Reply to "Comment on 'Energy balance for a dissipative system'"

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In a Comment by I. R. Senitzky [Phys. Rev. E 51, 5166 (1995)] on a recent paper by Li et al. [Phys. Rev. E 48, 1547 (1993)] dealing with energy balance for an oscillator coupled with a heat bath, it is claimed that the formula given there for the power supplied to the oscillator by the bath, while formally correct, is misleading, since it does not vanish at absolute zero. In reply, it is pointed out that different parts of the physical system, which is the oscillator plus the bath plus their coupling, can and do exchange energy, even at absolute zero.

PACS number(s): 05.30.-d, 05.40.+j

In a recent paper [1] on energy balance for a dissipative system, we discussed the case of an oscillator coupled to a heat bath and used the quantum Langevin equation to obtain a formula for the rate work is done by the bath on the oscillator. In his Comment [2], Senitzky asserts that, while our results are correct, they " ... are misleading." He goes on to claim that the quantum fluctuations at zero temperature "... cannot do work." In this Reply, we describe what appears to us to be the essential point: the physical system is the oscillator coupled to a heat bath, not the uncoupled oscillator. Different parts of this system can and do exchange energy, even at zero temperature.

First, however, we cannot let pass the fact that the Comment repeats an old mistake: the proposed power spectrum of the fluctuating force is that of white noise (independent of frequency) and not the Planck spectrum of quantum noise. So far as we know, a correct formulation of the quantum Langevin equation was first given in the Ford, Kac, and Mazur paper [3], but its form and the basis for obtaining the equation have by now been understood from a variety of points of view [4,5]. For the Ohmic case of a frequency-independent friction constant, the case treated in the Comment, the correct quantum Langevin equation for a particle of mass m in an external potential V(x) takes the form [4]

$$m\ddot{x} + \zeta \dot{x} + V'(x) = F(t). \tag{1}$$

Here F(t) is a Gaussian random operator force with mean zero and correlation

$$\frac{1}{2}\langle F(t)F(t')+F(t')F(t)\rangle=\int_{0}^{\infty}d\omega P(\omega)\cos[\omega(t-t')],$$

where $P(\omega)$ is the power spectrum, given by

$$P(\omega) = rac{\zeta}{\pi} \hbar \omega \coth(\hbar \omega / 2kT) = rac{2\zeta}{\pi} \left(rac{\hbar \omega}{2} + rac{\hbar \omega}{e^{\hbar \omega / kT} - 1}
ight).$$

The commutator of the random force is

$$[F(t), F(t')] = \frac{2\hbar\zeta}{i\pi} \int_0^\infty d\omega \omega \sin[\omega(t - t')]$$
$$= 2i\hbar\zeta \delta'(t - t'), \tag{4}$$

where δ' is the derivative of the delta function. Note that the correlation and commutator are both proportional to the friction constant ζ and that their form is independent of the external potential energy V(x). These are direct consequences of the fluctuation-dissipation theorem [6]. In particular, we emphasize that the power spectrum of the random force is the Planck spectrum, with the addition of the contribution of the zero-point fluctuations. Only in the classical limit, $\hbar \to 0$, does the spectrum become the flat spectrum of white noise.

The form of the correlation given in Eq. (3b) of the Comment, which is taken from Eq. (7) of the second of Refs. [2] of the Comment does not satisfy any of the criteria noted above. The same form appears in each of Refs. [2-4] of the Comment. One might ask how such an error could have arisen and, indeed, persist in the literature? The answer, we believe, is that people had in mind the case of an oscillator, for which the potential is of the form $V(x) = \frac{1}{2}m\omega_0^2x^2$ and the Langevin equation takes the form

$$m\ddot{x} + \zeta \dot{x} + m\omega_0^2 x = F(t). \tag{5}$$

In this case, the correlation function for the oscillator displacement can easily be computed and, with the correct form (2) for the force correlation, the result is

