Quantum thermodynamic functions for an oscillator coupled to a heat bath

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Small systems (of interest in the areas of nanophysics, quantum information, etc.) are particularly vulnerable to environmental effects. Thus, we determine various thermodynamic functions for an oscillator in an arbitrary heat bath at arbitrary temperatures. Explicit results are presented for the most commonly discussed heat bath models: Ohmic, single relaxation time, and blackbody radiation.

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I. INTRODUCTION

Heat bath models are of topical interest especially in areas such as quantum information and nanophysics. Thus, it is important to develop realistic calculations that can be used to make contact with experiments. Here, we wish to examine the effects of a heat bath on various thermodynamic functions such as entropy, partition function, average energy, specific heat, and heat capacity. Our starting point is based on an exact result which we have previously derived for the free energy of an oscillator in an arbitrary heat bath, in terms of a single integral involving the generalized susceptibility[1] arising from the associated quantum Langevin equation.[2] This result was used in a series of papers to obtain free energy shifts of atomic levels in a blackbody radiation field; the effect of a heat bath on the magnetic moment of an electron gas,[3] based on a generalization of our previous work to include a magnetic field; a proof that the third (Nernst's) law of thermodynamics is valid in the presence of a heat bath;[4] and a demonstration that a supposed violation of the second law is only apparent.[5] Thus, because of its wide applicability, we are motivated to systematically develop explicit results for the most commonly discussed heat bath models. Hence, in Sec. II, we review our starting-point Hamiltonian describing an oscillator in an arbitrary heat bath at temperature T which enabled us to obtain the equation of motion of the oscillator in terms of a quantum Langevin equation which, in turn, led us to an exact expression for the free energy of an oscillator in an arbitrary heat bath. Next, we use this general result to consider in detail the most commonly discussed heat bath models, obtaining results for the free energy $F(T)$ which incorporates the Ohmic, single relaxation time, and blackbody radiation models in a form which is very similar for all cases, involving the Stieltjes J function, whose properties we present in the Appendix. This enables us to obtain a simple expression in terms of the J function for the free energy $F(T)$ which incorporates the Ohmic, single relaxation time, and blackbody radiation models. This expression for $F(T)$ is then used to obtain explicit results, both for low temperature and high temperature, for various thermodynamic functions such as the specific heat, the energy, and the heat capacity; these results are presented in Sec. III (for the Ohmic model) and Sec. IV (for the single relaxation and blackbody radiation

models). Results for the $T=0$ case are given in Sec. V. We conclude with a brief summary and discussion in Sec. VI.

II. FREE ENERGY

The most general coupling of a quantum particle coupled to a linear passive heat bath is equivalent to an independent-oscillator model,[1,2] which is described by the Hamiltonian

$$H = \frac{p^2}{2m} + V(x) + \sum_j \left(\frac{p_j^2}{2m_j} + \frac{1}{2} m_j \omega_j^2 (q_j - x)^2 \right). \quad (2.1)$$

Here x and p are the particle coordinate and momentum operators and $V(x)$ is the potential energy of an external force. The jth independent oscillator has coordinate q_j and momentum p_j, and the generality of the model arises from the infinity of oscillators with an arbitrary choice of the mass m_j and frequency ω_j for each.

Use of the Heisenberg equations of motion leads to the quantum Langevin equation

$$m\ddot{x} + \int_{-\infty}^{t} dt' \mu(t - t') \dot{x}(t') + V'(x) = F(t), \quad (2.2)$$

where $\mu(t)$ is the so-called memory function. $F(t)$ is the random (fluctuation or noise) operator force with mean $\langle F(t) \rangle = 0$. The quantities $\mu(t)$ and $F(t)$ describe the properties of the heat bath and are independent of the external force.

