Independent Oscillator Model of a Heat Bath: Exact Diagonalization of the Hamiltonian

G. W. Ford,[1] **J. T. Lewis,**[2] **and R. F. O'Connell**[3]

The problem of a quantum oscillator coupled to an independent-oscillator model of a heat bath is discussed. The transformation to normal coordinates is explicitly constructed using the method of Ullersma. With this transformation an alternative derivation of an exact formula for the oscillator free energy is constructed. The various contributions to the oscillator energy are calculated, with the aim of further understanding this formula. Finally, the limitations of linear coupling models, such as that used by Ullersma, are discussed in the form of some critical remarks.

1. INTRODUCTION

In recent publications we have shown that the quantum Langevin equation affords a powerful and physically appealing approach to the problem of an atom in a blackbody radiation field.[1,2] This problem goes back to van Kampen's thesis,[3] where a nonrelativistic atom interacting via dipole coupling with the electromagnetic field was first discussed with modern methods. There, too, he first pointed out that the problem of a har- monically bound electron (oscillator) is exactly soluble and provides an instructive model for real atoms. Some years later, in a classic series of four papers,[4] his student P. Ullersma discussed the general model of an

---

[1] Department of Physics, University of Michigan, Ann Arbor, Michigan 48109-1120.
[2] School of Theoretical Physics, Dublin Institute for Advanced Studies, Dublin 4, Ireland.
[3] Department of Physics and Astronomy, Louisiana State University, Baton Rouge, Louisiana 70803-4001.

oscillator linearly coupled to a bath of independent oscillators. This linear coupling model has the defect that it is unphysical in the sense that for the free particle there is no lower bound on the energy of the system.[2] Ullersma was well aware of this defect and handled it by placing a requirement [ref. 4, p. 33, Eq. (19)] that the oscillator force constant be sufficiently large that the system is physical. Unfortunately, later authors have not always been so careful and the result has been confusion and error in the subsequent literature. Indeed, Ullersma himself, in his application of his results to the oscillator coupled to the radiation field, obtained incorrect results.

Our purpose here is to apply Ullersma's methods to the independent oscillator (IO) model of a heat bath. The point is that this model, in contrast to the linear coupling model, has a lower bound on the energy and is therefore unique and physically correct.[2] In Section 2 we describe this model, find the normal modes, and construct the explicit transformation to normal coordinates. Then, in Section 3 we form the operator Hamiltonian for the system and use the canonical transformation to normal coordinates to obtain a remarkable formula for the oscillator energy, a formula we have obtained earlier by other methods.[1,5] In Section 4 we use this same transformation to calculate the thermal expectation of various contributions to the Hamiltonian for the system, with the aim of understanding the remarkable formula. Finally, in Section 5 we make some concluding remarks.

2. THE IO MODEL

The IO model is a very simple model in which the quantum particle is surrounded by a large (eventually infinite) number of heat bath particles, each attached to it by a spring. The Lagrangian for an oscillator coupled to an IO heat bath with N bath oscillators is therefore

$$L = \tfrac{1}{2}m\dot{x}^2 - \tfrac{1}{2}Kx^2 + \sum_{j=1}^{N} \left[\tfrac{1}{2}m_j\dot{q}_j^2 - \tfrac{1}{2}m_j\omega_j^2(q_j - x)^2 \right] \tag{2.1}$$

This is the Lagrangian for a set of coupled oscillators. According to a well-known theorem of mechanics,[6,7] the potential and kinetic energies for such a system can be simultaneously brought to diagonal form by an orthogonal coordinate transformation. In the remainder of this section we do this explicitly by first finding the normal modes of the system and then constructing the transformation.

2.1. Normal Modes

The equations of motion according to the Lagrangian (2.1) take the form

$$m\ddot{x} + Kx = \sum_{j=1}^{N} m_j \omega_j^2 (q_j - x) \qquad (2.2)$$

$$\ddot{q}_j + \omega_j^2 q_j = \omega_j^2 x \qquad (2.3)$$

We seek normal mode solutions of the form

$$x(t) = X_0(\omega) e^{-i\omega t}; \qquad q_j(t) = X_j(\omega) e^{-i\omega t}, \qquad j = 1, 2,\ldots \qquad (2.4)$$

The equations of motion then become

$$(-m\omega^2 + K) X_0 = \sum_{j=1}^{N} m_j \omega_j^2 (X_j - X_0) \qquad (2.5)$$

$$(-\omega^2 + \omega_j^2) X_j = \omega_j^2 X_0, \qquad j = 1, 2,\ldots \qquad (2.6)$$

It follows from (2.6) that

$$X_j(\omega) = \frac{\omega_j^2}{-\omega^2 + \omega_j^2} X_0(\omega) \qquad (2.7)$$

Putting this in (2.5), that equation becomes

$$\left[-m\omega^2 + K + \sum_{j=1}^{N} m_j \omega_j^2 \frac{\omega^2}{\omega^2 - \omega_j^2} \right] X_0(\omega) = 0 \qquad (2.8)$$

There will therefore be a nontrivial normal mode solution if and only if the quantity in square brackets vanishes for some frequency ω. That is, if and only if

$$m\omega^2 - K = \sum_{j=1}^{N} m_j \omega_j^2 \frac{\omega^2}{\omega^2 - \omega_j^2} \qquad (2.9)$$

The solution of this equation is illustrated in Fig. 1, where the two sides are plotted as functions of ω^2. The abcissae of the points of intersection of the two graphs give the squares of the normal mode frequencies. The following points are worthy of particular attention.

