

Frequency Shifts and Master Equations for a Quantum Oscillator Coupled to a Reservoir

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Received April 14, 1998

For a quantum oscillator coupled to a reservoir, master equations obtained under the assumptions of weak coupling and use of a rotating-wave Hamiltonian (RWA) are known to give incorrect frequency shifts. Here, we show that a calculation which does not invoke the RWA gives results for the frequency shifts, which agree with exact results for Lamb-type (temperature $T=0$) shifts. However, for non-zero T , we point out that, in general, corresponding energy and free energy shifts for the system require exact treatments since off-resonant contributions (which are automatically excluded in weak coupling calculations) are important in the case of super-Ohmic reservoirs. © 1998 Academic Press

Master equations are pervasive in many areas of physics, particularly quantum optics. They give information, primarily, on the time dependence of the reduced density matrix but they also give information on energy shifts (i.e., Lamb-type shifts). Most derivations in the literature assume (a) weak coupling and (b) the rotating-wave approximation (RWA) but it is well-known that the energy shifts resulting from these calculations are not correct. In particular, Ackerhalt *et al.* [1], among others, have correctly pointed out that counter-rotating terms (which are dropped in the RWA) make a major contribution to the Lamb shift.

Recently, we have derived a master equation for an oscillator coupled to a very general dissipative environment (in particular, the electromagnetic field) without using the RWA [2]. As expected, the frequency shifts are different from the usual RWA results but the question still remains as to whether or not they are correct. This question can be answered by virtue of the fact that we have previously calculated the exact energy shift for the problem [3] and it is our purpose here to compare the various results.

The second-order master equation which we obtained [2] is the general form for any linear passive dissipation. It also has the *form* of the RWA master equation except that we have explicit expressions for the decay rate and the shift, ΔH_0 , in the free oscillator Hamiltonian, both of which are completely characterized by the spectral distribution $\text{Re } \tilde{\mu}(\omega + i0^+)$. Also $\tilde{\mu}(\omega)$ is the Fourier transform of $\mu(t)$, which appears in the corresponding generalized quantum Langevin equation for the coordinate operator. Explicitly, the decay rate is given by

$$\gamma(\omega_0) = \frac{1}{m} \text{Re } \tilde{\mu}(\omega_0 + i0^+), \quad (1)$$

and the oscillator frequency shift (corresponding to ΔH_0) by

$$\Delta\omega_0 = \frac{\omega_0}{\pi m} P \int_0^\infty d\omega \frac{\text{Re } \tilde{\mu}(\omega + i0^+)}{\omega_0^2 - \omega^2}, \quad (2)$$

where ω_0 is the oscillator frequency. Now, as we have already noted [4], $\tilde{\mu}(z)$ is analytic in the upper half-plane, it is a positive even function on the real axis and thus obeys the Stieltjes inversion theorem (essentially the Kramers–Kronig relation with at most one subtraction and the latter can be absorbed into the particle mass) so that we obtain

$$\Delta\omega_0 = \frac{1}{2m} \text{Im } \tilde{\mu}(\omega_0). \quad (3)$$

Such a strikingly simple result demands an insightful interpretation which can be gleaned by considering the expression for the generalized susceptibility $\alpha(\omega)$, a quantity which is fundamental for the calculation of all physical properties of an oscillator in a dissipative environment. In general [3, 4],

$$\begin{aligned} \alpha(\omega) &= -\{m(\omega^2 - \omega_0^2) + i\omega\tilde{\mu}(\omega)\}^{-1} \\ &= -\{m(\omega^2 - \omega_0^2) - \omega \text{Im } \tilde{\mu}(\omega) + i\omega \text{Re } \tilde{\mu}(\omega)\}^{-1}, \end{aligned} \quad (4)$$

so that

$$|\alpha(\omega)|^2 = \left\{ m^2 \left(\omega^2 - \omega_0^2 - \frac{\omega}{m} \text{Im } \tilde{\mu}(\omega) \right)^2 + (\omega \text{Re } \tilde{\mu}(\omega))^2 \right\}^{-1}. \quad (5)$$

In the weak coupling limit, which corresponds to $\text{Re } \tilde{\mu}(\omega)$, $\text{Im } \tilde{\mu}(\omega) \ll m\omega_0$, we see that $\text{Im } \alpha(\omega)$ or $|\alpha(\omega)|^2$, quantities involved in the calculation of correlation functions, energy shifts, etc., have poles at

$$\omega^2 - \omega_0^2 - \frac{\omega}{m} \text{Im } \tilde{\mu}(\omega) = 0, \quad (6)$$

and a width given to lowest order ($\omega = \omega_0$) by $(1/m) \text{Re } \tilde{\mu}(\omega_0)$.

Thus, to first order in weak coupling, we see from (6) that a pole occurs if

$$2m\omega(\omega - \omega_0) = \omega \operatorname{Im} \tilde{\mu}(\omega_0), \quad (7)$$

so that

$$\omega - \omega_0 = \frac{1}{2m} \operatorname{Im} \tilde{\mu}(\omega_0), \quad (8)$$

which is the same as (3) above. In other words, the frequency shift arising from the master equation approach (without invoking the RWA) is precisely the shift in the resonance frequency.

In the case of constant friction ($\tilde{\mu}(\omega) = m\gamma = \text{constant}$, so that $\operatorname{Im} \tilde{\mu}(\omega) = 0$), the so-called Ohmic model, we obtain a zero frequency shift (in contrast to the non-zero result found by use of the RWA [5]). This is consistent with a Bethe-type non-relativistic calculation of the Lamb shift for the oscillator [6]. In the case of the oscillator in a radiation field, we found [2] that the decay rate is again frequency independent leading again to a zero frequency shift.

Next, we address the question as to what happens with $T \neq 0$. As we have previously emphasized [7], when the interaction between the oscillator and field is included, so that the system is described by the full Hamiltonian, the spectrum (aside from the ground state) becomes purely continuous, no matter how weak the interaction. One says that the discrete eigenvalues at the excited atomic energy levels have been “absorbed” by the continuum. In their place are only local peaks in the density of continuum states. One can, however, introduce “pseudoeigenvalues” (associated with these peaks) which have both real and imaginary parts. However, since we are dealing with a thermodynamic system, the best way to proceed is to calculate the free energy due to the interaction [3] and we recall the familiar relation between free energy F , energy U , and entropy S ,

$$F = U - TS. \quad (9)$$

At zero temperature, free energy and energy are the same, but at finite temperature they are different. In particular, for our system there should be a contribution to the entropy arising from the population distribution over the *continuum* of energy levels.

The overall result [3] is that temperature-dependent shifts in both energy and free energy occur, which arise from off-resonant contributions, which are especially important for super-Ohmic reservoirs ($\operatorname{Re} \tilde{\mu}(\omega) \sim \omega^a$, where $a > 0$), such as the radiation reservoir ($\operatorname{Re} \tilde{\mu}(\omega) \sim \omega^2$). Such off-resonant contributions do not appear in weak coupling calculations. In summary, these T -dependent shifts do not result from a shift in the pseudoeigenvalues but rather represent a contribution from the background. This is made manifest by the fact that the T -dependent shifts do not depend on the oscillator frequency.

ACKNOWLEDGMENT

This work of R.F.O'C was supported in part by the U.S. Army Research Office under Grant DAAH04-94-G0333.

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