In the particular case of an oscillator potential,

$$V(x) = \frac{1}{2} K x^2 = \frac{1}{2} m \omega_0^2 x^2. \quad (2.3)$$

Substituting Eq. (2.3) into Eq. (2.2) enables us to obtain the explicit solution

$$x(t) = \int_{-\infty}^{t} dt' G(t - t') F(t'), \quad (2.4)$$

where G is the Green function. The Green function vanishes for negative times, and its Fourier transform

$$\alpha(\omega) = \int_0^\infty dt e^{i\omega t} G(t) \qquad (2.5)$$

is the familiar response function (generalized susceptibility). This is given by

$$\alpha(z) = \frac{1}{-mz^2 - iz\widetilde{\mu}(z) + K}, \qquad (2.6)$$

where $\widetilde{\mu}(z)$ is the Fourier transform of the memory function:

$$\widetilde{\mu}(z) = \int_0^\infty dt \mu(t) e^{izt}. \qquad (2.7)$$

Note that $\widetilde{\mu}(z)$ and, hence, also $\alpha(z)$ are analytic in the upper half plane.

The system of an oscillator coupled to a heat bath in thermal equilibrium at temperature T has a well-defined free energy. The free energy ascribed to the oscillator, $F(T)$, is given by the free energy of the system minus the free energy of the heat bath in the absence of the oscillator. This calculation was carried out by two different methods[2,6] leading to the "remarkable formula"

$$F(T) = \frac{1}{\pi} \int_0^\infty d\omega f(\omega, T) \text{Im} \left\{ \frac{d \ln \alpha(\omega + i0^+)}{d\omega} \right\}, \qquad (2.8)$$

where $f(\omega, T)$ is the free energy of a single oscillator of frequency ω, given by

$$f(\omega, T) = kT \ln[1 - \exp(-\hbar\omega/kT)]. \qquad (2.9)$$

Here the zero-point contribution ($\hbar\omega/2$) has been omitted, but in the brief section V we remark upon this contribution. We have referred to Eq. (2.8) as a "remarkable formula,"[2,6] in the sense that it displays a nontrivial dependence on the temperature T, in contrast with the corresponding classical formula. We have now all the basic tools at our disposal and we proceed to consider three cases of interest:

$$\widetilde{\mu}(z) = \zeta, \quad \text{Ohmic,}$$

$$\widetilde{\mu}(z) = \frac{\zeta}{1 - iz\tau}, \quad \text{single relaxation time,}$$

$$\widetilde{\mu}(z) = \frac{2e^2 z\Omega^2}{3c^3(z + i\Omega)}, \quad \text{quantum electrodynamics(QED).}$$

$$(2.10)$$

Here ζ is the Ohmic friction constant, while τ is the relaxation time. It is generally assumed that the relaxation time is small in the sense that $\tau \ll \zeta/m$. In the QED case, Ω is a high-frequency cutoff characterizing the electron form factor ($\Omega \to \infty$ corresponds to a point electron). The susceptibility for all three cases may be combined in a single expression

$$\alpha(z) = \frac{z + i\Omega}{-m(z + i\Omega')(z^2 + i\gamma z - \omega_0^2)}. \qquad (2.11)$$

For the single relaxation time model

$$\tau = \frac{1}{\Omega} = \frac{1}{\Omega' + \gamma}, \quad \frac{\zeta}{m} = \gamma \frac{\Omega'^2 + \gamma\Omega' + \omega_0^2}{(\Omega' + \gamma)^2}, \quad \frac{K}{m} = \omega_0^2 \frac{\Omega'}{\Omega' + \gamma}.$$

$$(2.12)$$

The Ohmic model corresponds to the limit of $\Omega' \to \infty$, in which case $\tau \to 0$, $\zeta/m \to \gamma$, and $K/m \to \omega_0^2$. For the QED model,

