Charged oscillator in a heat bath in the presence of a magnetic field

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We obtain the generalized susceptibility for the motion of a charged oscillator in a harmonic potential well in the presence of a uniform external magnetic field, and linearly coupled to a heat bath, by using the generalized quantum Langevin equation we obtained in an earlier paper. The result is then used to calculate the autocorrelation function of the position operator of the oscillator by the fluctuation-dissipation theorem. The free energy of the oscillator is then obtained in terms of the determinant of the susceptibility matrix. Applications are made to two types of heat baths: the Ohmic case and the case of blackbody radiation. As a special case (no heat bath) of our general formalism, a well-known eigenspectrum result is obtained but in a simple and rather novel fashion.

I. INTRODUCTION

The problem of a charged quantum particle moving in an external magnetic field $\mathbf{B}$ in an arbitrary potential $V(\mathbf{r})$, and linearly coupled to a passive heat bath (consisting of an infinite number of oscillators) has been formulated in terms of the quantum Langevin equation in an earlier paper.[1] The equation takes the form

$$m\ddot{\mathbf{r}}+\int_{-\infty}^{t} dt'\mu(t-t')\dot{\mathbf{r}}(t')+\nabla V(\mathbf{r})-\frac{e}{c}(\dot{\mathbf{r}}\times\mathbf{B})=\mathbf{F}(t)\ , \quad (1.1)$$

where the dot denotes differentiation with respect to t. The influence of the external magnetic field is solely represented by the quantum version of the Lorentz force term and both the operator-valued random force $\mathbf{F}(t)$ and the memory function $\mu(t)$ of the heat bath are unchanged by the magnetic field. In Ref. 1 we did not discuss susceptibilities, position autocorrelation functions, and free energies because their evaluation requires the specification of the potential. Here we discuss such quantities for the important case of a harmonic potential for which an exact analysis is possible.

In Sec. II we consider the problem of the response of the system to an external force $\mathbf{f}(t)$. In the case of a spatial harmonic potential, the problem is shown to be exactly solvable. The coefficient matrix of the response of the system to the perturbation, which is called the generalized susceptibility, plays an important role in determining the dynamics of the system. It is related to the correlation function of the position operator of the charged oscillator by the fluctuation-dissipation theorem. Furthermore, in the absence of the external force, it can be used to calculate the free energy of the oscillator in thermal equilibrium at temperature T, which is defined as the free energy of the system minus the free energy of the heat bath in the absence of the oscillator. The corresponding problem in the absence of a magnetic field has been considered by Ford, Lewis, and O'Connell.[2] They obtained this formula:

$$F_0(T)=\frac{1}{\pi}\int_0^{\infty} d\omega\, f(\omega,T)\mathrm{Im}\left[\frac{d}{d\omega}\ln\alpha^{(0)}(\omega)\right]\ , \quad (1.2)$$

where $f(\omega,T)$ is the free energy of a single oscillator of frequency ω at temperature T and $\alpha^{(0)}(\omega)$ is the scalar susceptibility in the absence of a magnetic field.[2] [It should be noted that, in Refs. 2 and 3, what we now call $\alpha^{(0)}(\omega)$ was referred to as $\alpha(\omega)$. The latter quantity now refers to the matrix of the elements $\alpha_{\rho\omega}(\omega)$ as discussed below.] In the presence of the external magnetic field, we shall show that the same formula holds only with $\alpha^{(0)}(\omega)$ replaced by the determinant of the generalized susceptibility matrix obtained in Sec. II. We will prove this in Sec. III by using the fluctuation-dissipation theorem. In the Appendix we present an alternative proof which is more succinct but perhaps less transparent. As we shall see, similar considerations apply to the case of the energy of the oscillator in thermal equilibrium at temperature T. In Sec. IV, we apply the general formulas obtained in Sec. III to two specific problems: the Ohmic and blackbody radiation heat baths. We shall see explicitly the diamagnetic behavior of the Ohmic heat bath at zero temperature. The blackbody radiation heat-bath problem is shown to be reducible to that of Ohmic heat bath plus a temperature-dependent shift in free energy. In Sec. V, we consider a special case (no heat bath) of our general formalism and obtain a well-known eigenspectrum result, but in a simple and rather novel fashion. Finally, in Sec. VI, we present our conclusions.

II. GENERALIZED SUSCEPTIBILITY FOR A HARMONIC POTENTIAL

In the presence of an external force,[3] the Hamiltonian has an added term $W=-\mathbf{r}\cdot\mathbf{f}(t)$, where $\mathbf{f}(t)$, the generalized force, is a given c-number function of time. This results in an added term $\mathbf{f}(t)$ on the right-hand side of (1.1). Thus, in a uniform external magnetic field and in a spatial harmonic potential well $[V(\mathbf{r})=\frac{1}{2}K\mathbf{r}^2]$, and in the presence of an external force $f(t)$, the generalized quantum Langevin equation takes the form

$$m\ddot{\mathbf{r}}+\int_{-\infty}^{t}dt'\mu(t-t')\dot{\mathbf{r}}(t')-\frac{e}{c}\dot{\mathbf{r}}\times\mathbf{B}+K\mathbf{r}=\mathbf{F}(t)+\mathbf{f}(t)\ , \tag{2.1}$$

which is now a linear differential equation in $\mathbf{r}$. Fourier transforming (2.1), we obtain

$$\left[(-m\omega^2-i\omega\tilde{\mu}+K)\delta_{\rho\sigma}+i\omega\frac{e}{c}\epsilon_{\rho\sigma\eta}B_\eta\right]\tilde{r}_\sigma(\omega)=\tilde{F}_\rho(\omega)+\tilde{f}_\rho(\omega)\ , \tag{2.2}$$

where

$$\tilde{\mu}(\omega)\equiv\int_0^\infty dt\, e^{i\omega t}\mu(t)\ , \tag{2.3}$$

$$\tilde{r}_\sigma(\omega)=\int_{-\infty}^{\infty}dt\, e^{i\omega t}r_\sigma(t)\ , \tag{2.4}$$

and so on, and where $\epsilon_{\rho\sigma\eta}$ is the Levi-Civita symbol, a totally antisymmetric tensor. Throughout this paper the Greek indices stand for three spatial directions (i.e., ρ,σ, etc. $=1,2,3$) and we adopt the Einstein summation convention for repeated Greek indices.

