There is No Quantum Regression Theorem

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The Onsager regression hypothesis states that the regression of fluctuations is governed by macroscopic equations describing the approach to equilibrium. It is here asserted that this hypothesis fails in the quantum case. This is shown first by explicit calculation for the example of quantum Brownian motion of an oscillator and then in general from the fluctuation-dissipation theorem. It is asserted that the correct generalization of the Onsager hypothesis is the fluctuation-dissipation theorem. [S0031-9007(96)00679-5]

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The regression hypothesis.—The regression theorem (or, more properly, hypothesis) of Onsager states that "…the average regression of fluctuations will obey the same laws as the corresponding macroscopic irreversible process" [1]. Thus, for example, the correlation of temperature fluctuations in a gas satisfies the Fourier equation of thermal diffusion [2]. The purpose of this Letter is to point out that, contrary to the number of assertions appearing in the literature [3–6], there is no quantum regression theorem in the sense of Onsager. Similar observations have been made in special cases (see, e.g., [7,8]), but here we investigate this question more generally. The essential point is made in our Eq. (25) below, which expresses the fact that the proper quantum generalization of the Onsager hypothesis is the fluctuation-dissipation theorem, not the so-called quantum regression theorem.

As a simple example, which is also that discussed most often in the literature, we first discuss the case of quantum Brownian motion of a harmonically bound particle (oscillator). This will allow an explicit demonstration of the nature and origin of the failure of the Onsager hypothesis in the quantum case. Then, in order to put the remarks in a general context, we quote the fluctuation-dissipation theorem of Callen and Welton in the form involving the relaxation function. This enables us to present a general analysis that is independent of the quantum Langevin equation. But, more important, this analysis applies to any quantum system (oscillator, two level atom, etc.). As a result, we shall see in general why the Onsager hypothesis fails in the quantum case.

Quantum Brownian motion.—The quantum Brownian motion of the oscillator is described by the quantum Langevin equation [9],

$$m\ddot{x} + \zeta\dot{x} + Kx = F(t), \tag{1}$$

where x is the displacement operator and $F(t)$ is an operator random force, a Gaussian operator with expected value zero and correlation

$$\frac{1}{2}\langle F(t)F(t') + F(t')F(t)\rangle = \frac{2\zeta}{\pi}\int_0^\infty d\omega\,\frac{\hbar\omega}{2}\coth\left(\frac{\hbar\omega}{2kT}\right) \times \cos[\omega(t-t')]. \tag{2}$$

The commutator of the random force, which will not be used in the following discussion, but which is needed for consistency, is

$$[F(t),F(t')] = \frac{\zeta}{i\pi}\int_0^\infty d\omega\,\hbar\omega\sin[\omega(t-t')]. \tag{3}$$

The parameters appearing in the quantum Langevin equation (1) are m, the oscillator mass, K, the spring constant, and ζ, the dissipative force constant. Note that the random force is independent of the oscillator parameters m and K. It depends only on the absolute temperature T and the constant ζ, which is a measure of the strength of the coupling to the random environment (in general, a field).

The stationary solution of the quantum Langevin equation is

$$x(t) = \frac{1}{m}\int_{-\infty}^{t} dt'\,e^{-\gamma(t-t')/2}\,\frac{\sin\omega_1(t-t')}{\omega_1}\,F(t'), \tag{4}$$

where we have introduced

$$\gamma = \zeta/m, \qquad \omega_1 = \sqrt{K/m - \gamma^2/4}. \tag{5}$$

The correlation of the displacement is defined to be

$$C(t-t') = \tfrac{1}{2}\langle x(t)x(t') + x(t')x(t)\rangle. \tag{6}$$

With the force correlation given in Eq. (2), it is a straightforward matter to obtain the following expression for this correlation,

$$C(t) = \frac{2\zeta}{\pi}\int_0^\infty d\omega\,\frac{(\hbar\omega/2)\coth(\hbar\omega/2kT)}{(K-m\omega^2)^2+\zeta^2\omega^2}\cos(\omega t). \tag{7}$$

Since the integrand is an even function of ω, we can also write

$$C(t) = \frac{\zeta}{\pi}\int_{-\infty}^{\infty} d\omega\,\frac{(\hbar\omega/2)\coth(\hbar\omega/2kT)}{(K-m\omega^2)^2+\zeta^2\omega^2}\,e^{-i\omega t}. \tag{8}$$

The equation describing the approach of a given mean displacement to its equilibrium value of zero is obtained by forming the expectation value of the quantum Langevin equation,

$$m\langle\ddot{x}\rangle + \zeta\langle\dot{x}\rangle + K\langle x\rangle = 0\,. \tag{9}$$

The Onsager hypothesis would state that for $t > 0$ the correlation $C(t)$ satisfies this same equation. But, using the expression (8) for $C(t)$, we see that

$$m\ddot{C} + \zeta\dot{C} + KC = \frac{\zeta}{\pi}\int_{-\infty}^{\infty} d\omega\, \frac{(\hbar\omega/2)\coth(\hbar\omega/2kT)}{K - m\omega^2 + i\zeta\omega} \times e^{-i\omega t}. \tag{10}$$