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

$$\frac{M}{m} = \frac{(\omega_0^2 + \gamma\Omega')(\Omega' + \gamma)}{\omega_0^2 \Omega'}, \qquad (2.13)$$

where m is the bare mass and

$$M = m + \frac{2e^2\Omega}{3c^3} \qquad (2.14)$$

is the renormalized (observed) mass. In this QED case, the limit $\Omega' \to \infty$ corresponds to the largest value of the cutoff Ω consistent with a positive bare mass; that is, in this limit $m = 0$, $K = M\omega_0^2$, and $\Omega = 1/\tau_e$, where

$$\tau_e = \frac{2e^2}{3Mc^3} = 6 \times 10^{-24} \text{ s.} \qquad (2.15)$$

With the general form (2.11) the free energy (2.8) can be written

$$F(T) = \frac{kT}{\pi} \int_0^\infty d\omega \ln(1 - e^{-\hbar\omega/kT}) \left(-\frac{\Omega}{\omega^2 + \Omega^2} + \frac{\Omega'}{\omega^2 + \Omega'^2} \right.$$
$$\left. + \frac{\omega^2 + \omega_0^2}{(\omega^2 - \omega_0^2)^2 + \gamma^2 \omega^2} \right). \qquad (2.16)$$

We use partial fractions in the third term by introducing

$$z_1 = \frac{\gamma}{2} + i\omega_1, \quad z_1^* = \frac{\gamma}{2} - i\omega_1, \quad \omega_1 = \sqrt{\omega_0^2 - \frac{\gamma^2}{4}},$$

$$(2.17)$$

and we note that, for the overdamped case $[(\gamma/2) > \omega_0]$, ω_1 is imaginary, in which case $z_1 = \frac{\gamma}{2} - |\omega_1|$ and $z_1^* = \frac{\gamma}{2} + |\omega_1|$. Hence

$$F(T) = \frac{kT}{\pi} \int_0^\infty d\omega \ln(1 - e^{-\hbar\omega/kT}) \left(-\frac{\Omega}{\omega^2 + \Omega^2} + \frac{\Omega'}{\omega^2 + \Omega'^2} \right.$$
$$\left. + \frac{z_1}{\omega^2 + z_1^2} + \frac{z_1^*}{\omega^2 + z_1^{*2}} \right)$$
$$= kT \left\{ J\left(\frac{\hbar\Omega}{2\pi kT} \right) - J\left(\frac{\hbar\Omega'}{2\pi kT} \right) - J\left(\frac{\hbar z_1}{2\pi kT} \right) - J\left(\frac{\hbar z_1^*}{2\pi kT} \right) \right\},$$

$$(2.18)$$

where $J(z)$ is the Stieltjes J function:

$$J(z) = -\frac{1}{\pi} \int_0^\infty dt \ln(1 - e^{-2\pi t}) \frac{z}{t^2 + z^2}, \quad \text{Im } z > 0.$$

(2.19)

In the next two sections, we consider the three specific models separately and in detail. For this purpose, we make extensive use of the J function, whose properties are discussed in detail in the Appendix.

III. OHMIC MODEL

Here

$$F(T) = -kT\left[J\left(\frac{\hbar z_1}{2\pi kT}\right) + J\left(\frac{\hbar z_1^*}{2\pi kT}\right) \right],$$

(3.1)

where in the expression (2.17) for z_1 and z_1^* we put $\omega_0 = \sqrt{K/m}$ and $\gamma = \zeta/m$.

A. Low-temperature expansion ($kT \ll \hbar\omega_0$)

In the low-temperature case we use the asymptotic expansion (A5) for J. With this we obtain for the free energy

$$F(T) = -\left[\frac{\pi(kT)^2\gamma}{6\hbar\omega_0^2} + \frac{\pi^3(kT)^4\gamma(3\omega_0^2 - \gamma^2)}{45\hbar^3\omega_0^6} \right.$$
$$\left. + \frac{8\pi^5(kT)^6\gamma(5\omega_0^4 - 5\gamma^2\omega_0^2 + \gamma^4)}{315\hbar^5\omega_0^{10}} + \cdots \right].$$ (3.2)