1. The normal mode frequencies are all real, even for a free particle ($K = 0$).

2. The number of distinct normal mode frequencies is one more than the number of distinct bath frequencies. We denote the normal mode frequencies by $\bar{\omega}_r$, $r = 0, 1,..., N$.

3. The normal mode frequencies $\bar{\omega}_r$ interleave the bath frequencies ω_j.

Figure 1 should be contrasted with the corresponding figure in Ullersma's first paper [see Fig. 1 and also Eq. (17) of ref. 4]. The essential difference is that for the linear coupling model there will be an unstable normal mode frequency for a free particle (in Ullersma's notation $m = 1$ and $K = \Omega_0^2$). We repeat that Ullersma was aware of this and imposed a requirement [Eq. (19) of ref. 4] on K such that there be no such unstable modes. However, in the subsequent literature this has led to much confusion.

Before we proceed, it will be useful to introduce some further notation. The (generalized) susceptibility is

$$\alpha(\omega) = \left[-m\omega^2 + K + \sum_{j=1}^{N} m_j \omega_j^2 \frac{\omega^2}{\omega^2 - \omega_j^2} \right]^{-1} \qquad (2.10)$$

This is the Fourier transform of the (retarded) Green function for the oscillator. More precisely, if a term $xf(t)$ is added to the Lagrangian (2.1), then an added term $f(t)$ will appear on the right-hand side of the oscillator
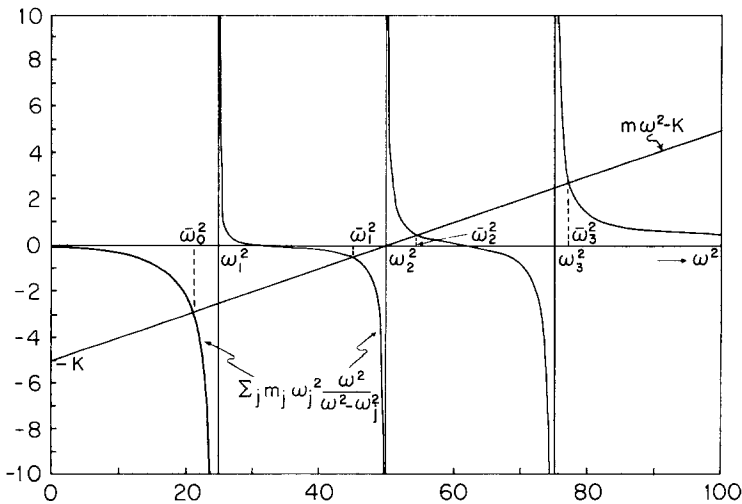

Fig. 1.   Plot of the functions $m\omega^2 - K$ and $\sum_{j=1}^{N} m_j \omega_j^2 [\omega^2/(\omega^2 - \omega_j^2)]$ as functions of ω^2. The abscissae of the points of intersection of the two graphs give the eigenvalues $\bar{\omega}_r^2$ $(r = 0, 1, 2,..., N)$ corresponding to the solutions of $\alpha^{-1}(\omega) = 0$.

equation of motion (2.2). The solution of the resulting equations of motion can be written

$$x(t) = \int_{-\infty}^{t} dt'\, G(t - t')\, f(t') \tag{2.11}$$

where, for $\text{Im}(\omega) > 0$,

$$\alpha(\omega) = \int_{0}^{\infty} dt\, e^{i\omega t} G(t) \tag{2.12}$$

We also write

$$\alpha(\omega) = [-m\omega^2 + K - i\omega\tilde{\mu}(\omega)]^{-1} \tag{2.13}$$

where

$$\tilde{\mu}(\omega) = \sum_{j=1}^{N} m_j \omega_j^2 \frac{i\omega}{\omega^2 - \omega_j^2} \tag{2.14}$$

is the Fourier transform of the memory function occurring in the Langevin equation for the 10 model.[2] It is clear from (2.10) that the bath frequencies $(\omega_j, j = 1, 2,..., N)$ are zeros of $\alpha(\omega)$ and that the normal mode frequencies $(\bar{\omega}_r, r = 0, 1,..., N)$ are poles of $\alpha(\omega)$. That is, we can write

$$\alpha(\omega) = -\frac{1}{m} \prod_{j=1}^{N} (\omega^2 - \omega_j^2) \Big/ \prod_{r=0}^{N} (\omega^2 - \bar{\omega}_r^2) \tag{2.15}$$

It is perhaps worth stressing that the zeros and poles of $\alpha(\omega)$ are all simple; if more than one bath oscillator has the same frequency, this is reflected in an increased strength of the contribution of that frequency to, say, $\tilde{\mu}(\omega)$, not in a multiplicity of the corresponding zero of the susceptibility.

