator U (I differ from [2] slightly at this point), we finally get

$$K(t) \approx K^{(0)}(t) - \mathrm{i}\alpha \int_{t_0}^{t} \mathrm{d}t''\, C(t,t'')Q(t''), \tag{22}$$

where (with $\tau = t + t'' - t'$)

$$C(t,t'') \equiv \frac{1}{\hbar}\int_{t''}^{t} \mathrm{d}\tau\, [K^{(0)}(t), \dot{K}^{(0)}(\tau)] = -\frac{1}{\hbar}[K^0(t), K^0(t'')]. \tag{23}$$

Equation (22) may now be inserted into (18) to obtain the approximate linear equations for Q and P:

$$\dot{P}(t) = -m\Omega^2 Q(t) + f(t) + \alpha K^0(t) - \mathrm{i}\alpha^2 \int_{t_0}^{t} \mathrm{d}t''\, C(t,t'')Q(t''),$$

$$\dot{Q}(t) = \frac{1}{m}P(t). \tag{24}$$

Here the K^0 term may be interpreted as quantum noise, and the C term contains a dissipative part.

At this stage, C in (23) is a quantum operator not a c-number, and it is in general a function of the two variables t, t'' not just their difference. In the special case when H_B is quadratic and K is linear (the oscillator case), C is a c-number and is a function only of $t - t''$, and is independent of T. But the question is whether (24) can be simplified for a general H_B and K.

At this point, Senitzky [2] makes the approximation of replacing C by its expectation value:

$$C(t-t'') \approx \mathrm{tr}\{\rho C(t,t'')\} \equiv c(t-t'',T), \tag{25}$$

where now

$$\rho = \frac{\exp(-H_B^{(0)}/kT)}{\mathrm{tr}\exp(-H_B^{(0)}/kT)}. \tag{26}$$

Notice that this ρ is not quite the same as that defined in the previous section in (2).

In justification of this approximation, Senitzky [2] writes 'we ignore the quantum-mechanical properties of the loss-mechanism [that is, the bath] in terms of higher order than the second', and 'all our final results (but not necessarily the intermediate steps) will be expectation values with respect to the loss-mechanism; and since the term affected involves only second and higher order interactions, only the higher order quantum mechanical effects are neglected in the final result'. I have not understood the distinction between higher order effects (higher order in α) and higher order quantum mechanical effects. It seems that the terms neglected in the approximation (24) are not of higher order in α or in $\hbar$ than the terms retained.

If we make the approximation (25) and insert it into (24), we obtain an equation of Langevin type. If we choose $t_0 = -\infty$ and take Fourier transforms (denoted by $\tilde{Q}$ etc), we obtain

$$[m(\Omega^2 - \omega^2) + G(\omega,T)]\tilde{Q}(\omega) \equiv \mathrm{i}\omega Z(\omega,T)\tilde{Q}(\omega) = \alpha\tilde{K}(\omega) + \tilde{F}(\omega), \tag{27}$$

where

$$G(\omega, T) = \alpha^2 \int \mathrm{d}\omega' \, \frac{1}{\omega' - \omega - \mathrm{i}\epsilon} \tilde{c}(\omega', T), \tag{28}$$

where $\tilde{c}$ is the Fourier transform of c defined in (25). So, in this approximation, there does exist a c-number impedance Z and $\tilde{Z}$ is the inverse of the susceptibility $\tilde{\chi}$ defined in section 2 in equation (5). The real part of $\tilde{Z}$ is the resistance giving the dissipation. But, without the approximation (25), the C term in the equation of motion is a quantum operator.