The entropy is

$$S(T) = -\frac{\partial F(T)}{\partial T}$$
$$= k\left[\frac{\pi kT\gamma}{3\hbar\omega_0^2} + \frac{4\pi^3(kT)^3\gamma(3\omega_0^2 - \gamma^2)}{45\hbar^3\omega_0^6} \right.$$
$$\left. + \frac{16\pi^5(kT)^5\gamma(5\omega_0^4 - 5\gamma^2\omega_0^2 + \gamma^4)}{105\hbar^5\omega_0^{10}} + \cdots \right]$$
$$+ \frac{16\pi^5(kT)^6\gamma(5\omega_0^4 - 5\gamma^2\omega_0^2 + \gamma^4)}{105\hbar^5\omega_0^{10}}$$
$$- \frac{8\pi^5(kT)^6\gamma(5\omega_0^4 - 5\gamma^2\omega_0^2 + \gamma^4)}{315\hbar^5\omega_0^{10}}.$$ (3.3)

The energy is

$$U(T) = F + TS$$
$$= \frac{\pi(kT)^2\gamma}{6\hbar\omega_0^2} + \frac{\pi^3(kT)^4\gamma(3\omega_0^2 - \gamma^2)}{15\hbar^3\omega_0^6}$$
$$+ \frac{8\pi^5(kT)^6\gamma(5\omega_0^4 - 5\gamma^2\omega_0^2 + \gamma^4)}{63\hbar^5\omega_0^{10}} + \cdots.$$ (3.4)

The specific heat is

$$C(T) = T\frac{\partial S}{\partial T}$$
$$= k\left[\frac{\pi kT\gamma}{3\hbar\omega_0^2} + \frac{4\pi^3(kT)^3\gamma(3\omega_0^2 - \gamma^2)}{15\hbar^3\omega_0^6} \right.$$
$$\left. + \frac{16\pi^5(kT)^5\gamma(5\omega_0^4 - 5\gamma^2\omega_0^2 + \gamma^4)}{21\hbar^5\omega_0^{10}} + \cdots \right].$$

(3.5)

As a check, we note that the leading term in Eq. (3.2) agrees with the result obtained by us in Ref. 4 while the leading term in Eq. (3.3) agrees with our earlier results[4] as well as a recent result of Hanggi and Ingold.[7] In addition, the first two terms in Eq. (3.5) agree with the results obtained in Ref. 7.

B. High-temperature expansion ($kT \gg \hbar\omega_0$)

In the high-temperature case we use the small argument expansion (A4) for J, with the result

$$F(T) = -kT \ln\frac{kT}{\hbar\omega_0} - \frac{\hbar\gamma}{2\pi} \ln\frac{2\pi kT}{\hbar\omega_0} - \frac{\hbar\omega_1}{\pi}\arccos\frac{\gamma}{2\omega_0}$$
$$- \frac{\hbar\gamma}{2\pi}(1 - \gamma_E) - 2kT\sum_{n=2}^\infty (-)^n \frac{\zeta(n)}{n}\left(\frac{\hbar\omega_0}{2\pi kT}\right)^n$$
$$\times \cos\left(n\arccos\frac{\gamma}{2\omega_0}\right).$$ (3.6)

As a check we consider the uncoupled oscillator. Forming the limit $\gamma \to 0$, we find

$$F(T) \to -kT \ln\frac{kT}{\hbar\omega_0} - \frac{\hbar\omega_0}{2} + kT\sum_{n=1}^\infty \frac{\zeta(2n)}{n}\left(\frac{\hbar\omega_0}{2\pi kT}\right)^{2n}$$
$$= kT \ln(1 - e^{-\hbar\omega_0/kT}),$$ (3.7)

which is the familiar result (2.9) for the uncoupled oscillator. Here we have used the formula[8]

$$\ln(1 - e^{-z}) = \ln z - \frac{1}{2} + \sum_{n=1}^\infty (-)^{n+1}\frac{\zeta(2n)}{n}\left(\frac{z}{2\pi}\right)^n.$$ (3.8)