For $t > 0$ we can complete the contour with a large arc in the lower half plane, where the integrand vanishes. The denominator in the integrand has zeros only in the upper half plane, while the numerator has poles at $\omega = -in\Omega$, where n is a positive integer and

$$\Omega = \frac{2\pi kT}{\hbar}\,. \tag{11}$$

The integral is therefore equal to $-2\pi i$ times the sum of the residues at these poles. The result is

$$m\ddot{C} + \zeta\dot{C} + KC = -2\zeta kT\sum_{n=1}^{\infty}\frac{n\Omega e^{-n\Omega t}}{mn^2\Omega^2 + \zeta n\Omega + K}\,. \tag{12}$$

This, being a sum of positive terms, does not vanish. Therefore, the correlation does not satisfy the macroscopic equation (9) and the Onsager hypothesis is not satisfied.

In the classical limit ($\hbar \to 0$ or, equivalently, $\Omega \to \infty$) the right-hand side of (12) vanishes identically, and the Onsager hypothesis is satisfied. This same result can be seen directly from the integral on the right-hand side of (10). There the only place the Planck constant $\hbar$ occurs is in the numerator in the integrand, which is the average energy of a quantum oscillator of frequency ω,

$$u(\omega) = \frac{\hbar\omega}{2}\coth\frac{\hbar\omega}{2kT}\,. \tag{13}$$

In the classical limit this average energy goes to the classical equipartition value kT, independent of frequency. The integrand is then analytic in the lower half plane and therefore the integral vanishes for $t > 0$. Thus, we see that the failure of the Onsager hypothesis is precisely due to the deviation of the quantum oscillator energy from its classical equipartition value. This deviation has two aspects: a high frequency linear divergence due to the quantum zero-point oscillations and a cutoff of the finite-temperature contribution at frequencies of the order of Ω.

The effect of the zero-point oscillations is obtained by evaluating the sum on the right-hand side of (12) in the limit $T \to 0$. This is easily done if we recognize that in this limit there will be very many terms in the sum, which may then be approximated by an integral. The result is

$$m\ddot{C} + \zeta\dot{C} + KC = -\frac{\hbar\zeta}{\pi}\int_0^{\infty} dy\,\frac{ye^{-yt}}{my^2 + \zeta y + K}\,. \tag{14}$$

This integral can be expressed in terms of the error integral function [10], but it will be sufficient for our purpose to exhibit the short and long time behavior, which correspond, respectively, to the large and small y behavior of the integrand. The result is

$$m\ddot{C} + \zeta\dot{C} + KC = \frac{\hbar\gamma}{\pi}\times\begin{cases}\ln(\omega_0 t), & t\to 0\,,\\ -\frac{1}{(\omega_0 t)^2}, & t\to\infty\,,\end{cases} \tag{15}$$

where $\omega_0 = \sqrt{K/m}$ is the natural frequency of the undamped oscillator. Thus we see that, far from vanishing, the right-hand side is logarithmically divergent at short times.

The short time logarithmic divergence remains at finite temperature, since the above argument replacing the sum by an integral requires only that the product Ωt be small. On the other hand, at finite temperature the long time power-law decay is replaced by an exponential decay. Thus, if $\Omega t \gg 1$, one can replace the sum by its first term. In this way, we obtain at finite temperature the result

$$m\ddot{C} + \zeta\dot{C} + KC = \frac{\hbar\gamma}{\pi}\times\begin{cases}\ln(\Omega t), & t\to 0\,,\\ -\frac{e^{-\Omega t}}{1+\gamma/\Omega+K/m\Omega^2}, & t\to\infty\,.\end{cases} \tag{16}$$

This qualitative change in the long time behavior, from a power-law decay at $T = 0$ to an exponential decay at $T > 0$, is a typical quantum phenomenon.

The fluctuation-dissipation theorem.—The theorem deals with a system with Hamiltonian H in equilibrium at temperature T. The expectation of an operator $\mathcal{O}$ in the Hilbert space of H is defined to be

$$\langle\mathcal{O}\rangle \equiv \frac{\mathrm{Tr}\{\mathcal{O}\,e^{-H/kT}\}}{\mathrm{Tr}\{e^{-H/kT}\}}\,. \tag{17}$$

We shall also use the notation,

$$\mathcal{O}(t) \equiv e^{iHt/\hbar}\mathcal{O}e^{-iHt/\hbar}. \tag{18}$$

Here $\mathcal{O}(t)$ is the (Heisenberg) operator that evolves in time t from the operator $\mathcal{O}$.