We now construct the matrix of transformation to normal coordinates, introducing

$$X_{0r} \equiv X_0(\bar{\omega}_r) \tag{2.16}$$

and, using (2.7),

$$X_{jr} \equiv X_j(\bar{\omega}_r) = \frac{\omega_j^2}{-\bar{\omega}_r^2 + \omega_j^2} X_{0r}, \qquad j = 1, 2,..., N \tag{2.17}$$

We require the normalization condition

$$mX_{0r}^2 + \sum_{j=1}^{N} m_j X_{jr}^2 = 1, \qquad r = 0, 1,..., N \tag{2.18}$$

It follows that

$$X_{0r}^2 = \left[m + \sum_{j=1}^{N} m_j \omega_j^4 / (\bar{\omega}_r^2 - \omega_j^2)^2 \right]^{-1}$$

$$= -\{ [d\alpha^{-1}(\omega)/d\omega^2]_{\omega = \bar{\omega}_r} \}^{-1} \tag{2.19}$$

Here the second form tells us that $-X_{0r}^2$ is the residue of the pole of $\alpha(z^{1/2})$ at $z = \bar{\omega}_r^2$; we shall find this a useful result. In the sequel it will be convenient to put $m_0 = m$ and to extend the values of the index j to include zero. We can then write the orthogonality relation for the transformation matrix X_{jr} in the form

$$\sum_{j=0}^{N} m_j X_{jr} X_{js} = \delta_{rs}, \qquad r, s = 0, 1, ..., N \tag{2.20}$$

The completeness relation takes the form

$$\sum_{r=0}^{N} X_{jr} X_{kr} = \frac{1}{m_j} \delta_{ij}, \qquad j, k = 0, 1, ..., N \tag{2.21}$$

The orthogonality and completeness relations follow from the general theory,[6,7] but it is straightforward to derive them from the relations we have given. Thus, for $r = s$ the orthogonality relation (2.20) is just the normalization condition (2.18), while for $r \neq s$ we can use (2.17) to write

$$\sum_{j=0}^{N} m_j X_{jr} X_{js} = \left[m + \sum_{j=1}^{N} m_j \frac{\omega_j^4}{(-\bar{\omega}_r^2 + \omega_j^2)(-\bar{\omega}_s^2 + \omega_j^2)} \right] X_{0r} X_{0s}$$

$$= \frac{1}{\bar{\omega}_r^2 - \bar{\omega}_s^2} \left[m\bar{\omega}_r^2 - \sum_{j=1}^{N} m_j \omega_j^2 \frac{\bar{\omega}_r^2}{\bar{\omega}_r^2 - \omega_j^2} \right.$$

$$\left. - m\bar{\omega}_s^2 + \sum_{j=1}^{N} m_j \omega_j^2 \frac{\bar{\omega}_s^2}{\bar{\omega}_s^2 - \omega_j^2} \right] X_{0r} X_{0s}$$

$$= 0, \qquad r \neq s \tag{2.22}$$

Here the second step is a simple identity, while the final step follows from (2.9). The proof of the completeness relation (2.21) is equally straightforward, but we omit it here.

2.2. Transformation to Normal Mode Coordinates

We introduce normal mode coordinates through the relation

$$Q_r = mX_{0r}x + \sum_{j=1}^{N} m_j X_{jr} q_j \tag{2.23}$$

The inverse of this transformation is

$$x = \sum_{r=0}^{N} X_{0r} Q_r, \qquad q_j = \sum_{r=0}^{N} X_{jr} Q_r \qquad (2.24)$$

Putting this in the Lagrangian (2.1), we get

$$L = \tfrac{1}{2} \sum_{r=0}^{N} \sum_{s=0}^{N} \left\{ X_{0r} X_{0s} (m \dot{Q}_r \dot{Q}_s - K Q_r Q_s) \right.$$
$$\left. + \sum_{j=1}^{N} \left[m_j X_{jr} X_{js} \dot{Q}_r \dot{Q}_s - m_j \omega_j^2 (X_{jr} - X_{0r})(X_{js} - X_{0s}) Q_r Q_s \right] \right\} \qquad (2.25)$$

Now we first use (2.17) in the one factor $(X_{jr} - X_{0r})$ in the last term, but not in the other factor $(X_{js} - X_{0s})$, to write

$$(X_{jr} - X_{0r}) = \frac{\bar{\omega}_r^2}{\omega_j^2} X_{jr} \qquad (2.26)$$

With a little rearrangement of the terms, the Lagrangian can then be written in the form (note that the sums over j now extend over $j = 0$):

$$L = \sum_{r=0}^{N} \sum_{s=0}^{N} \left[\left(\sum_{j=0}^{N} m_j X_{jr} X_{js} \right) (\tfrac{1}{2} \dot{Q}_r \dot{Q}_s - \tfrac{1}{2} \bar{\omega}_r^2 Q_r Q_s) \right.$$
$$\left. + \left(-K X_{0r} + \bar{\omega}_r^2 \sum_{j=0}^{N} m_j X_{jr} \right) X_{0s} \right] \qquad (2.27)$$