Returning to the expansion (3.6), we obtain explicit expressions for the first few terms,

$$F(T) = -kT \ln\frac{kT}{\hbar\omega_0} - \frac{\hbar\gamma}{2\pi} \log\frac{2\pi kT}{\hbar\omega_0} - \frac{\hbar\omega_1}{\pi}\arccos\frac{\gamma}{2\omega_0}$$
$$- \frac{\hbar\gamma}{2\pi}(1 - \gamma_E) + \frac{\hbar^2(2\omega_0^2 - \gamma^2)}{48kT} - \frac{\zeta(3)\hbar^3\gamma(3\omega_0^2 - \gamma^2)}{24\pi^3(kT)^2}$$
$$+ \cdots.$$ (3.9)

With this, the entropy, energy, and specific heat are given, respectively, by

$$S(T) = -\frac{\partial F(T)}{\partial T}$$

$$= k\left(\ln\frac{kT}{\hbar\omega_0} + 1\right) + \frac{\hbar\gamma}{2\pi T}$$

$$- 2k\sum_{n=2}^{\infty}(-)^n\frac{(n-1)\zeta(n)}{n}\left(\frac{\hbar\omega_0}{2\pi kT}\right)^n$$

$$\times\cos\left(n\arccos\frac{\gamma}{2\omega_0}\right).$$

$$= k\left(\ln\frac{kT}{\hbar\omega_0} + 1\right) + \frac{\hbar\gamma}{2\pi T} + k\frac{\hbar^2(2\omega_0^2 - \gamma^2)}{48(kT)^2}$$

$$- k\frac{\zeta(3)}{12\pi^3}\frac{\hbar^3\gamma(3\omega_0^2 - \gamma^2)}{(kT)^3}, \tag{3.10}$$

$$U(T) = F + TS$$

$$= kT - \frac{\hbar\gamma}{2\pi}\left(\ln\frac{2\pi kT}{\hbar\omega_0} - \gamma_E\right) - \frac{\hbar\omega_1}{\pi}\arccos\frac{\gamma}{2\omega_0}$$

$$- 2kT\sum_{n=2}^{\infty}(-)^n\zeta(n)\left(\frac{\hbar\omega_0}{2\pi kT}\right)^n\cos\left(n\arccos\frac{\gamma}{2\omega_0}\right)$$

$$= kT - \frac{\hbar\gamma}{2\pi}\left(\ln\frac{2\pi kT}{\hbar\omega_0} - \gamma_E\right) - \frac{\hbar\omega_1}{\pi}\arccos\frac{\gamma}{2\omega_0}$$

$$+ \frac{\hbar^2(2\omega_0^2 - \gamma^2)}{24kT} - \frac{\zeta(3)}{8\pi^3}\frac{\hbar^3\gamma(3\omega_0^2 - \gamma^2)}{(kT)^2}, \tag{3.11}$$

and

$$C(T) = T\frac{\partial S}{\partial T}$$

$$= k - \frac{\hbar\gamma}{2\pi T} + 2k\sum_{n=2}^{\infty}(-)^n(n-1)\zeta(n)$$

$$\times\left(\frac{\hbar\omega_0}{2\pi kT}\right)^n\cos\left(n\arccos\frac{\gamma}{2\omega_0}\right)$$

$$= k - \frac{\hbar\gamma}{2\pi T} - k\frac{\hbar^2(2\omega_0^2 - \gamma^2)}{24(kT)^2} + k\frac{\zeta(3)}{4\pi^3}\frac{\hbar^3\gamma(3\omega_0^2 - \gamma^2)}{(kT)^3}. \tag{3.12}$$

Note that all these results apply to the overdamped case with the prescription

$$\omega_1\arccos\frac{\gamma}{2\omega_0} \rightarrow |\omega_1|\ln\left(\frac{\gamma}{2\omega_0} - \frac{|\omega_1|}{\omega_0}\right).$$

Also, we again have a check in that the first three terms in the specific heat agree with the results obtained in Ref. 7 for the Ohmic model.