(2)

$$\frac{1}{2}\langle x(t)x(t')+x(t')x(t)\rangle$$

$$= \int_0^\infty d\omega \mid \alpha(\omega) \mid^2 P(\omega) \cos[\omega(t - t')], \quad (6)$$

where $\alpha(\omega)$ is the oscillator susceptibility (response function), given by

$$\alpha(\omega) = \frac{1}{-m\omega^2 - i\omega\zeta + m\omega_0^2}.$$
 (7)

So far this is an exact result, consistent with the correlation (2). It can also be obtained directly, without reference to the form of the random force, using the fluctuation-dissipation theorem [7,8]. Note that we use the word fluctuation in the sense of Refs. [7] and [8], to include both thermal and quantum fluctuations. Next, we use the fact that in those early works people restricted consideration to the zero coupling limit: $\zeta \to 0$. In this limit one can easily show that

$$\zeta \mid \alpha(\omega) \mid^2 \to \frac{\pi}{2m\omega_0^2} \delta(\omega - \omega_0).$$
 (8)

With this we obtain the familiar result for the correlation of the free oscillator [9],

$$\frac{1}{2}\langle x(t)x(t')+x(t')x(t)\rangle$$

$$\rightarrow \frac{\hbar \coth(\hbar\omega_0/2kT)}{2m\omega_0}\cos[\omega_0(t-t')]. \quad (9)$$

The fact that in this limit the oscillator response function gives rise to a δ function at the oscillator frequency ω_0 means that one could replace $P(\omega)$ with the constant $P(\omega_0)$ in the expression (6) for the correlation of x and still get the correct expression for the free oscillator correlation in the zero coupling limit. On the other hand, if one makes the same replacement in the force correlation (2), which is what is done in Refs. [2] and [4] of the Comment, one gets the δ function correlation of white noise. This is clearly in contradiction with the general form (2) for the correlation of the random force and is wrong. In this connection, we should mention the important paper of Benguria and Kac [10], who showed that for the nonlinear oscillator one gets in the zero coupling limit the correct form of the correlation only with the correct forms (3) and (4) for the power spectrum and commutator. Thus, even in the zero coupling limit, the form of the force correlation given in the Comment is wrong.

We turn now to a discussion of the energy balance, using the above results. Here it is important to recognize that the physical system is that of an oscillator coupled to a heat bath (what in the Comment is called the loss mechanism). The microscopic Hamiltonian for this system is of the form

$$H = H_{\rm osc} + H_{\rm bath} + H_{\rm coupling}, \tag{10}$$

with the three terms corresponding to the oscillator, heat bath, and coupling terms in the system Hamiltonian. This is a system with an infinite number of degrees of freedom, each with its corresponding zero-point oscillation. At absolute zero this system is in its ground state and, trivially, there is no work done on or by the system. But, for any finite coupling, no matter how weak, $H_{\rm osc}$ does not commute with H. Therefore, the ground state of H is not the ground state of $H_{\rm osc}$ and, even at absolute zero, the oscillator energy must fluctuate. To be specific, the mean square fluctuation of $H_{\rm osc}$ is not zero,

$$\Delta H_{\rm osc}^2 = \langle H_{\rm osc}^2 \rangle - \langle H_{\rm osc} \rangle^2 \neq 0. \tag{11}$$

Again, this fluctuation does not vanish at absolute zero and no matter how weak the coupling. The point of the paper of Li et al. [1] is that this fluctuation is driven by a fluctuating force exerted by the bath. The work done per unit time by this force is, of course, balanced by the dissipative loss, so there is no net work done on the oscillator.