If we denote the matrix in front of $\tilde{r}$ on the left-hand side of (2.2) by $D_{\rho\sigma}(\omega)$ and then solve for its inverse matrix, we get

$$\tilde{r}_\rho(\omega)=\alpha_{\rho\sigma}(\omega)[\tilde{f}_\sigma(\omega)+\tilde{F}_\sigma(\omega)]\ , \tag{2.5}$$

where

$$\alpha_{\rho\sigma}\equiv[D(\omega)^{-1}]_{\rho\sigma}=\left[\lambda^2\delta_{\rho\sigma}-\left[\omega\frac{e}{c}\right]^2B_\rho B_\sigma-\epsilon_{\rho\sigma\eta}B_\eta\lambda i\omega\frac{e}{c}\right]\Big/\det D(\omega)\ , \tag{2.6}$$

with

$$\det D(\omega)=\lambda\left[\lambda^2-\left[\omega\frac{e}{c}\right]^2\mathbf{B}^2\right] \tag{2.7}$$

and

$$\lambda(\omega)=-m\omega^2+K-i\omega\tilde{\mu}(\omega)\equiv[\alpha^{(0)}(\omega)]^{-1}\ . \tag{2.8}$$

Using the fact that $\tilde{\mu}(\omega)^*=\tilde{\mu}(-\omega)$, we deduce that $\alpha_{\rho\sigma}$ given by (2.6) has the following properties:

$$\alpha_{\rho\sigma}(-\omega)=\alpha^*_{\rho\sigma}(\omega)\ , \tag{2.9}$$

$$\alpha_{\rho\sigma}(\omega,\mathbf{B})=\alpha_{\sigma\rho}(\omega,-\mathbf{B})\ . \tag{2.10}$$

Now let us introduce the position autocorrelation functions

$$\psi_{\rho\sigma}(t)\equiv\tfrac{1}{2}\langle r_\rho(t)r_\sigma(0)+r_\sigma(0)r_\rho(t)\rangle=\frac{1}{2\pi}\int_{-\infty}^{\infty}d\omega\, e^{-i\omega t}\tilde{\psi}_{\rho\sigma}(\omega)\ . \tag{2.11}$$

Then, in the case of weak external forces (linear response theory), the Fourier transform $\tilde{\psi}_{\rho\sigma}(\omega)$ is related to $\alpha_{\rho\sigma}(\omega)$ by the fluctuation-dissipation theorem [see (A.14) of Ref. 3]

$$\tilde{\psi}_{\rho\sigma}(\omega)=\frac{\hbar}{2i}\coth\left[\frac{\hbar\omega}{2kT}\right]\times[\alpha_{\rho\sigma}(\omega+i0^+)-\alpha^*_{\sigma\rho}(\omega+i0^+)]\ . \tag{2.12}$$

From (2.6), one can decompose $\alpha_{\rho\sigma}(\omega)$ into symmetric and antisymmetric parts:

$$\alpha_{\rho\sigma}(\omega)=\alpha^s_{\rho\sigma}(\omega)+\alpha^a_{\rho\sigma}(\omega)\ , \tag{2.13}$$

with

$$\alpha^s_{\rho\sigma}(\omega)=\left[\lambda^2\delta_{\rho\sigma}-\left[\omega\frac{e}{c}\right]^2B_\rho B_\sigma\right]\Big/\det D(\omega) \tag{2.14}$$

and

$$\alpha^a_{\rho\sigma}(\omega)=\left[-\epsilon_{\rho\sigma\eta}B_\eta\lambda i\omega\frac{e}{c}\right]\Big/\det D(\omega)\ . \tag{2.15}$$

Thus

$$\begin{aligned}\alpha_{\rho\sigma}(\omega)-\alpha^*_{\sigma\rho}(\omega)&=[\alpha^s_{\rho\sigma}(\omega)-\alpha^s_{\rho\sigma}(\omega)^*]+[\alpha^a_{\rho\sigma}(\omega)+\alpha^a_{\rho\sigma}(\omega)^*]\\&=2i\,\mathrm{Im}\alpha^s_{\rho\sigma}(\omega)+2\,\mathrm{Re}\alpha^a_{\rho\sigma}(\omega)\ .\end{aligned} \tag{2.16}$$

Combining (2.11), (2.12), and (2.16), and noting that $\mathrm{Im}\alpha^s_{\rho\sigma}(\omega)$ is an odd function of ω while $\mathrm{Re}\alpha^a_{\rho\sigma}(\omega)$ is an even function of ω, we have, finally,

$$\begin{aligned}\tfrac{1}{2}\langle r_\rho(t)r_\sigma(t')+r_\sigma(t')r_\rho(t)\rangle=&\frac{\hbar}{\pi}\int_0^\infty d\omega\,\mathrm{Im}[\alpha^s_{\rho\sigma}(\omega+i0^+)]\coth\left[\frac{\hbar\omega}{2kT}\right]\cos[\omega(t-t')]\\&-\frac{\hbar}{\pi}\int_0^\infty d\omega\,\mathrm{Re}[\alpha^a_{\rho\sigma}(\omega+i0^+)]\coth\left[\frac{\hbar\omega}{2kT}\right]\sin[\omega(t-t')]\ .\end{aligned} \tag{2.17}$$

III. FREE ENERGY OF THE OSCILLATOR

The Hamiltonian leading to (2.1) in the case where $\mathbf{f}(t)$ is zero is

$$H_0=\frac{1}{2m}\left[\mathbf{p}-\frac{e}{c}\mathbf{A}\right]^2+\tfrac{1}{2}K\mathbf{r}^2+\sum_j\left[\frac{\mathbf{p}_j^2}{2m_j}+\tfrac{1}{2}m_j\omega_j^2(\mathbf{q}_j-\mathbf{r})^2\right] . \tag{3.1}$$

