Quantum Oscillator in a Blackbody Radiation Field

G. W. Ford[a]

Institut Laue-Langevin, 38042 Grenoble Cedex, France

J. T. Lewis

School of Theoretical Physics, Dublin Institute for Advanced Studies, Dublin 4, Ireland

and

R. F. O'Connell

Department of Physics and Astronomy, Louisiana State University, Baton Rouge, Louisiana 70803

The quantum Langevin equation is used to calculate an *exact* expression for the *free energy* of a quantum oscillator interacting, via dipole coupling, with a blackbody radiation field. In particular, we obtain a temperature-dependent shift in the free energy. This result may then be used to obtain corresponding results for the energy, the partition function, and other thermodynamic quantities.

We consider the problem of determining the free energy of a quantum oscillator in thermal equilibrium with the radiation field at temperature T. In the weak-coupling limit the free energy is given by the Planck formula. Our purpose here is to give, within the dipole approximations, an exact formula for this free energy. (The reason that we stress the calculation of the free energy rather than the internal energy is that the former is a thermodynamic potential from which the other thermodynamic functions can be derived.) Our result is that, in addition to a modification of the Planck formula due to the finite linewidth, there is a positive shift $\Delta F_0(T) = \pi e^2 (kT)^2 / 9\hbar Mc^3$ which is of quantum electrodynamic origin.

Problems involving the interaction of a quantum system with a heat bath are receiving increasing attention in areas such as condensed matter[1] and quantum optics.[2, 3] Our purpose here is to show that statistical methods which make use of the quantum Langevin equation can be a powerful tool for attacking such problems. The correct form of the quantum Langevin equation for a particular model of a heat bath was given by Ford, Kac, and Mazur.[4] Here we use this equation for the case in which the heat bath is the radiation field.

The quantum Langevin equation takes the general form

$$m\ddot{x} + \int_{-\infty}^{t} dt' \, \mu(t - t')\dot{x}(t') + Kx = F(t). \qquad (1)$$

This is an equation for the time-dependent Heisenberg operator $x(t)$. The coupling with the radiation field is described by two terms: the radiation reaction term characterized by the memory function $\mu(t)$, and the fluctuating term characterized by the operator-valued random force $F(t)$. For our purposes we need this equation only to extract the generalized susceptibility, which is done by forming the Fourier transform of (1) and writing the result in the form

$$\tilde{x}(\omega) = \alpha(\omega)\tilde{F}(\omega), \qquad (2)$$

where we use the superposed tilde to denote the Fourier transform, e.g., $\tilde{x}(\omega)$ is the Fourier transform of the operator $x(t)$. Here $\alpha(\omega)$ is the generalized susceptibility (a c-number) given by

$$\alpha(\omega) = [-m\omega^2 + K - i\omega\tilde{\mu}(\omega)]^{-1}, \qquad (3)$$

where

$$\tilde{\mu}(\omega) = \int_0^{\infty} dt \, \mu(t)e^{i\omega t}, \quad \text{Im}\,\omega > 0, \qquad (4)$$

is the Fourier transform of the memory function.

Clearly $\tilde{\mu}(\omega)$ is analytic in the upper-half ω plane. In addition, energy considerations require that the real part of $\tilde{\mu}(\omega)$ be positive on the real axis. Functions satisfying these two requirements are termed positive functions.[5, 6] This condition of positivity is of fundamental physical importance; its violation is tantamount to a violation of the second law of thermodynamics (see Ref. 5, and references therein). It is also very restrictive: Positive functions have neither zeros nor poles in the upper-half plane, on the real axis they can have only simple zeros with negative imaginary coefficient and simple poles with positive imaginary residues, the reciprocal of a positive function is a positive function, etc.

The system of oscillator coupled to the radiation field in thermal equilibrium at temperature T has a well-defined free energy. The free energy ascribed to the oscillator, $F_0(T)$, is the free energy of this system minus the free energy of the radiation field in the absence of the oscillator. For this free energy we have

the remarkable formula

$$F_0(T) = \frac{1}{\pi} \int_0^{\infty} d\omega \, f(\omega, T) \, \text{Im} \left[\frac{d \ln\alpha(\omega)}{d\omega} \right], \quad (5)$$

where $f(\omega, T)$ is the free energy of a single oscillator of frequency ω, given by the familiar formula (see, e.g., Landau and Lifshitz,[7] especially Secs. 49 and 61),

$$f(\omega, T) = kT \ln[1 - \exp(-\hbar\omega/kT)]. \quad (6)$$

Note that we discard the $T = 0$ contributions since our interest is in the temperature-dependent effects.