This fluctuation can be calculated explicitly and without any assumption about the strength of the coupling. First of all, the oscillator energy operator takes the form

$$H_{\rm osc} = \frac{1}{2}m\dot{x}^2 + \frac{1}{2}m\omega_0^2 x^2. \tag{12}$$

If one makes the identification $q = (m/\hbar\omega_0)^{1/2}\dot{x}$ and $p = -(m\omega_0/\hbar)^{1/2}x$, which is implied by the "solution" given in Eqs. (2) of the Comment, this operator is identical with that given in Eq. (1) of the Comment. Next, the exact expression (6) for the correlation of x can be used to calculate $\langle x^2 \rangle$ and $\langle \dot{x}^2 \rangle$ at absolute zero. With these we obtain an exact expression for the mean of the oscillator energy at T=0:

$$\langle H_{\rm osc} \rangle = \frac{\hbar}{\pi} \left(\omega_0^2 - \frac{\zeta^2}{4m^2} \right)^{1/2} \cos^{-1} \left(\frac{\zeta}{2m\omega_0} \right) + \frac{\hbar \zeta}{2\pi m} \ln \left(\frac{\omega_c}{\omega_0} \right), \tag{13}$$

where ω_c is a high frequency cutoff. Since x and \dot{x} are Gaussian operators with mean zero, the mean of the square of $H_{\rm OSC}$ can be expressed in terms of products of $\langle x^2 \rangle$ and $\langle \dot{x}^2 \rangle$. The resulting expression is, however, rather complicated, so we will not display it here. Instead, we follow the Comment in making the weak coupling approximation, $\zeta \ll m\omega_0$. In this approximation, the result (13) takes the simple form

$$\langle H_{\rm osc} \rangle \cong \frac{\hbar \omega_0}{2} + \frac{\hbar \zeta}{2\pi m} \ln(\omega_c/\omega_0),$$
 (14)

and the mean square fluctuation becomes

$$\Delta H_{\rm OSC}^2 = \langle H_{\rm OSC} \rangle \frac{\hbar \zeta}{\pi m} \ln(\omega_c/\omega_0). \tag{15}$$

Thus we see explicitly, even in the weak coupling approximation, that the mean of the oscillator energy is above its ground state energy and that the fluctuations in this energy do not vanish. In this sense, we feel it is wrong to say that the fluctuations at T=0 "... cannot do work"

and that the bath (loss mechanism) "... cannot, in reality, provide energy at T=0." One part of a physical system in its ground state can and does exchange energy with another part. Perhaps the difficulty here is a confusion of the weak coupling approximation ($\zeta \ll m\omega_0$) with the zero coupling limit ($\zeta \to 0$). Of course, the uncoupled oscillator in its ground state cannot give up energy. The results we have exhibited are consistent with this.

Finally, we consider the form of the energy balance. Forming the time derivative of $H_{\rm osc}$, using the quantum Langevin equation for the oscillator and then forming the expectation, one can readily show that

$$\frac{d}{dt}\langle H_{\rm osc}\rangle + \zeta \langle \dot{x}^2 \rangle = \frac{1}{2}\langle \dot{x}F + F\dot{x}\rangle. \tag{16}$$

We emphasize that this is an exact equation; we have not made the weak coupling approximation. It corresponds to Eq. (4) of the Comment, but is not quite equivalent with that equation, even in the weak coupling approximation. The differences, however, are not crucial. Now, each of the expectations occurring in this equation is an equal-time expectation and must be independent of time

as a consequence of the time-displacement invariance of the system. Therefore the time derivative of $\langle H_{\rm osc} \rangle$ must be zero and the remaining terms must be equal. In our paper [1], we evaluated the right hand side (actually for the more general case of a frequency-dependent friction constant) which we interpreted as the rate work is done by the fluctuating force acting on the oscillator. In the Comment it is objected that this interpretation is "unphysical," since this power does not vanish at absolute zero, when the system is in its ground state. We feel that this objection is met by our remarks above. On the other hand, one could simply subtract the zero-point contribution from each term in the energy balance equation (16), which would remove the objection by sleight of hand. This, in effect, is what is is done in the Comment. But the zero-point fluctuations are real and it is of interest to see that the energy balance holds even at absolute

This work was supported in part by the National Science Foundation under Grant No. INT-9204411 and by the U.S. Army Research Office under Grant No. DAAHO4-94-G-0333

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