This is the interacting oscillator (IO) model in the presence of an external magnetic field $\mathbf{B}$, considered in an earlier paper,[1] where e, m, $\mathbf{p}$, and $\mathbf{r}$ are the charge, mass, momentum, and position of the oscillator, respectively, and the corresponding quantities with the lower indices j refer to the jth heat-bath oscillator. The vector potential $\mathbf{A}$ is related to the magnetic field $\mathbf{B}$ through the equation

$$\mathbf{B}(\mathbf{r})=\nabla\times\mathbf{A}(\mathbf{r}) . \tag{3.2}$$

To calculate the mean energy $\langle H_0\rangle$ by the fluctuation-dissipation theorem, we are led, following Ford, Lewis, and O'Connell,[3] to consider the Hamiltonian

$$H=H_0-\mathbf{r}\cdot\mathbf{f}(t)-\sum_j\mathbf{q}_j\cdot\mathbf{f}_j(t) , \tag{3.3}$$

where $\mathbf{f}(t)$ and $\mathbf{f}_j(t)$ are c-number functions of time.

The Heisenberg equations of motion for the charged oscillator from (3.3) are

$$\dot{\mathbf{r}}=[\mathbf{r},H]/i\hbar=\left[\mathbf{p}-\frac{e}{c}\mathbf{A}\right]\Big/m , \tag{3.4}$$

$$\dot{\mathbf{p}}=[\mathbf{p},H]/i\hbar=-K\mathbf{r}+\sum_j m_j\omega_j^2(\mathbf{q}_j-\mathbf{r})+\frac{e}{c}(\dot{\mathbf{r}}\times\mathbf{B})+\frac{e}{c}(\dot{\mathbf{r}}\cdot\nabla)\mathbf{A}+\frac{i\hbar e}{2mc}\nabla(\nabla\cdot\mathbf{A})+\mathbf{f} . \tag{3.5}$$

For the heat-bath oscillators

$$\dot{\mathbf{q}}_j=[\mathbf{q}_j,H]/i\hbar=\mathbf{p}_j/m_j , \tag{3.6}$$

$$\dot{\mathbf{p}}_j=[\mathbf{p}_j,H]/i\hbar=-m_j\omega_j^2(\mathbf{q}_j-\mathbf{r})+\mathbf{f}_j . \tag{3.7}$$

Eliminating the momentum variables, (3.4) and (3.5) combine to give

$$m\ddot{\mathbf{r}}=-K\mathbf{r}+\sum_j m_j\omega_j^2(\mathbf{q}_j-\mathbf{r})+\frac{e}{c}\dot{\mathbf{r}}\times\mathbf{B}+\mathbf{f} . \tag{3.8}$$

Similarly, (3.6) and (3.7) yield

$$m_j\ddot{\mathbf{q}}_j=-m_j\omega_j^2\mathbf{q}_j+m_j\omega_j^2\mathbf{r}+\mathbf{f}_j . \tag{3.9}$$

For a detailed derivation of the Lorentz term $(e/c)(\dot{\mathbf{r}}\times\mathbf{B})$ in (3.8) we refer to Eqs. (7)–(15) of Ref. 1. Note that without $\mathbf{f}$ and $\mathbf{f}_j$, (3.8) and (3.9) are just Eqs. (15) and (5) of Ref. 1, respectively. Using (3.4) and (3.6), and rearranging some terms, (3.1) can be written in the form

$$H_0=\left[\tfrac{1}{2}m\dot{\mathbf{r}}^2+\tfrac{1}{2}\left[K+\sum_j m_j\omega_j^2\right]\mathbf{r}^2\right]+\sum_j(\tfrac{1}{2}m_j\dot{\mathbf{q}}_j^2+\tfrac{1}{2}m_j\omega_j^2\mathbf{q}_j^2)-\sum_j m_j\omega_j^2\mathbf{q}_j\cdot\mathbf{r} . \tag{3.10}$$

We now turn to an evaluation of the ensemble average of H_0, which is the mean energy of the system of the oscillator interacting with the heat bath in thermal equilibrium at temperature T. First, taking Fourier transforms, (3.8) and (3.9) become

$$\left[\delta_{\rho\sigma}\left[-m\omega^2+K+\sum_j m_j\omega_j^2\right]+i\omega\frac{e}{c}\epsilon_{\rho\sigma\eta}B_\eta\right]\tilde{r}_\sigma-\sum_j m_j\omega_j^2\tilde{q}_{j\rho}=\tilde{f}_\rho , \tag{3.11}$$

$$m_j(-\omega^2+\omega_j^2)\tilde{q}_{j\rho}-m_j\omega_j^2\tilde{r}_\rho=\tilde{f}_{j\rho} . \tag{3.12}$$

The solutions of these equations are

$$\tilde{r}_\rho=\alpha_{\rho\sigma}\tilde{f}_\sigma+\sum_j\beta_{j,\rho\sigma}\tilde{f}_{j\sigma} , \tag{3.13}$$

$$\tilde{q}_{j\rho}=\beta_{j,\rho\sigma}\tilde{f}_\sigma+\sum_i\gamma_{ji,\rho\sigma}\tilde{f}_{i\sigma} , \tag{3.14}$$

where $\alpha_{\rho\sigma}(\omega)$, the oscillator susceptibility, is given by (2.6),

$$\beta_{j,\rho\sigma}(\omega)\equiv\frac{\omega_j^2}{-\omega^2+\omega_j^2}\alpha_{\rho\sigma}(\omega) \tag{3.15}$$

is the cross susceptibility, and

$$\gamma_{ji,\rho\sigma}(\omega)\equiv\frac{\omega_i^2\omega_j^2}{(\omega^2-\omega_j^2)(\omega^2-\omega_i^2)}\alpha_{\rho\sigma}(\omega)+\frac{\delta_{ij}\delta_{\rho\sigma}}{m_j(-\omega^2+\omega_j^2)} \tag{3.16}$$

is the heat-bath oscillator susceptibility. Since $\alpha_{\rho\sigma}^a(\omega)=0$ if $\rho=\sigma$, from (2.17) we immediately get

$$\tfrac{1}{2}\langle\mathbf{r}(t)\cdot\mathbf{r}(t')+\mathbf{r}(t')\cdot\mathbf{r}(t)\rangle=\frac{\hbar}{\pi}\int_0^\infty d\omega\,\mathrm{Im}[\alpha_{\rho\rho}(\omega+i0^+)]\times\coth\left[\frac{\hbar\omega}{2kT}\right]\cos[\omega(t-t')] , \tag{3.17}$$

which, of course, is a special case of (2.17). Differentiating with respect to t and t' and then setting t' equal to t, we have

$$\langle\dot{\mathbf{r}}^2\rangle=\frac{\hbar}{\pi}\int_0^\infty d\omega\coth\left[\frac{\hbar\omega}{2kT}\right]\mathrm{Im}[\alpha_{\rho\rho}(\omega+i0^+)]\omega^2 . \tag{3.18}$$