In the second line, we can again use (2.17) to write

$$-K X_{0r} + \bar{\omega}_r^2 \sum_{j=0}^{N} m_j X_{jr} = \left(-K + m \bar{\omega}_r^2 - \sum_{j=1}^{N} m_j \omega_j^2 \frac{\bar{\omega}_r^2}{\omega_j^2 - \bar{\omega}_r^2} \right) X_{0r} \qquad (2.28)$$

which vanishes on account of (2.9). We can therefore drop the second line in (2.27). In the first line we use the orthogonality relation (2.20) to get the final result:

$$L = \sum_{r=0}^{N} (\tfrac{1}{2} \dot{Q}_r^2 - \tfrac{1}{2} \bar{\omega}_r^2 Q_r^2) \qquad (2.29)$$

This is the Lagrangian for a set of $N + 1$ independent oscillators.

3. THE MEAN ENERGY

The Hamiltonian operator for the oscillator coupled to an IO heat bath is obtained from the Lagrangian (2.1) by standard methods. The result is

$$H = \frac{p^2}{2m} + \frac{1}{2}Kx^2 + \sum_{j=1}^{N}\left[\frac{1}{2m_j}p_j^2 + \frac{1}{2}m_j\omega_j^2(q_j - x)^2\right] \tag{3.1}$$

This is brought to diagonal form by the canonical transformation corresponding to (2.23). That is, one puts

$$Q_r = mX_{0r}x + \sum_{j=1}^{N} m_j X_{jr}q_j, \qquad P_r = X_{0r}p + \sum_{j=1}^{N} X_{jr}p_j \tag{3.2}$$

whose inverse is

$$x = \sum_{r=0}^{N} X_{0r}Q_r, \qquad q_j = \sum_{r=0}^{N} X_{jr}Q_r$$

$$p = m\sum_{r=0}^{N} X_{0r}P_r, \qquad p_j = m_j\sum_{r=0}^{N} X_{jr}P_r \tag{3.3}$$

By an argument identical to that used to obtain the form (2.28) for the Lagrangian, this transformation brings the Hamiltonian (3.1) to the diagonal form

$$H = \sum_{r=0}^{N} (\tfrac{1}{2}P_r^2 + \tfrac{1}{2}\bar\omega_r^2 Q_r^2) \tag{3.4}$$

This is the Hamiltonian for a set of $N+1$ independent oscillators. It follows that, if we define the thermal expectation of an operator $\mathcal{O}$ by

$$\langle \mathcal{O} \rangle = \mathrm{Tr}[\mathcal{O}\exp(-H/kT)]/\mathrm{Tr}[\exp(-H/kT)] \tag{3.5}$$

(here T is the temperature and k is Boltzmann's constant), then

$$\langle Q_r Q_s \rangle = (\hbar/2\bar\omega_r)\coth(\hbar\bar\omega_r/2kT)\,\delta_{rs}$$

$$\langle P_r P_s \rangle = (\hbar\bar\omega_r/2)\coth(\hbar\bar\omega_r/2kT)\,\delta_{rs} \tag{3.6}$$

These are the chief results that will be used in the rest of this paper.

We now turn to the calculation of the oscillator energy at temperature T. First we form $U(T)$, the energy of the system of oscillator coupled to the heat bath. This is just the thermal average of the Hamiltonian (3.1) itself. Using the above results, we see that

$$U(T) \equiv \langle H \rangle = \sum_{r=0}^{N} u(\bar\omega_r, T) \tag{3.7}$$

where $u(\omega, T)$ is the energy, including rest energy, of a single oscillator of frequency ω at temperature T,

$$u(\omega, T) = (\hbar\omega/2) \coth(\hbar\omega/2kT) \tag{3.8}$$

We must compare this with $U_B(T)$, the energy of the heat bath in the absence of the oscillator. The Hamiltonian for this system of bath alone is

$$H_B = \sum_{j=1}^{N} \left(\frac{1}{2m_j} p_j^2 + \frac{1}{2} m_j \omega_j^2 q_j^2 \right) \tag{3.9}$$

Therefore, repeating the argument for this system, we have

$$U_B(T) \equiv \mathrm{Tr}[H_B \exp(-H_B/kT)]/\mathrm{Tr}[\exp(-H_B/kT)]$$

$$= \sum_{j=1}^{N} u(\omega_j, T) \tag{3.10}$$

Now for N large, to leading order, $U(T)$ and $U_B(T)$ are the same. The point is that the frequencies ω_j and the frequencies $\bar{\omega}_r$ interleave and therefore for large N and when they are densely distributed, they have the same distribution. However, if we form the difference

$$U_O(T) = U(T) - U_B(T) \tag{3.11}$$

the leading order cancels and we obtain a finite result. This is the energy we ascribe to the oscillator. It is the energy one would obtain, say, in a *gedanken* experiment in which one measured the difference in weights of the coupled system and the system of bath alone.