IV. SINGLE RELAXATION TIME AND NONRELATIVISTIC QED MODELS

The free energy is now of the general form (2.18), which can be written

$$F(T) = F_{\text{Ohmic}}(T) + kT\left[J\left(\frac{\hbar\Omega}{2\pi kT}\right) - J\left(\frac{\hbar\Omega'}{2\pi kT}\right)\right]. \tag{4.1}$$

We argue that Ω and Ω' will always be large compared with kT, so it is appropriate to use the low-temperature expansion and then only the first term. The result is

$$F(T) = F_{\text{Ohmic}}(T) + \frac{\pi(kT)^2}{6\hbar}\left(\frac{1}{\Omega} - \frac{1}{\Omega'}\right). \tag{4.2}$$

For the single relaxation time case, it is clear from Eqs. (2.12) that the second term in Eq. (4.2) is very small so that the results in this case are essentially the same as for the Ohmic case. However, for the QED case,

$$\frac{1}{\Omega} = \frac{1}{\Omega'} + \frac{\gamma}{\omega_0^2}, \tag{4.3}$$

so

$$F(T) = F_{\text{Ohmic}}(T) + \frac{\pi(kT)^2\gamma}{6\hbar\omega_0^2}. \tag{4.4}$$

A. Low-temperature expansion ($kT \ll \hbar\omega_0$)

The second term in Eq. (4.4) is exactly the negative of the leading term in the low-temperature expansion ($kT \ll \hbar\omega_0$) for the Ohmic case, given in Eq. (3.2). In other words, the T^2 term vanishes and the leading term is the T^4 term. The result is that

$$F_{\text{QED}}(T) = -\left[\frac{\pi^3(kT)^4\gamma(3\omega_0^2 - \gamma^2)}{45\hbar^3\omega_0^6} + \frac{8\pi^5(kT)^6\gamma(5\omega_0^4 - 5\gamma^2\omega_0^2 + \gamma^4)}{315\hbar^5\omega_0^{10}} + \cdots\right], \tag{4.5}$$

$$S_{\text{QED}}(T) = k\left[\frac{4\pi^3(kT)^3\gamma(3\omega_0^2 - \gamma^2)}{45\hbar^3\omega_0^6} + \frac{16\pi^5(kT)^5\gamma(5\omega_0^4 - 5\gamma^2\omega_0^2 + \gamma^4)}{105\hbar^5\omega_0^{10}} \cdots\right], \tag{4.6}$$

$$U_{\text{QED}}(T) = \frac{\pi^3(kT)^4\gamma(3\omega_0^2 - \gamma^2)}{15\hbar^3\omega_0^6} + \frac{8\pi^5(kT)^6\gamma(5\omega_0^4 - 5\gamma^2\omega_0^2 + \gamma^4)}{63\hbar^5\omega_0^{10}} + \cdots, \tag{4.7}$$

and

$$C_{\text{QED}}(T) = k \left[\frac{4\pi^3 (kT)^3 \gamma (3\omega_0^2 - \gamma^2)}{15\hbar^3 \omega_0^6} + \frac{16\pi^5 (kT)^5 \gamma (5\omega_0^4 - 5\gamma^2 \omega_0^2 + \gamma^4)}{21\hbar^5 \omega_0^{10}} + \cdots \right].$$

(4.8)

We note that, in the large cutoff limit,[9] $\gamma = \omega_0^2 \tau_e$, where τ_e is given in Eq. (2.15). In this limit and with $\gamma \ll \omega_0$, we have a check in that the leading terms in the free energy and the entropy agree with the results obtained earlier by us.[4]