Similar expressions hold for $\langle\mathbf{q}_j^2\rangle$ and $\langle\dot{\mathbf{q}}_j^2\rangle$, with $\alpha_{\rho\rho}$ being replaced by $\gamma_{jj,\rho\rho}$ in (3.17) and (3.18). For $\langle\mathbf{q}_j\cdot\mathbf{r}\rangle$, noting the symmetry of the cross susceptibility $\beta_{j,\rho\sigma}$ in (3.13) and (3.14), we have a similar result with $\beta_{j,\rho\rho}$ replacing $\alpha_{\rho\rho}$:

$$\langle\mathbf{q}_j\cdot\mathbf{r}\rangle=\frac{\hbar}{\pi}\int_0^\infty d\omega\coth\left[\frac{\hbar\omega}{2kT}\right]\mathrm{Im}[\beta_{j,\rho\rho}(\omega+i0^+)] . \tag{3.19}$$

The second group of terms in (3.10) is the Hamiltonian of the heat bath in the absence of the oscillator. We denote it as H_B. Its mean value is given by

$$\begin{aligned}\langle H_B\rangle &= \sum_j \frac{\hbar}{\pi}\int_0^\infty d\omega \coth\left[\frac{\hbar\omega}{2kT}\right]\frac{1}{2}m_j(\omega^2+\omega_j^2)\mathrm{Im}[\gamma_{jj,\rho\rho}(\omega+i0^+)] \\ &= \frac{\hbar}{2\pi}\int_0^\infty d\omega \coth\left[\frac{\hbar\omega}{2kT}\right]\mathrm{Im}\left[\sum_j m_j(\omega^2+\omega_j^2)\left[\frac{\omega_j^4}{(\omega^2-\omega_j^2)^2}\alpha_{\rho\rho}+\frac{3}{m_j(-\omega^2+\omega_j^2)}\right]\right] \\ &= \frac{\hbar}{2\pi}\int_0^\infty d\omega \coth\left[\frac{\hbar\omega}{2kT}\right]\mathrm{Im}\left[\sum_j \frac{m_j(\omega^2+\omega_j^2)\omega_j^4}{(\omega^2-\omega_j^2)^2}\alpha_{\rho\rho}\right] \\ &\quad+\frac{\hbar}{2\pi}\sum_j\int_0^\infty d\omega \coth\left[\frac{\hbar\omega}{2kT}\right]\mathrm{Im}\left\{\frac{3(\omega^2+\omega_j^2)}{\omega+\omega_j}\left[\mathrm{P}\left[\frac{1}{\omega_j-\omega}\right]+i\pi\delta(\omega_j-\omega)\right]\right\} \\ &= \frac{\hbar}{2\pi}\int_0^\infty d\omega \coth\left[\frac{\hbar\omega}{2kT}\right]\mathrm{Im}\left[\sum_j \frac{m_j(\omega^2+\omega_j^2)\omega_j^4}{(\omega^2-\omega_j^2)^2}\alpha_{\rho\rho}\right]+3\sum_j\frac{\hbar\omega_j}{2}\coth\left[\frac{\hbar\omega_j}{2kT}\right]. \end{aligned} \tag{3.20}$$

In the second line, we have used (3.16) to calculate the trace $\gamma_{jj,\rho\rho}$, while the fourth line follows from the identity

$$\frac{1}{\omega-\omega_j+i0^+}=\mathrm{P}\left[\frac{1}{\omega-\omega_j}\right]-i\pi\delta(\omega-\omega_j)\ , \tag{3.21}$$

where P denotes principal value. (Remember that ω in the integral is approached from above the real axis, i.e., $\omega\to\omega+i0^+$.) The last term of (3.20) is readily recognized as the mean energy of the free heat bath in the absence of the oscillator, which we will denote as $U_B(T)$, as in Ref. 3.

Combining the results (3.17)–(3.20) and using (3.10), we find the oscillator energy, which is defined to be the mean energy of the system of the oscillator interacting with the heat bath minus the mean energy of the heat bath in the absence of the oscillator:

$$\begin{aligned}U_0(T,B)\equiv\langle H_0\rangle-U_B(T)&=\frac{\hbar}{\pi}\int_0^\infty d\omega\coth\left[\frac{\hbar\omega}{2kT}\right]\left[\mathrm{Im}(\alpha_{\rho\rho})\frac{1}{2}\left[m\omega^2+K+\sum_j m_j\omega_j^2\right]\right. \\ &\qquad\left.+\frac{1}{2}\sum_j\mathrm{Im}\left[\frac{m_j(\omega^2+\omega_j^2)\omega_j^4}{(\omega^2-\omega_j^2)^2}\alpha_{\rho\rho}\right]-\sum_j m_j\omega_j^2\mathrm{Im}(\beta_{j,\rho\rho})\right] \\ &=\frac{\hbar}{2\pi}\int_0^\infty d\omega\coth\left[\frac{\hbar\omega}{2kT}\right]\mathrm{Im}\left[\alpha_{\rho\rho}\left[m\omega^2+K+\sum_j\frac{\omega^2+\omega_j^2}{(\omega^2-\omega_j^2)^2}\omega^2 m_j\omega_j^2\right]\right].\end{aligned} \tag{3.22}$$

The last equation follows from (3.15).