For this oscillator energy we have a remarkable formula, which we obtain by the following argument. Using the two expressions (2.19) for X_{0r},[2] we can write the expression (3.7) for $U(T)$ in the form

$$U(T) = -\sum_{r=0}^{N} u(\bar{\omega}_r, T) \left(m + \sum_{j=1}^{N} \frac{m_j \omega_j^4}{(\bar{\omega}_r^2 - \omega_j^2)^2} \right) \left\{ \left[\frac{d\alpha^{-1}(\omega)}{d\omega^2} \right]_{\omega = \bar{\omega}_r} \right\}^{-1} \tag{3.12}$$

As we have noted, this last factor is the residue of the pole of $\alpha(z^{1/2})$ at $z = \bar{\omega}_r^2$. We therefore can use the residue theorem to write

$$U(T) = \frac{1}{2\pi i} \int_{C''} dz \, u(z^{1/2}, T) \left[m + \sum_{j=1}^{N} m_j \omega_j^4/(z - \omega_j^2)^2 \right] \alpha(z^{1/2}) \tag{3.13}$$

Here the contour C'' encloses all the poles of $\alpha(z^{1/2})$ but excludes all other poles of the integrand, as shown in Fig. 2. We now deform the contour into the contour C enclosing all the poles of the integrand on the positive real
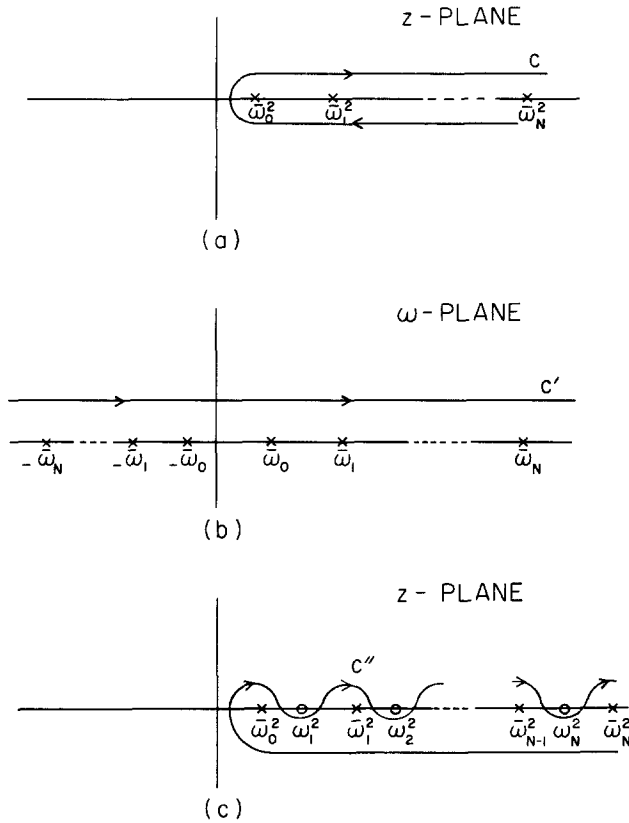
Fig. 2. Illustration of the contours of integration.

axis. In the process we pick up the residues of the integrand at the poles $z = \omega_j^2$, $j = 1, 2, ..., N$. Using the expression (2.10) for $\alpha(\omega)$, we see that the residue of the integrand at $z = \omega_j^2$ is just $-u(\omega_j, T)$. Therefore, we can write

$$U(T) = (1/2\pi i) \int_C dz\, u(z^{1/2}, T) \left[m + \sum_{j=1}^{N} m_j \omega_j^4/(z - \omega_j^2)^2 \right] \alpha(z^{1/2})$$

$$+ \sum_{j=1}^{N} u(\omega_j, T) \tag{3.14}$$

Next we use once again the identity of the two expressions (2.19) to write

$$\left[m + \sum_{j=1}^{N} m_j \omega_j^4/(z - \omega_j^2)^2 \right] \alpha(z^{1/2}) = -\frac{d\alpha^{-1}(z^{1/2})}{dz} \alpha(z^{1/2})$$

$$= \frac{d \ln[\alpha(z^{1/2})]}{dz} \tag{3.15}$$

Using this in the integrand of (3.14) and recognizing the sum as $U_B(T)$, we see that the oscillator energy (3.11) can be written

$$U_O(T) = \frac{1}{2\pi i} \int_C dz\, u(z^{1/2}, T) \frac{d\ln[\alpha(z^{1/2})]}{dz} \tag{3.16}$$

The contour C can now be deformed slightly into a contour completely enclosing the real axis in the z plane. Since there is no singularity of the integrand at $z = 0$, there is no change in the above expression. We now make the change of variable $z = \omega^2$. The contour enclosing the real axis in the z plane becomes a contour just above the real axis in the ω plane. We therefore can write

$$U_O(T) = \frac{1}{2\pi i} \int_{-\infty}^{\infty} d\omega\, u(\omega, T) \frac{d\ln[\alpha(\omega + i0^+)]}{d\omega} \tag{3.17}$$