Formula (5) is striking because it expresses the free energy of the *interacting* oscillator in terms of the susceptibility (3) alone. It can be derived explicitly for general microscopic heat-bath models which lead to a quantum Langevin equation, but the following simple argument contains the essence of the proof. From (3) it is not difficult to see that $-i\omega\alpha(\omega)$ is a positive function provided that $\tilde{\mu}(\omega)$ is a positive function and that m and K are positive. If the normal modes are discrete, $\alpha(\omega)$ will have poles on the real axis at the normal-mode frequencies of the interacting system and zeros at the normal-mode frequencies of the radiation field in the absence of the oscillator. This should be apparent from (2): If $\alpha(\omega) = 0$ there can be a fluctuating force with no $\tilde{x}$, while if $\alpha(\omega)^{-1} = 0$ there can be a motion of $\tilde{x}$ with no force. Therefore, one can write

$$\alpha(\omega) \propto \prod_i (\omega^2 - \omega_i^2)/\prod_j (\omega^2 - \bar{\omega}_j^2), \quad \text{Im}\,\omega > 0, \quad (7)$$

where the numerator is the product over normal modes of the free radiation field, and the denominator is the product over those of the interacting system. In (5) it is understood that $\alpha(\omega)$ is the boundary value as ω approaches the real axis from above. If, therefore, one recalls the well-known formula $1/(x + i0^+) = P(1/x) - i\pi\delta(x)$, one sees that

$$\pi^{-1} \text{Im}[d \ln\alpha(\omega)/d\omega] = \sum_j [\delta(\omega - \bar{\omega}_j) + \delta(\omega + \bar{\omega}_j)] - \sum_j [\delta(\omega - \omega_j) + \delta(\omega + \omega_j)]. \quad (8)$$

When this is put into (5) the result can be written as

$$F_0(T) = \sum_j f(\bar{\omega}_j, T) - \sum_i f(\omega_i, T), \quad (9)$$

where the first sum is clearly the free energy of the interacting field, and the second that of the free field. This demonstrates our assertion.

To apply the formula (5) we must have an expression for the generalized susceptibility or, equivalently, the function $\tilde{\mu}(\omega)$. The form of this function is implicit in any discussion of electromagnetic radiation reaction, but we have been unable to find a convenient reference in which an explicit form is given, and so we will sketch a derivation. In the dipole approximation the Hamiltonian for the oscillator interacting with the radiation field is[8, 9]

$$H = (1/2m)[p_x - (e/c)A_x]^2 + \tfrac{1}{2}Kx^2 + \sum_{\mathbf{k},s} \hbar c k a_{\mathbf{k},s}^{\dagger} a_{\mathbf{k},s}, \quad (10)$$

where the vector potential is given by

$$A_x = \sum_{\mathbf{k},s} (2\pi\hbar c/kV)^{1/2}(f_k^* a_{\mathbf{k},s} \hat{e}_{\mathbf{k},s} \cdot \hat{x} + f_k a_{\mathbf{k},s}^{\dagger} \hat{e}_{\mathbf{k},s}^* \cdot \hat{x}), \quad (11)$$

where f_k is the electron form factor, $\hat{e}$ is the polarization vector, and V is the volume. The Heisenberg equations of motion obtained from (10) are

$$\dot{x} = (1/m)[p_x - (e/c)A_x], \quad \dot{p}_x = -Kx, \quad \dot{a}_{\mathbf{k},s} = -icka_{\mathbf{k},s} + i(2\pi e^2/\hbar ckV)^{1/2} f_k \hat{x} \cdot \hat{e}_{\mathbf{k},s}^* \dot{x}. \quad (12)$$

Integrating the last of these equations we find

$$a_{\mathbf{k},s}(t) = a_{\mathbf{k},s}^f(t) + i(2\pi e^2/\hbar ckV)^{1/2} f_k \hat{x} \cdot \hat{e}_{\mathbf{k},s}^* \int_{-\infty}^t dt' \exp[-i\omega(t - t')]\dot{x}(t'), \quad (13)$$

where $a_{\mathbf{k},s}^f(t)$ is the free-field Heisenberg operator. We now put this expression into (11) to obtain an expression for $A_x(t)$. By use of this, the first two of Eqs. (12) can be cast into the form (1) with

$$\mu(t) = (8\pi e^2/3V) \sum_{\mathbf{k}} |f_{\mathbf{k}}|^2 \cos(ckt), \quad (14)$$

and with $F(t) = -(e/c)\dot{A}_x^f(t)$. Our results are insensitive to the detailed shape of the form factor, $f_{\mathbf{k}}$; for convenience of calculation we choose

$$|f_{\mathbf{k}}|^2 = \Omega^2/(\Omega^2 + c^2 k^2), \quad (15)$$

where Ω is a large cutoff frequency. Then (4) gives, upon passing to the limit of infinite volume V,

$$\tilde{\mu}(\omega) = 2e^2\Omega^2\omega/3c^3(\omega + i\Omega). \quad (16)$$

Note that this is a positive function. It does not show the pole structure on the real axis evoked in the argument of the previous paragraph because in the infinite-volume limit the normal-mode frequencies of the radiation field are continuously distributed. In this

case the real axis becomes a branch cut and the pole of (16) in the lower half-plane is on the "unphysical sheet" reached by analytical continuation through the cut. When (16) is put into (3) one gets

$$\alpha(\omega) = \frac{\omega + i\Omega}{-m\omega^3 - iM\Omega\omega^2 + K(\omega + i\Omega)}, \tag{17}$$

where M is the renormalized electron mass,

$$M = m + 2e^2\Omega/3c^3. \tag{18}$$

The denominator in (17) can be factored to write

$$\alpha(\omega) = \frac{(\omega + i\Omega)}{m(\omega + i\Omega')(\omega_0^2 - \omega^2 - i_{\gamma\omega})}. \tag{19}$$