Since the memory function of the heat bath associated with the Hamiltonian (3.1) is[3]

$$\tilde{\mu}(\omega)=\frac{i}{2}\sum_j m_j\omega_j^2\left[\frac{1}{\omega-\omega_j}+\frac{1}{\omega+\omega_j}\right], \tag{3.23}$$

thus

$$\frac{d\tilde{\mu}}{d\omega}=-i\sum_j m_j\omega_j^2\frac{\omega^2+\omega_j^2}{(\omega^2-\omega_j^2)^2}\ . \tag{3.24}$$

Substituting (3.24) into (3.22), we have

$$U_0(T,B)=\frac{\hbar}{2\pi}\int_0^\infty d\omega\coth\left[\frac{\hbar\omega}{2kT}\right]\mathrm{Im}\left[\alpha_{\rho\rho}\left[m\omega^2+K+i\omega^2\frac{d\tilde{\mu}}{d\omega}\right]\right]. \tag{3.25}$$

This equation can be simplified further. From (2.6), the trace of $\alpha(\omega)$ is

$$\alpha_{\rho\rho}(\omega)=\left[3\lambda^2-\left[\omega\frac{e}{c}\right]^2\mathbf{B}^2\right]\Big/\det D(\omega) \tag{3.26}$$

and, from (2.6) and (2.7), the determinant of $\alpha(\omega)$ is

$$\det\alpha(\omega)=[\det D(\omega)]^{-1}=\left\{\lambda\left[\lambda^2-\left[\omega\frac{e}{c}\right]^2\mathbf{B}^2\right]\right\}^{-1}, \tag{3.27}$$

where [rewriting (2.8) for convenience]

$$\lambda(\omega)=[\alpha^{(0)}(\omega)]^{-1}=-m\omega^2+K-i\omega\tilde{\mu}(\omega)\ . \tag{3.28}$$

Hence

$$\begin{aligned}\omega\frac{d}{d\omega}\{\ln[\det\alpha(\omega)]\}&=-\omega\left\{\frac{d\lambda}{d\omega}\left[3\lambda^2-\left[\omega\frac{e}{c}\right]^2\mathbf{B}^2\right]-2\omega\lambda\left[\frac{e}{c}\right]^2\mathbf{B}^2\right\}\Big/\det D(\omega)\\&=-3+\left[\lambda-\omega\frac{d\lambda}{d\omega}\right]\left[3\lambda^2-\left[\omega\frac{e}{c}\right]^2\mathbf{B}^2\right]\Big/\det D(\omega)\\&=-3+\left[\lambda-\omega\frac{d\lambda}{d\omega}\right]\alpha_{\rho\rho}(\omega)\ .\end{aligned} \tag{3.29}$$

By (3.28)

$$\lambda-\omega\frac{d\lambda}{d\omega}=m\omega^2+K+i\omega^2\frac{d\tilde{\mu}}{d\omega}\ . \tag{3.30}$$

Thus

$$\left[m\omega^2+K+i\omega^2\frac{d\tilde{\mu}}{d\omega}\right]\alpha_{\rho\rho}(\omega)=3+\omega\frac{d}{d\omega}\{\ln[\det\alpha(\omega)]\}\ . \tag{3.31}$$

Substituting (3.31) in (3.25), we finally obtain

$$U_0(T,B)=\frac{1}{\pi}\int_0^\infty d\omega\, u(\omega,T)\mathrm{Im}\left[\frac{d}{d\omega}\ln[\det\alpha(\omega+i0^+)]\right]\ , \tag{3.32}$$

where $u(\omega,T)$ is the Planck energy (including zero-point energy) of a free oscillator of frequency ω:

$$u(\omega,T)\equiv\frac{\hbar\omega}{2}\coth\left[\frac{\hbar\omega}{2kT}\right]\ , \tag{3.33}$$

and $\det\alpha(\omega)$ is given by (3.27) and (3.28). The corresponding formula for the free energy of the oscillator takes the form

$$F_0(T,B)=\frac{1}{\pi}\int_0^\infty d\omega\, f(\omega,T)\mathrm{Im}\left[\frac{d}{d\omega}\ln[\det\alpha(\omega+i0^+)]\right]\ , \tag{3.34}$$

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

$$f(\omega,T)=kT\ln[2\sinh(\hbar\omega/2kT)]\ . \tag{3.35}$$

Equations (3.32) and (3.34) represent extensions, to $B\neq0$, of the "remarkable formulas" given in Ref. 2 for the case $B=0$. It will be noticed that the corresponding results in Ref. 2 [see also (1.2) above] have $\alpha^{(0)}(\omega)$, the scalar susceptibility in the absence of a magnetic field, instead of $\det\alpha(\omega)$. To make the role of the magnetic field more explicit, we now use (3.27) and (3.28) to write

$$\det\alpha(\omega)=[\alpha^{(0)}(\omega)]^3\left[1-\left[\frac{eB\omega}{c}\right]^2[\alpha^{(0)}(\omega)]^2\right]^{-1} \tag{3.36}$$

so that

$$F_0(T,B)=F_0(T,0)+\Delta F_0(T,B)\ , \tag{3.37}$$

where

$$F_0(T,0)=\frac{3}{\pi}\int_0^\infty d\omega\, f(\omega,T)\mathrm{Im}\left[\frac{d}{d\omega}\ln\alpha^{(0)}(\omega)\right] \tag{3.38}$$

is the free energy of the oscillator in the absence of the magnetic field [in agreement with Eq. (5) of Ref. 2, except for the extra factor of 3 which results from our consideration here of three dimensions] and the correction due to the magnetic field is given by

$$\Delta F_0(T,B)=-\frac{1}{\pi}\int_0^\infty d\omega\, f(\omega,T)\mathrm{Im}\left\{\frac{d}{d\omega}\ln\left[1-\left[\frac{eB\omega}{c}\right]^2[\alpha^{(0)}(\omega)]^2\right]\right\}\ , \tag{3.39}$$

where $\alpha^{(0)}(\omega)$ is defined in (2.8). Our basic result (3.34) may also be derived (see the Appendix) using a succinct (but perhaps a less transparent) method, which is a natural generalization of the method given in Ref. 2 for the $B=0$ situation.