This formula can be simplified somewhat if we note that $u(\omega, T)$ is an odd function of ω, while $\alpha(\omega + i0^+)$ satisfies the reality condition

$$\alpha(-\omega + i0^+) = \alpha(\omega + i0^+)^* \tag{3.18}$$

Therefore, we may write

$$U_O(T) = \frac{1}{\pi} \int_0^{\infty} d\omega\, u(\omega, T) \,\mathrm{Im}\, \frac{d\ln[\alpha(\omega + i0^+)]}{d\omega} \tag{3.19}$$

This is the remarkable formula for the oscillator energy.

The reason we say this formula is remarkable is that it expresses the oscillator energy, including the energy of interaction with the heat bath, in terms of the oscillator susceptibility alone. Moreover, it stands outside the usual formulas and prescriptions of stochastic processes, which in general are limited to expressions for expectations of functions of the system variables (in our example the oscillator coordinate x) alone. This formula says something about the heat bath. It is an essentially quantum mechanical formula. In the classical limit $(\hbar \to 0)$ the single-oscillator energy $u(\omega, T) \to kT$, and, since the phase of the polarizability $\alpha(\omega + i0^+)$ goes through π as ω goes from $+\infty$ to $-\infty$, we see that $U_O(T) \to kT$. This is just the classical equipartition energy for an oscillator and should be obvious from the beginning, since there is one additional oscillator in the coupled system.

For completeness we give the formula for the oscillator free energy. This is defined to be

$$F_O(T) \equiv F(T) - F_B(T)$$

$$= -kT \ln\{\text{tr}[\exp(-H/kT)]\}$$

$$+ kT \ln\{\text{tr}[\exp(-H_B/kT)]\}$$

$$= \sum_{r=0}^{N} f(\bar{\omega}_r, T) - \sum_{j=1}^{N} f(\omega_j, T) \qquad (3.20)$$

where $f(\omega, T)$ is the free energy of a single oscillator, including zero-point energy,

$$f(\omega, T) = kT \ln[2 \sinh(\hbar\omega/2kT)] \qquad (3.21)$$

The oscillator free energy has the physical interpretation of the work done when at constant temperature the oscillator is coupled to the heat bath. The formula for this free energy, obtained in exactly the same way as that for the energy is

$$F_O(T) = \frac{1}{\pi} \int_0^{\infty} d\omega\, f(\omega, T) \, \text{Im} \frac{d\ln[\alpha(\omega + i0^+)]}{d\omega} \qquad (3.22)$$

Of course, the two formulas are related by the thermodynamic identity

$$U = F - T\, \partial F/\partial T \qquad (3.23)$$

Perhaps, before closing this section, we should remark that a simple, direct proof of this formula for the free energy, based on the form (2.15) for the susceptibility, is given in ref. 1.

4. CONTRIBUTIONS TO THE MEAN ENERGY

Here we evaluate the various contributions to the energy, with the aim of elucidating the remarkable formula (3.19). The Hamiltonian (3.1) can be written

$$H = H_O + H_B + H_{\text{INT}} + R \qquad (4.1)$$

Here H_O is the Hamiltonian for the free oscillator, H_B is the bath Hamiltonian (3.9), H_{INT} is the interaction energy in the linear coupling model used by Ullersma, and R is the remainder (sometimes termed the self-interaction energy),

$$H_O = \frac{p^2}{2m} + \frac{1}{2} Kx^2 = \frac{1}{2} m\dot{x}^2 + \frac{1}{2} Kx^2$$

$$H_{\text{INT}} = -\sum_{j=1}^{N} m_j \omega_j^2 q_j x \qquad (4.2)$$

$$R = \sum_{j=1}^{N} \frac{1}{2} m_j \omega_j^2 x^2$$

The thermal expectation of each of these quantities can be formed using the same method as used in Section 3 to derive the formula for the oscillator energy.

As an illustration, consider the thermal average of the square of the oscillator displacement,

$$\langle x^2 \rangle = \sum_{r=0}^{N} (\hbar/2\bar{\omega}_r) \coth(\hbar\bar{\omega}_r/2kT) \, X_{0r}^2$$

$$= (1/2\pi i) \int_C dz \, (\hbar/2z^{1/2}) \coth(\hbar z^{1/2}/2kT) \, \alpha(z^{1/2}) \qquad (4.3)$$

Here, the first line is obtained using (3.3) and (3.6), while the second line follows from (2.19) and the interpretation of $-X_{0r}^2$ as the residue of $\alpha(z^{1/2})$ at its pole at $z = \bar{\omega}_r^2$. In this integral the contour C is that shown in Fig. 2a. Again, we must deform this contour slightly into a contour completely enclosing the real axis in the z plane. This time there is a contribution, since the integrand has a pole at the origin. On the contour enclosing the real axis we can make the substitution $z = \omega^2$ to get

$$\langle x^2 \rangle = (\hbar/2\pi i) \int_{C'} d\omega \, \coth(\hbar\omega/2kT) \, \alpha(\omega) + kT\alpha(0) \qquad (4.4)$$