The point here is that $\alpha(\omega)$ has three poles, all in the lower half-plane in accord with the positivity condition. Equating coefficients in the denominators of (17) and (19), we find the relations

$$\frac{1}{\Omega} = \frac{1}{\Omega'} + \frac{\gamma}{\omega_0^2}, \quad \frac{K}{M} = \frac{\omega_0^2\Omega'}{\Omega' + \gamma},$$

$$\frac{M}{m} = \frac{(\omega_0^2 + \gamma\Omega')(\Omega' + \gamma)}{\omega_0^2\Omega'}. \tag{20}$$

Alternatively, one can view these as expressions for the parameters Ω, K, and M in terms of the parameters Ω', ω_0, and γ which when substituted into (17) give (19).

With the form (19) we see that

$$\text{Im}\left[\frac{d\ln\alpha(\omega)}{d\omega}\right] = \frac{\gamma(\omega_0^2 + \omega^2)}{(\omega^2 - \omega_0^2)^2 + \gamma^2\omega^2} + \frac{\Omega'}{\omega^2 + \Omega'^2} - \frac{\Omega}{\omega^2 + \Omega^2}. \tag{21}$$

When this is put into (5) we can then pass to the limit of large cutoff, assuming $kT/\hbar\Omega \ll 1$. Then using the first of the relations (20) we obtain the following exact expression for the oscillator free energy:

$$F_0(T) = \frac{1}{\pi}\int_0^\infty d\omega\, f(\omega, T)\left[\frac{\gamma(\omega_0^2 + \omega^2)}{(\omega_0^2 - \omega^2)^2 + \omega^2\gamma^2} - \frac{\gamma}{\omega_0^2}\right]. \tag{22}$$

In this result the parameters ω_0 and γ are to be taken in the large-cutoff limit, which from (18) and (20) can be shown to give

$$\omega_0 = (K/M)^{1/2}, \quad \gamma = 2e^2\omega_0^2/3Mc^3. \tag{23}$$

The result (22) can be written

$$F_0(T) = F_0'(T) + \Delta F_0(T), \tag{24}$$

where the first term,

$$F_0'(T) = \frac{1}{\pi}\int_0^\infty d\omega\, f(\omega, T)\frac{\gamma(\omega_0^2 + \omega^2)}{(\omega_0^2 - \omega^2)^2 + \gamma^2\omega^2}, \tag{25}$$

should be recognized as the free energy of an oscillator with natural frequency ω_0 and width γ, and the second term,

$$\Delta F_0(T) = -\frac{\gamma}{\omega_0^2\pi}\int_0^\infty d\omega\, f(\omega, T)$$

$$= \frac{\pi e^2(kT)^2}{9\hbar Mc^3}, \tag{26}$$

is a quantum electrodynamic correction.

The expression (25) is exactly what one would obtain if in (5) one were to use (3) with $\tilde{\mu} = m\gamma$ a constant (the friction constant) and with $K = m\omega_0^2$. In this connection it is instructive to form the corresponding energy, by use of the familiar thermodynamic relation between energy, U, and free energy, F:

$$U = F - T\,\partial F/\partial T. \tag{27}$$

In the weak-coupling limit ($\gamma \to 0$),

$$U_0'(T) \to \hbar\omega_0[\exp(\hbar\omega_0/kT) - 1]^{-1}. \tag{28}$$

This is just the Planck energy of the quantum oscillator. Thus, $F_0'(T)$ corresponds to the Planck energy, including the effect of finite width of the oscillator levels. Therefore, the additional term $\Delta F_0(T)$ is to be interpreted as a temperature-dependent *shift* in free energy of each level. The corresponding energy level shift,

$$\Delta U_0(T) = -\pi e^2(kT)^2/9\hbar Mc^3, \tag{29}$$

is negative. We emphasize that for the oscillator this is an *exact* result. It follows that previous perturbation calculations,[2,3] which when applied to the oscillator lead to a positive energy shift, are not correct as they stand and must be reinterpreted. In a subsequent publication we will show how this can be done in the framework of thermodynamic perturbation theory.

(a)Permanent address: Department of Physics, The University of Michigan, Ann Arbor, Mich. 48109.

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