IV. OHMIC AND BLACKBODY RADIATION HEAT BATHS

In this section, we will apply the formula derived in Sec. III to two types of heat baths.

A. Ohmic heat bath

In the case of the Ohmic heat bath, $\tilde{\mu}(\omega)=m\gamma$, a constant, which is the simplest memory function one can choose. Thus making use of (3.27) and (3.28), (3.34) becomes

$$F_0(T,B)=\frac{1}{\pi}\int_0^\infty d\omega\, f(\omega,T)\left[\frac{\gamma(\omega^2+\omega_0^2)}{(\omega^2-\omega_0^2)^2+\omega^2\gamma^2}+\frac{\gamma(\omega^2+\omega_0^2)}{(\omega^2-\omega_0^2+\omega_c\omega)^2+\omega^2\gamma^2}+\frac{\gamma(\omega^2+\omega_0^2)}{(\omega^2-\omega_0^2-\omega_c\omega)^2+\omega^2\gamma^2}\right], \tag{4.1}$$

where $\omega_0=(K/m)^{1/2}$. For the internal energy $U_0(T,B)$, we see from a comparison of (3.32) and (3.34) that one need only replace $f(\omega,T)$ in (4.1) by $u(\omega,T)$, which is given by (3.33). In the high-temperature limit

$$u(\omega,T)=\frac{\hbar\omega}{2}\coth\left[\frac{\hbar\omega}{2kT}\right]\to kT\ , \tag{4.2}$$

and, using the method of contour integration, one can show that

$$\begin{aligned}U_0(T,B)&=\frac{kT}{\pi}\int_0^\infty d\omega\left[\frac{\gamma(\omega^2+\omega_0^2)}{(\omega^2-\omega_0^2)^2+\omega^2\gamma^2}+\frac{\gamma(\omega^2+\omega_0^2)}{(\omega^2-\omega_0^2+\omega_c\omega)^2+\omega^2\gamma^2}+\frac{\gamma(\omega^2+\omega_0^2)}{(\omega^2-\omega_0^2-\omega_c\omega)^2+\omega^2\gamma^2}\right]\\&=\begin{cases}3kT & \text{if } \omega_0\neq 0\\ \frac{3}{2}kT & \text{if } \omega_0=0\ .\end{cases}\end{aligned} \tag{4.3}$$

This is classical result, which we note is independent of B.

At $T=0$ K, $f(\omega,T)=u(\omega,T)\to\hbar\omega/2$ and thus both $F_0(0,B)$ and $U_0(0,B)$ are logarithmically divergent. That is due to the contribution of the zero-point energy, which is of no physical significance. However, the difference $\Delta F_0(0,B)=F_0(0,B)-F_0(0,B=0)$ is finite. From (3.39), we have

$$\Delta F_0(0,B)=\frac{\hbar}{2\pi}\int_0^\infty d\omega\,\omega\left[\frac{\gamma(\omega^2+\omega_0^2)}{(\omega^2-\omega_0^2+\omega_c\omega)^2+\omega^2\gamma^2}+\frac{\gamma(\omega^2+\omega_0^2)}{(\omega^2-\omega_0^2-\omega_c\omega)^2+\omega^2\gamma^2}-\frac{2\gamma(\omega^2+\omega_0^2)}{(\omega^2-\omega_0^2)^2+\omega^2\gamma^2}\right], \tag{4.4}$$

which is a function of ω_c^2. This integral can be expressed in closed form:

$$\begin{aligned}\Delta F_0(0,B)=\frac{\hbar}{\pi}\Bigg\{&2\left[\frac{b+a}{2}\right]^{1/2}\tan^{-1}\left[\frac{2}{\gamma}\left[\frac{b+a}{2}\right]^{1/2}\right]-\left[\frac{b-a}{2}\right]^{1/2}\ln\left[\frac{\gamma/2+\sqrt{(b-a)/2}}{\gamma/2-\sqrt{(b-a)/2}}\right]\\&-2\left[\omega_0^2-\frac{\gamma^2}{4}\right]^{1/2}\tan^{-1}\left[\frac{2}{\gamma}\left[\omega_0^2-\frac{\gamma^2}{4}\right]^{1/2}\right]\Bigg\},\end{aligned} \tag{4.5}$$

where

$$b=\left\{\left[\left[\frac{\omega_c}{2}\right]^2+\left[\omega_0+\frac{\gamma}{2}\right]^2\right]\left[\left[\frac{\omega_c}{2}\right]^2+\left[\omega_0-\frac{\gamma}{2}\right]^2\right]\right\}^{1/2}$$

and

$$a=\left[\frac{\omega_c}{2}\right]^2+\omega_0^2-\frac{\gamma^2}{4}\ . \tag{4.6}$$

Taking the derivative of $\Delta F_0(0,B)$ with respect to $(\omega_c/2)^2$ (denoted by z), we get

$$\frac{d}{dz}\Delta F_0(0,B)=\frac{\hbar}{\pi b}\left\{\frac{[(b+a)/2]+\gamma^2/4}{\sqrt{(b+a)/2}}\tan^{-1}\left[\frac{2}{\gamma}\left[\frac{b+a}{2}\right]^{1/2}\right]-\frac{\gamma^2/4-[(b-a)/2]}{2\sqrt{(b-a)/2}}\ln\left[\frac{\gamma/2+\sqrt{(b-a)/2}}{\gamma/2-\sqrt{(b-a)/2}}\right]\right\}. \tag{4.7}$$

By virtue of the inequalities $\tan^{-1}x>x/(1+x^2)$ $(x>0)$ and $\frac{1}{2}\ln[(1+x)/(1-x)]<x/(1-x^2)$ $(0<x<1)$, one can show that

$$\frac{(b+a)/2+\gamma^2/4}{\sqrt{(b+a)/2}}\tan^{-1}\left[\frac{2}{\gamma}\left[\frac{b+a}{2}\right]^{1/2}\right]>\frac{\gamma}{2} \tag{4.8}$$

and

$$\frac{\gamma^2/4-[(b-a)/2]}{2\sqrt{(b-a)/2}}\ln\left[\frac{\gamma/2+\sqrt{(b-a)/2}}{\gamma/2-\sqrt{(b-a)/2}}\right]<\frac{\gamma}{2}\ . \tag{4.9}$$

Hence

$$\frac{d}{dz}\Delta F_0(0,B)>0\ , \tag{4.10}$$

which means that $\Delta F_0(0,B)$ is a monotonically increasing function of ω_c^2. This diamagnetic behavior is what we would expect from the orbital origin of the magnetism (since spin has been neglected).