Here the added term is the contribution of the pole in the integrand of (4.3) at the origin in the z plane, and the contour C' in the ω plane is that shown in Fig. 2b. We now displace this contour down onto the real axis. In doing this, we use the identity

$$\coth[\hbar(\omega + i0^+)/2kT] = P \coth(\hbar\omega/2kT) - i(2\pi kT/\hbar) \, \delta(\omega) \qquad (4.5)$$

where P denotes principal value. The contribution of the δ-function exactly cancels the added term in (4.4) and we obtain the result

$$\langle x^2 \rangle = (\hbar/2\pi i) P \int_{-\infty}^{\infty} d\omega \, \coth(\hbar\omega/2kT) \, \alpha(\omega) \qquad (4.6)$$

where the principal value prescription is only at the origin. As a final step we use the fact that $P \coth(\hbar\omega/2kT)$ is an odd function of ω, together with the reality condition $\alpha(-\omega + i0^+) = \alpha(\omega + i0^+)^*$, to write

$$\langle x^2 \rangle = (\hbar/\pi) \int_0^{\infty} d\omega \, \coth(\hbar\omega/kT) \, \mathrm{Im}[\alpha(\omega + i0^+)] \qquad (4.7)$$

Here we have dropped the principal value prescription, since $\mathrm{Im}[\alpha(\omega + i0^+)]$, being an odd function of ω, vanishes at $\omega = 0$.

Consider now the thermal expectation of the free-oscillator Hamiltonian. Using the methods illustrated above, we find

$$\langle H_O \rangle = (\hbar/\pi) \int_0^\infty d\omega \, \coth(\hbar\omega/2kT) \tfrac{1}{2}(m\omega^2 + K) \, \text{Im}[\alpha(\omega + i0^+)] \quad (4.8)$$

One might be tempted to identify this expectation with the oscillatory energy, but this would not be correct. We have seen that the oscillator energy $U_O(T)$ given by (3.19) has the physical interpretation of the difference in energy of the system of oscillator coupled to the bath and that of the bath alone. There is no such simple interpretation for $\langle H_O \rangle$. It is instructive to form the difference $U_O - \langle H_O \rangle$. Using (3.19), (4.8), and the expression (2.13) for $\alpha(\omega)$, we find

$$U_O - \langle H_O \rangle = \frac{\hbar}{2\pi} \int_0^\infty d\omega \, \coth\left(\frac{\hbar\omega}{2kT}\right) \text{Re}\left[\omega^2 \alpha(\omega) \frac{d\tilde{\mu}(\omega)}{d\omega}\right] \quad (4.9)$$

We see here that except for the case where the spectrum of the bath oscillators is such that $\tilde{\mu}(\omega)$ is a constant, independent of ω, the expectation of the free-oscillator Hamiltonian will differ from the oscillator energy. This is just the case of Ohmic friction, where $\tilde{\mu}(\omega) = \zeta$, the friction constant.

Next consider the thermal expectation of the remainder term R in (4.1). From the expression (2.14) for $\tilde{\mu}(\omega)$ we see that [recall $1/(x + i0^+) = P(1/x) - i\pi\delta(x)$]

$$\text{Re}[\tilde{\mu}(\omega + i0^+)] = \frac{\pi}{2} \sum_{j=1}^N m_j \omega_j^2 [\delta(\omega - \omega_j) + \delta(\omega + \omega_j)] \quad (4.10)$$

With this we see that we can write

$$\langle R \rangle = \frac{1}{\pi} \int_0^\infty d\omega \, \text{Re}[\tilde{\mu}(\omega + i0^+)]\langle x^2 \rangle \quad (4.11)$$

Since on general grounds we know that $\text{Re}[\tilde{\mu}(\omega + i0^+)]$ must be positive,[2] we see that this quantity can never be zero. It is never correct to neglect it, as is frequently done in discussions based on linear coupling models. Indeed, in the case of Ohmic friction the integral is linearly divergent.

The expectations of the remaining terms in (4.1) can be obtained by the same methods. With a little rearrangement the results can be expressed in terms of the expections we have already obtained. One finds

$$\langle H_B \rangle = U_B + U_O - 3\langle H_O \rangle + 2K\langle x^2 \rangle + \langle R \rangle$$
$$\langle H_{\text{INT}} \rangle = 2\langle H_O \rangle - 2K\langle x^2 \rangle - 2\langle R \rangle \quad (4.12)$$

Note that the expectation of the remainder term, neglected in linear coupling theories, is present in each of these expressions. As we have remarked above, this term is divergent for the case of Ohmic friction, as well as for most physically meaningful cases. When, however, these results are combined to form $U \equiv \langle H \rangle$, this term cancels and we once again obtain

$$U \equiv \langle H \rangle = \langle H_O \rangle + \langle H_B \rangle + \langle H_{\text{INT}} \rangle + \langle R \rangle = U_B + U_O \quad (4.13)$$

as in (3.11). We should emphasize that all four contributions play a role in this check. It would be an error to identify U_O and $\langle H_O \rangle$, except in the case of Ohmic friction. It would be an error to identify U_B and $\langle H_B \rangle$ in any case. Finally, it would be an error to neglect R, since its contribution must delicately cancel among those of the last three terms in (4.1).