B. High-temperature expansion ($kT \gg \hbar\omega_0$)

With the high-temperature expansion (3.9) for F_{Ohmic} we find from the general expression (4.4)

$$F_{QED}(T) = -kT \ln \frac{kT}{\hbar\omega_0} + \frac{\pi (kT)^2 \gamma}{6\hbar\omega_0^2} + \cdots, \qquad (4.9)$$

$$S_{QED}(T) = k \left\{ \left(\ln \frac{kT}{\hbar\omega_0} + 1 \right) - \frac{\pi (kT) \gamma}{3\hbar\omega_0^2} + \cdots \right\}, \quad (4.10)$$

$$U_{QED}(T) = kT - \frac{\pi\gamma}{3\hbar\omega_0^2}(kT)^2 + \cdots, \qquad (4.11)$$

and

$$C_{QED}(T) = k \left\{ \frac{4\pi^3 (kT)^3 \gamma (3\omega_0^2 - \gamma^2)}{15\hbar^3 \omega_0^6} + \cdots \right\}. \quad (4.12)$$

We note that these results agree with the corresponding results in Ref. 1.

V. ZERO-POINT ENERGY

Since $F = U + TS$, the zero-point free energy is always identical with the zero-point energy. The zero-point free energy is obtained by replacing $f(\omega, T) \rightarrow \hbar\omega/2$ in the formula (2.8). The resulting expression diverges for the QED model, whatever the cutoff. For the single relaxation time model it is finite for finite relaxation time,

$$\begin{aligned}
(F)_{\text{zero-point}} &= \frac{\hbar}{2\pi} \int_0^\infty d\omega \left\{ -\frac{\Omega\omega}{\omega^2 + \Omega^2} + \frac{\Omega'\omega}{\omega^2 + \Omega'^2} + \frac{z_1\omega}{\omega^2 + z_1^2} \right. \\
&\quad \left. + \frac{z_1^*\omega}{\omega^2 + z_1^{*2}} \right\} \\
&= \frac{\hbar}{2\pi} \{ \Omega \ln \Omega - \Omega' \ln \Omega' - z_1 \ln z_1 - z_1^* \ln z_1^* \} \\
&= \frac{\hbar}{2\pi} \left\{ \Omega' \ln \frac{\Omega' + \gamma}{\Omega'} + \gamma \ln \frac{\Omega' + \gamma}{\omega_0} \right. \\
&\quad \left. + 2\omega_1 \arccos \frac{\gamma}{2\omega_0} \right\}.
\end{aligned}$$

(5.1)

In the Ohmic limit this is logarithmically divergent,

$$(F)_{\text{zero-point}} \sim \frac{\hbar}{2\pi} \left\{ \gamma (1 - \ln \omega_0 \tau) + 2\omega_1 \arccos \frac{\gamma}{2\omega_0} \right\}.$$

(5.2)

VI. CONCLUSIONS

Motivated by the fact that environmental effects play an important role in many topical areas of physics, where dissipation and fluctuation effects often play a significant role, we have presented an *exact* calculation of quantum thermodynamic functions for an oscillator in an arbitrary heat bath at arbitrary temperatures. Explicit results were obtained for both high and low temperatures. Since we are dealing with *nonadditivity of entropies*,[4] we use a method based on Eq. (2.8), which is an exact result for the free energy of an oscillator which takes into account interaction effects. In the Introduction, we have already given examples of its application.[3–5] However, there are many other possible topics where such results are likely to be applicable. For example, Jordan and Buttiker[10] have demonstrated the relation between entanglement (due to the heat bath) and energy fluctuations and concluded that large entanglement implies large energy fluctuations. Since their work was confined to zero temperature, it would be of interest to extend it to nonzero temperatures. In a similar vein, the decrease of the coherence length of an Aharonov-Bohm-like interferometer due to interaction with the environment was examined but again it was confined to zero temperature.[11]

Finally, we turn to a very different area where thermodynamic considerations play a vital role—i.e., the study of black holes. Following the remarkable results of Bekenstein,[12] there has been continuing interest in developing a microscopic theory for the entropy of a black hole and, in particular, the fact that it depends on the area of the event horizon. As an example, we mention the work of Bombelli *et al.*[13] and Srednicki,[14] where the use of partial traces and reduced density matrices played a crucial role. Since, in general, such techniques lead to results different from those obtained by the method discussed above, we feel that it would be worthwhile to apply our approach to the study of the thermodynamic properties of black holes.