In the weak-field limit ($B\to 0$), (4.5) can be expanded as a series of ω_c^2:

$$\Delta F_0(0,B)=\begin{cases}\dfrac{\hbar}{2\pi}\left[\dfrac{2\omega_0^2}{(\omega_0^2-\gamma^2/4)^{1/2}}\tan^{-1}\left[\dfrac{2}{\gamma}(\omega_0^2-\gamma^2/4)^{1/2}\right]-\gamma\right]\dfrac{(\omega_c/2)^2}{\omega_0^2-(\gamma^2/4)} & \text{if } \omega_c^2\ll\left|\omega_0^2-\dfrac{\gamma^2}{4}\right| \\ \dfrac{\hbar}{3\pi\gamma}\omega_c^2 \quad \text{if } \omega_0=\dfrac{\gamma}{2}\ . \end{cases} \tag{4.11}$$

The omitted terms are of order of ω_c^4. In both (4.5) and (4.11), $2(\omega_0^2-\gamma^2/4)^{1/2}\tan^{-1}[(2/\gamma)(\omega_0^2-\gamma^2/4)^{1/2}]$ should be replaced by

$$-\left[\frac{\gamma^2}{4}-\omega_0^2\right]^{1/2}\ln\left[\frac{\gamma/2+(\gamma^2/4-\omega_0^2)^{1/2}}{\gamma/2-(\gamma^2/4-\omega_0^2)^{1/2}}\right]$$

when $\omega_0<\gamma/2$. This is due to the identity

$$\tan^{-1}(ix)=\frac{i}{2}\ln|(1+x)/(1-x)|\ .$$

We note that the coefficients in front of ω_c^2 in (4.11) are positive because of the inequalities in (4.8) with $\omega_c=0$. As a final comment, we note that no mass renormalization is necessary, in contrast to what we will find in the next example.

B. Blackbody radiation heat bath

In this case, the associated memory function is[2]

$$\tilde{\mu}(\omega)=2e^2\Omega^2\omega/3c^3(\omega+i\Omega)\ , \tag{4.12}$$

where Ω is a cutoff frequency.

Thus

$$\begin{aligned}\lambda\pm\frac{eB\omega}{c}&=-m\omega^2+K-i\omega\tilde{\mu}\pm\frac{eB\omega}{c}\\ &=\frac{m}{\omega+i\Omega}\left[-\omega^3-\left[i\frac{\Omega M}{m}\mp\frac{eB}{mc}\right]\omega^2\right.\\ &\qquad\left.+\left[\frac{K}{m}\pm i\frac{eB}{mc}\Omega\right]\omega+i\frac{\Omega K}{m}\right]\ ,\end{aligned} \tag{4.13}$$

where

$$M=m+2e^2\Omega/3c^3 \tag{4.14}$$

is the renormalized mass. In the limit of large cutoff ($\Omega\to\infty$ and $m\to 0$), the numerator in (4.13) can be factored to give

$$\lambda\pm\frac{eB\omega}{c}=\frac{m}{m+i\Omega}\left[\omega+i\frac{\Omega M}{m}\right][-\omega^2+\omega_0^2\mp i\omega_c\tau_e\omega_0^2 -i\tau_e(\omega_c^2+\omega_0^2)\omega\pm\omega_c\omega]\ , \tag{4.15}$$

where $\omega_0^2=K/M$, $\omega_c=eB/Mc$, and $\tau_e=2e^2/3Mc^3\simeq 6\times 10^{-24}$ sec. Because $\omega_c=1.76\times 10^{11}$ ($B/10^4$ G) Hz and the atomic unit of frequency is 4×10^{16}, we see that typically

$$\tau_e\omega_c\ll 1,\quad \tau_e\omega_0\ll 1\ . \tag{4.16}$$

Also, if we assume that $\omega_c\ll\omega_0$, then (4.15) can be simplified to

$$\lambda\pm\frac{eB\omega}{c}=\frac{M}{1-i\tau_e\omega}(-\omega^2+\omega_0^2-i\omega\tau_e\omega_0^2\pm\omega_c\omega)\ . \tag{4.17}$$

Thus

$$\begin{aligned}\det\alpha(\omega)&=\frac{1}{\lambda[\lambda^2-(\omega e/c)^2B^2]}\\ &=\frac{1-i\tau_e\omega}{M(-\omega^2+\omega_0^2-i\omega\tau_e\omega_0^2)}\\ &\quad\times\frac{1-i\tau_e\omega}{M(-\omega^2+\omega_0^2-i\omega\tau_e\omega_0^2+\omega_c\omega)}\\ &\quad\times\frac{1-i\tau_e\omega}{M(-\omega^2+\omega_0^2-i\omega\tau_e\omega_0^2-\omega_c\omega)}\ .\end{aligned} \tag{4.18}$$

Substituting (4.18) into (3.34) and using (4.16), as well as the fact that $\hbar\tau_e^{-1}\gg kT$, we obtain the expression for the oscillator free energy

$$F_0(T,B)=\frac{1}{\pi}\int_0^\infty d\omega\, f(\omega,T)\left[\frac{\gamma(\omega^2+\omega_0^2)}{(\omega^2-\omega_0^2)^2+\omega^2\gamma^2}+\frac{\gamma(\omega^2+\omega_0^2)}{(\omega^2-\omega_0^2+\omega_c\omega)^2+\omega^2\gamma^2}+\frac{\gamma(\omega^2+\omega_0^2)}{(\omega^2-\omega_0^2-\omega_c\omega)^2+\omega^2\gamma^2}\right]+\frac{\pi e^2(kT)^2}{3\hbar Mc^3}\ , \qquad (4.19)$$

where $\gamma=\omega_0^2\tau_e$. The first term corresponds to the result given in (4.1) for the case of $\tilde{\mu}(\omega)=m\gamma$. The second term is the familiar temperature dependent shift,[2] which is independent of the magnetic field.