The term $\alpha\tilde{K}$ in (27) is interpreted as noise and plays the role of the force fluctuation f hypothesized at the end of section 2. The noise spectrum is (choosing the symmetrized product)

$$S^{(f)}_{\mathrm{sym}}(\omega, T) = \frac{\alpha^2}{4\pi} \int \mathrm{d}t \, \exp(-\mathrm{i}\omega t) \, \mathrm{tr}\{\rho(K(0)K(t) + K(t)K(0)\}, \tag{29}$$

where the superfix (f) denotes the noise in f as opposed to Q. Then the fluctuation–dissipation theorem (*if* the approximation (25) were valid) would be

$$S^{(f)}_{\mathrm{sym}}(\omega, T) = \frac{1}{\pi}[\mathrm{Re}\, Z(\omega, T)]N(T, \omega), \tag{30}$$

where N is the Bose function defined in (12). The theorem could alternatively be expressed in terms of the fluctuation Q produced by the noise K, by using

$$\mathrm{i}\omega Z(\omega)\tilde{Q} = \alpha\tilde{K}(\omega),$$

where Z is defined in (27).

4. The argument of Feynman and Hibbs

A fluctuation–dissipation theorem is derived in section 12.9 of [4] (see also [14]). The argument is very similar to that of Senitsky except that it uses Feynman's path integrals instead of Heisenberg equations of motion. It assumes that the Lagrangian is of second degree (so that the bath degrees of freedom can be explicitly integrated out). Feynman and Hibbs appear to argue that such a second degree Lagrangian is very general.

5. The master equation

A different approach to the same physical problem is via the master equation for the density operator ρ (see for example [5], chapter 5). For a critique of this method in the quantum case see [9].

Using now the interaction picture (instead of the Heisenberg picture), the density operator obeys the equation

$$\hbar\dot{\rho}(t) = -\mathrm{i}[H_{\mathrm{int}}(t), \rho(t)], \tag{31}$$

where H_{int} is defined in (17). Iterating this equation,

$$\dot{\rho}(t) = -\frac{\mathrm{i}}{\hbar}[H_{\mathrm{int}}(t), \rho(t_0)] - \frac{1}{\hbar^2}\int_{t_0}^{t} \mathrm{d}t' \, [H_{\mathrm{int}}(t), [H_{\mathrm{int}}(t'), \rho(t')]]. \tag{32}$$

We assume the initial condition that the density operator factorizes into a bath part and a system part

$$\rho(t_0) = \rho_{\mathrm{B}} \otimes \rho_{\mathrm{S}}. \tag{33}$$

We would normally choose ρ_{B} to be the Boltzmann distribution.

From (32) we can deduce equations for expectation values of operators. For example

$$\frac{\mathrm{d}}{\mathrm{d}t}\,\mathrm{tr}\{\rho(t)P(t)\} = -m\Omega^2\,\mathrm{tr}\{\rho(t)Q(t)\} + \alpha\,\mathrm{tr}\{\rho(t_0)K(T)\}\dot{P}(t) + \frac{\mathrm{i}\alpha^2}{\hbar}\int_{t_0}^{t}\mathrm{d}t'\,\mathrm{tr}\{\rho(t')[K(t),\,K(t')]Q(t')\}, \tag{34}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\,\mathrm{tr}\{\rho(t)Q(t)\} = \frac{1}{m}\,\mathrm{tr}\{\rho(t)P(t)\}. \tag{35}$$

If the loss mechanism consists of a set of oscillators, and if K is linear in these oscillator operators, then the commutator $[K(t),\,K(t')]$ in (34) is a c-number. In that case, the last term on the right in (34) contributes a dissipative term to the equations of motion for the expectation values of Q and P, consistently with the expectation value of the Langevin equation (24) in section 3.

In many cases (for instance for the oscillator model), the expectation value of the noise term (the second term on the right) in (34) vanishes. But we may look for the effect of noise by taking expectation values of products of two operators. For example, we could obtain a differential equation like (34) for

$$\mathrm{tr}\{\rho(t)P(t)P(t)\}, \tag{36}$$

and this would include expectation values of terms bilinear in K which would not vanish. However, from solutions of the Langevin equations (24), one could get (in the Heisenberg picture) expectation values like

$$\mathrm{tr}\{\rho_{\mathrm{H}}P_{\mathrm{H}}(t_1)P_{\mathrm{H}}(t_2)\} \tag{37}$$

(where the suffix H emphasizes the Heisenberg picture). Such unequal time correlators seem to appear less naturally in the master equation formalism (see for example section 5.2.1 of [5]).