5. CONCLUSION

We have used Ullersma's method to explicitly diagonalize the Hamiltonian for the IO model. With this we could give an alternate derivation of the formulas for the oscillator energy and free energy we had previously obtained with other methods. As we have earlier remarked,[2] any linear passive heat bath is equivalent to an IO model, so this is a general result.

With this explicit diagonalization we were able to evaluate the various contributions to the oscillator energy and thus to elucidate the various contributions. In particular, we were critical of the linear coupling model used by Ullersma and, indeed, by a number of earlier authors.[8-11] The basic difficulty with the linear coupling model is that there is no lower bound on the energy. This is a grave defect, since the bath is not passive, meaning that there is no thermal equilibrium state and the second law of thermodynamics is violated.[2] Ullersma was aware of this and attempted to correct the defect with a constraint on the oscillator force constant, but there remains some awkwardness and confusion, as is illustrated in the contrast between our Fig. 1 and the corresponding figure in Ullersma's paper. Another illustration is found in Eq. (17) of ref. 4, which in our notation would read

$$\alpha(\omega) = [-m\omega^2 + K - i\omega\tilde{\mu}_{LC}(\omega)]^{-1} \quad (5.1)$$

where, in place of (2.14),

$$\tilde{\mu}_{LC}(\omega) = \sum_{j=1}^{N} m_j \omega_j^2 \frac{i\omega_j^2}{\omega(\omega^2 - \omega_j^2)} \quad (5.2)$$

As in (4.10), from this we see that

$$\mathrm{Re}[\tilde{\mu}_{LC}(\omega + i0^+)] = \frac{\pi}{2} \sum_{j=1}^{N} m_j \omega_j^2 [\delta(\omega - \omega_j) + \delta(\omega + \omega_j) - 2\delta(\omega)] \quad (5.3)$$

This is obviously not a positive distribution, as is the corresponding quantity (4.10) for the IO model. But we know on the basis of fundamental principles that $\mathrm{Re}[\tilde{\mu}(\omega + i0^+)]$ must be a positive distribution.[2]

This serious defect of the linear coupling models must somehow be repaired. One at times sees this repair effected by a "force constant renormalization,"

$$K \to K + \sum_{j=1}^{N} m_j \omega_j^2 \quad (5.4)$$

This has the effect of replacing the linear coupling model with an IO model, i.e., of replacing the susceptibility (5.3) with the IO susceptibility (2.13). However, this repair is not unique; one can add terms to the linear coupling Hamiltonian so as to get *any* IO model. Surely it is better to start with a physically sensible and unique IO model which has no need of repair.

Finally, we would like to end with some remarks about van Kampen's original problem of the oscillator coupled to the blackbody radiation field, which acts as a heat bath. Here the confusion in the literature has come to the point that it is necessary to point out that the "coupling constant renormalization" discussed above is not the mass renormalization of quantum electrodynamics. We hope that the present paper will help clarify the situation. In any event, in our opinion, van Kampen's original formulation of the problem is still basic to any proper discussion.

ACKNOWLEDGMENTS

REFERENCES

1. G. W. Ford, J. T. Lewis, and R. F. O'Connell, *Phys. Rev. Lett.* **55**:2273 (1985).
2. G. W. Ford, J. T. Lewis, and R. F. O'Connell, *Phys. Rev. A* **38**:4419 (1988).
3. N. G. van Kampen, *K. Dan. Videnskab. Selsk. Mat. Fys. Medd.* **26**(15) (1951).

4. P. Ullersma, *Physica* **32**:27, 56, 74, 90 (1966).
5. G. W. Ford, J. T. Lewis, and R. F. O'Connell, *Ann. Phys. (N.Y.)* **185**:270 (1988).
6. E. T. Whittaker, *Analytical Dynamics*, 4th ed. (Cambridge University Press, Cambridge, 1937), Chapter VII.
7. H. Goldstein, *Classical Mechanics*, 2nd ed. (Addison-Wesley, Reading, Massachusetts, 1980), Chapter 6.
8. V. B. Magalinskij, *Zh. Eksp. Teor. Fiz.* **36**:1942 (1959) [*Sov. Phys. JETP* **9**:1381 (1959)].
9. R. P. Feynman and F. L. Vernon, *Ann. Phys. (N.Y.)* **24**:118 (1963).
10. F. Schwabl and W. Thirring, *Ergeb. Exakt. Naturwiss.* **36**:219 (1964).
11. J. Meixner, in *Statistical Mechanics of Equilibrium and Nonequilibrium*, J. Meixner, ed. (North-Holland, Amsterdam, 1965).