V. ABSENCE OF A HEAT BATH

The limit of no dissipation (no heat bath) is simply obtained by taking $\tilde{\mu}(\omega)=0$. Thus writing $K\equiv m\omega_0^2$, we see from (3.28) that

$$\lambda(\omega)=[\alpha^{(0)}(\omega)]^{-1}\to -m(\omega^2-\omega_0^2) \qquad (5.1)$$

and

$$\left[1-\left[\frac{eB\omega}{c}\right]^2[\alpha^{(0)}(\omega)]^2\right]\to\frac{1}{(\omega^2-\omega_0^2)^2}[(\omega^2-\omega_0^2)^2-(\omega\omega_c)^2]\ , \qquad (5.2)$$

where

$$\omega_c=eB/mc \qquad (5.3)$$

is the cyclotron frequency. These results, when substituted into (3.38) and (3.39), lead to

$$F_0(T,0)=3f(\omega_0,T) \qquad (5.4)$$

and

$$\Delta F_0(T,B)=f(\omega_1,T)+f(\omega_2,T)-2f(\omega_0,T)\ , \qquad (5.5)$$

where

$$\omega_{1,2}=\pm(\omega_c/2)+[(\omega_c/2)^2+\omega_0^2]^{1/2}\ , \qquad (5.6)$$

and $f(\omega,T)$ is given by (3.35). Hence, from (3.37),

$$F_0(T,B)=\sum_{i=0,1,2}f(\omega_i,T)\ . \qquad (5.7)$$

Similarly

$$U_0(T,B)=\sum_{i=0,1,2}u(\omega_i,T)\ , \qquad (5.8)$$

where $u(\omega,T)$ is given by (3.33). It immediately follows that the eigenspectrum of a charged oscillator in a magnetic field is given by

$$E=\sum_{i=0,1,2}\hbar\omega_i(n_i+\tfrac{1}{2})\quad\text{where } n_i=0,1,2.\ .\ .\ . \qquad (5.9)$$

This is a well-known result,[4] but it is interesting that we have obtained it in a rather novel fashion as a special case of our general formalism.

In fact, an even simpler derivation of (5.9) follows from the fact (see the Appendix) that the poles of $\alpha(\omega)$ occur for ω values equal to the normal mode frequencies of the interacting system (ϖ_j say). Hence from (3.27), we have

$$\lambda(\varpi_j)[\lambda^2(\varpi_j)-(m\varpi_j\omega_c)^2]=0\ . \qquad (5.10)$$

In the case where $\tilde{\mu}(\omega)=0$, we have from (3.28) that

$$\lambda(\varpi_j)=m(\omega_0^2-\varpi_j^2)\ . \qquad (5.11)$$

Thus (5.10) and (5.11) imply ϖ_j values equal to ω_0, ω_1, and ω_2 as before, so that Eqs. (5.7)–(5.9) again follow.

VI. CONCLUSIONS

We have shown that the problem of a charged oscillator moving in a harmonic potential well and an uniform external magnetic field, and coupled to an arbitrary physical heat bath can be solved exactly using the generalized quantum Langevin equation. The free energy (3.34) together with the explicit expression for $\det\alpha(\omega)$, given in (3.27) and (3.28), can in principle determine all the relevant quantities of the problem.

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APPENDIX: ALTERNATIVE DERIVATION OF EQ. (3.34)

Our method is a generalization of the method given in Ref. 2 for the case of zero magnetic field. We start with Eq. (2.5) in the absence of an external field:

$$\tilde{r}_\rho(\omega)=\alpha_{\rho\sigma}(\omega)\tilde{F}_\sigma(\omega)\ . \qquad (A1)$$

Thus the necessary and sufficient condition that there be a fluctuating force in the absence of a displacement $[\tilde{r}(\omega)=0]$ is that

$$\det\alpha(\omega)=0\ . \qquad (A2)$$

It follows that the zeros of $\det\alpha(\omega)$ occur for ω values equal to the normal-mode frequencies of the radiation field in the absence of the oscillator (ω_i say). In a similar manner, we note that if we invert (A1) to write

$$[\alpha(\omega)^{-1}]_{\rho\sigma}\tilde{r}_\sigma(\omega)=\tilde{F}_\rho(\omega)\ , \qquad (A3)$$

then it follows that there can be a nonzero displacement with no force $[\tilde{F}_\sigma(\omega)=0]$ if

$$\det\alpha(\omega)^{-1}=1/\det\alpha(\omega)=0 \ . \tag{A4}$$

Hence the poles of $\det\alpha(\omega)$ occur for ω values equal to the normal-mode frequencies of the interacting system ($\overline{\omega}_j$ say). Therefore one can write

$$\det\alpha(\omega)\propto \prod_i(\omega^2-\omega_i^2)\Big/\prod_j(\omega^2-\overline{\omega}_j^2), \quad \mathrm{Im}\omega>0 \ . \tag{A5}$$

Now, recalling the identity

$$\frac{1}{x+i0^+}=P\left[\frac{1}{x}\right]-i\pi\delta(x) \ , \tag{A6}$$

we see that

$$\pi^{-1}\mathrm{Im}[d\ln\det\alpha(\omega)/d\omega] =\sum_j[\delta(\omega-\overline{\omega}_j)+\delta(\omega+\overline{\omega}_j)] -\sum_j[\delta(\omega-\omega_j)+\delta(\omega+\omega_j)] \ . \tag{A7}$$

When this is put into (3.34), the result can be written as

$$F_0(T)=\sum_j f(\overline{\omega}_j,T)-\sum_i f(\omega_i,T) \ , \tag{A8}$$

which is precisely the definition of the free energy of the oscillator, where the first sum on the right-hand side of (A8) is clearly the free energy of the interacting system and the second is that of the free field. This demonstrates the correctness of (3.34).

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