Consider now a dynamical variable y, i.e., a self-adjoint operator in the Hilbert space of H. For convenience we assume, and it can always be arranged, that the expectation of y is zero,

$$\langle y\rangle = 0\,. \tag{19}$$

The correlation function of y is defined to be

$$C(t - t') = \tfrac{1}{2}\langle y(t)y(t') + y(t')y(t)\rangle. \tag{20}$$

The relaxation function is defined in terms of the perturbed Hamiltonian,

$$H_f = H - fy\,, \tag{21}$$

where f is a real c-number constant. One imagines that f is fixed in the distant past and the system is allowed to come to equilibrium at temperature T. Then at $t = 0$, f is set equal to zero, and the system evolves in time according to the Hamiltonian H. The expectation value of y is then

$$\langle y(t)\rangle_f \equiv \frac{\mathrm{Tr}\{y(t)e^{-(H-fy)/kT}\}}{\mathrm{Tr}\{e^{-(H-fy)/kT}\}}. \tag{22}$$

Here $y(t)$, given by the definition (18), is the Heisenberg operator evolving in time under the unperturbed Hamiltonian H. Finally, we assume f is small and expand

$$\langle y(t)\rangle_f = A(t)f + \cdots. \tag{23}$$

The function $A(t)$ thus defined is the relaxation function (sometimes also called the after-effect function). Note that, according to the definitions (22) and (23), the relaxation function is defined for both positive and negative times. This is adopted as a convention.

We introduce now the time Fourier transform of these functions

$$\tilde{A}(\omega) = \int_{-\infty}^{\infty} dt\, e^{i\omega t}A(t) \tag{24}$$

and similarly for $\tilde{C}(\omega)$. It can be shown in general that these are connected by the relation

$$\tilde{C}(\omega) = u(\omega)\tilde{A}(\omega), \tag{25}$$

where $u(\omega)$ is the free oscillator energy (13). This is the fluctuation-dissipation theorem [11,12].

In the classical limit $u(\omega) \rightarrow kT$, independent of frequency. Therefore, in this limit the fluctuation-dissipation theorem states that $C(t)$ and $A(t)$ are proportional. But this is the Onsager hypothesis since, if $\langle y(t)\rangle$ is a macroscopic variable, the relaxation function $A(t)$ will be a solution of a (linearized) macroscopic equation describing the approach to equilibrium. Thus, in the classical limit and for macroscopic variables corresponding to a dynamical variable of the system, the fluctuation-dissipation theorem is a proof of the Onsager regression hypothesis. On the other hand, in the quantum case, where $\hbar$ is not zero, the factor $u(\omega)$ is a nontrivial function of frequency. As we have seen in the case of Brownian motion, this leads to a failure of the Onsager hypothesis. Rather than to speak of failure, we would ourselves prefer to say that the proper quantum generalization of the Onsager hypothesis is the fluctuation-dissipation theorem.

It would perhaps be of interest to see exactly how the results obtained above for quantum Brownian motion follow from the fluctuation-dissipation theorem. The addition of a term $-fx$ to the Hamiltonian for the oscillator coupled to the heat reservoir clearly will result in a term f on the right-hand side of the macroscopic equation (9). The equilibrium solution with this term present is $\langle x\rangle = f/K$. The solution of Eq. (9) with this initial value is

$$\langle x(t)\rangle_f = \frac{f}{K} e^{-\gamma|t|/2}\left[\cos(\omega_1 t) + \frac{\gamma}{2\omega_1}\sin(\omega_1|t|)\right] \equiv fA(t). \tag{26}$$

The Fourier transform of the relaxation function is therefore

$$\tilde{A}(\omega) = \frac{2\zeta}{(K - m\omega^2)^2 + \zeta^2\omega^2}. \tag{27}$$

Putting this in the fluctuation-dissipation theorem (25) and forming the inverse Fourier transform, we obtain exactly the expression (8) for the correlation function. Note that this affords a direct calculation of that correlation, without reference to the quantum Langevin equation (1) or to the form (2) of the random force correlation.

Concluding remarks.—One can ask why it is that, despite the fact that there is no quantum regression theorem, there seem to be no flagrant errors in its application. The answer, we believe, is that in most applications in the field of quantum optics the random environment is the radiation field, which is coupled only weakly to the atomic system. Indeed, for the oscillator coupled to the radiation field $\zeta = K\tau_e$, where $\tau_e = 2e^2/3mc^3 \cong 6.24 \times 10^{-24}$ sec is a very short time on the atomic scale [13]. Since the right-hand side of, say, Eq. (10) is proportional to ζ, one can argue that in the weak coupling approximation one makes a small error in neglecting it.

But in the same order of weak coupling in which one would neglect the right-hand side of Eq. (10), one should also neglect the term proportional to ζ on the left-hand side. Thus, in fact, what is being considered is the correlation of the free oscillator, in which the coupling to the random environment is neglected. While in some applications this might be a reasonable approximation, it does not require the formalism and apparatus of quantum dissipation.

In conclusion, we would once again strongly emphasize that the fluctuation-dissipation theorem, either in the relaxation function form (25) or in the more often useful response function form [12], is the correct quantum generalization of the regression theorem. This is a simple and correct statement of the relation between the correlation of fluctuations and the macroscopic description of the approach to equilibrium. It does not require a weak coupling assumption.

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