The question at issue in this paper is whether one can obtain an approximate Langevin-like equation when the commutator $[K(t),\,K(t')]$ in (34) is *not* a c-number. This would be possible if the density matrix factorized (approximately) at all times:

$$\rho(t) \approx \rho_S(t) \otimes \rho_{\mathrm{B}}(t), \tag{38}$$

where the suffixes refer to *simple system* and *bath* respectively. To investigate the validity of this approximation, we can insert (38) into (31) and trace over the bath variables, to get (with the Hamiltonian (16))

$$\hbar\dot{\rho}_S(t) \approx -\mathrm{i}\,\mathrm{tr}_{\mathrm{B}}(\rho_{\mathrm{B}}K)[Q,\,\rho_S]. \tag{39}$$

In many cases, in particular in the simple case when the bath is a set of oscillators and K is linear in these variables (which is the simplest possible case, and for which the method of section 3 succeeds), the trace on the right-hand side of (39) is zero. This means that $\rho_S(t) \approx \rho_S(t_0)$. If it were legitimate to insert this approximation into the last term in (32), we would get no integral equation for $\rho_B(t)$ at all. Thus the approximation (38) seems to be inconsistent.

6. Comments

As mentioned in section 1, the quantum fluctuation–dissipation relation has been referred to in connection with experiments which might be thought to be sensitive to vacuum energy [11, 12]. I have argued in this paper that one should not appeal to the quantum fluctuation–dissipation relation without checking if it is valid for the case in point, and this requires some information about the dissipation mechanism.

What is the interpretation of the Bose distribution function (12) appearing in the fluctuation–dissipation relations? First of all, it is present only if the symmetrized product (11) is used (see [10]). In the ideal case where the equations of motions are linear, and so the commutator C in (23) is a c-number and the dissipation is independent of T, the Bose function (12) gives the complete temperature dependence of the noise spectrum (30). In this case, there is little doubt that (10) corresponds to the oscillators in the bath. If these are three dimensional, we would expect the dissipation in G in (27) to be proportional to ω^2.

Beyond this special case, the situation is less clear. I have argued above that the Langevin equation has not been proved in general. But even if we *assume* that the approximation (25) is justified, the factor N in (12) does not give the T-dependence of the noise spectrum, because the dissipation itself will in general be T-dependent. *If* the fluctuation–dissipation relation (11) had been justified generally, it would cover cases where the dissipation and noise were due to a bath of fermionic systems, and then the Bose factor N in (12) could not possibly represent the physics of the bath.

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References

[1] Callen H B and Welton T A 1951 *Phys. Rev.* **83** 34
[2] Senitzky I R 1960 *Phys. Rev.* **119** 670
[3] Landau L D and Lifshitz E M 1980 *Statistical Physics* (Oxford: Pergamon) Part I, paragraphs 123, 124
[4] Feynman R P and Hibbs A R 1965 *Quantum Mechanics and Path Integrals* (New York: McGraw-Hill)
[5] Gardiner C W and Zoller P 2000 *Quantum Noise* (Berlin: Springer)
[6] Kogan Sh 1996 *Electronic Noise and Fluctuations in Solids* (Cambridge: Cambridge University Press)
[7] Balescu R 1975 *Equilibrium and Nonequilibrium Statistical Mechanics* (New York: Wiley)
[8] Kreuzer H J 1981 *Nonequilibrium Thermodynamics and its Statistical Foundations* (Oxford: Clarendon)
[9] van Kampen N G 2001 *Fluctuations Noise Lett.* **1** C7
[10] Gavish U, Imry Y and Levinson Y 2000 *Phys. Rev.* B **62** R10637
[11] Koch R H, Van Harlingen D J and Clarke J 1982 *Phys. Rev.* **26** 74
[12] Beck C and Mackey M C 2005 *Phys. Lett.* B **605** 295
[13] Levinson Y 2003 *Phys. Rev.* B **67** 18504
[14] Schmid A 1982 *J. Low Temp. Phys.* **49** 609