APPENDIX: THE STIELTJES J FUNCTION

The Stieltjes J function is introduced by the integral[15]

$$J(z) = -\frac{1}{\pi} \int_0^\infty dt \ln(1 - e^{-2\pi t}) \frac{z}{z^2 + t^2}, \quad \text{Re}\{z\} > 0.$$

(A1)

The imaginary axis is a "natural boundary" of $J(z)$. That is, the analytic continuation of $J(z)$ into the left half plane is not given by the analytic continuation of the integrand.

This analytic continuation is based on the identity[15]

$$J(z) = \ln[\Gamma(z+1)] - \ln \sqrt{2\pi} - \left(z + \frac{1}{2} \right) \ln(z) + z. \quad (A2)$$

Since $\Gamma(z)$ is analytic in the entire plane except for poles at $z = 0, -1, -2, \ldots$, we can use this form throughout the z plane

cut along the negative real axis. It is then a simple matter to show that the continued J function is given by

$$J(ze^{\pm i\pi}) = -J(z) - \ln(1 - e^{\mp 2\pi iz}), \quad \text{Re}(z) > 0. \quad \text{(A3)}$$

For $|z| < 1$, we have the expansion[14]

$$J(z) = -\ln\sqrt{2\pi} - (z + 1/2)\ln z + z - \gamma_E z + \sum_{n=2}^{\infty} \frac{(-)^n \zeta(n)}{n} z^n, \quad \text{(A4)}$$

where $\gamma_E = 0.577\,215\,7$ is Euler's constant and $\zeta(n)$ is the Riemann zeta function. For large z we have the asymptotic expansion[16]

$$J(z) = \sum_{n=0}^{\infty} \frac{B_{2n+2}}{(2n+1)(2n+2)} \frac{1}{z^{2n+1}}, \quad \text{(A5)}$$

where the Bernoulli numbers are

$$B_2 = \frac{1}{6}, \quad B_4 = -\frac{1}{30}, \quad B_6 = \frac{1}{42}, \quad B_8 = -\frac{1}{30},$$

$$B_{10} = \frac{5}{66}, \quad B_{12} = -\frac{691}{2730}, \quad B_{14} = \frac{7}{6}, \quad B_{16} = -\frac{3617}{510},$$

$$B_{18} = \frac{43867}{798}, \quad B_{20} = -\frac{174611}{330}, \quad B_{22} = \frac{854513}{138}, \quad \dots. \quad \text{(A6)}$$

Very useful for numerical computation is the Lanczos formula[17,18]

$$J(z) = \left(z + \frac{1}{2}\right)\ln\frac{z + \gamma + \frac{1}{2}}{z} - \gamma - \frac{1}{2} + \ln\left\{d_0 + \sum_{n=1}^{N} \frac{d_n}{z + n}\right\}, \quad \text{Re}\, z > 0, \quad \text{(A7)}$$

where, for $N = 6$, $\gamma = 5$, and

$$d_0 = 1.000000000190015, \quad d_1 = 76.18009172947146,$$

$$d_2 = -86.50532032941677, \quad d_3 = 24.01409824083091,$$

$$d_4 = -1.231739572450155, \quad d_5 = 0.001208650973866179,$$

$$d_6 = -0.000005395239384953. \quad \text{(A8)}$$

The numerical error is small (less than 1 part per 10^9) everywhere in the right half plane.

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