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04/09/2026

Damped simple harmonic oscillator in quantum mechanics

Here we follow closely the first 16 pages of *Statistical Methods in Quantum Optics* by H. J. Carmichael to write an equation that describes the time dependence a simple harmonic oscillator coupled to a heat bath. Following Carmichael we will assume that this coupling is weak so that the time scale for the effects on the oscillator is large compared to its period and the time scale $\hbar/(kT)$ of the heat bath where T is the temperatur of the heat bath.

1 Formulation using second-order time-dependent perturbation theory

We first consider a general self-contain quantum mechanics problem of a combined "system" and "reservior" described a Hamiltonian H that is the sum of three operators:

$$H = H_S + H_R + H_{RS} \tag{1}$$

where H_S and H_R depend only on system and reservoirvariables respectively while H_{RS} couple the system and reservoirand is assumed to be small. We treat the sum $H_0 = H_S + H_R$ as the unperturbed Hamiltonian and H_{SR} as the perturbation and work in the interaction picture in which the time dependence generated by H_0 is removed from the states and instead included by working with time-dependent operators: $\widetilde{O}(t) = e^{+iH_0t/\hbar}Oe^{-iH_0t/\hbar}$ where the tilde indicates an operator expressed in the interaction picture. If χ is the density matrix for the combined system+reservoirthen in this interaction picture it will obey the Schrodinger equation

$$\dot{\widetilde{\chi}}(t) = -\frac{i}{\hbar}\left[\widetilde{H}_{SR}(t), \widetilde{\chi}(t)\right]. \tag{2}$$

Similar to the Wigner-Weiskopt treatment of unstable particle decay, the "Lindblad" treatment of this problem writes an exact time-dependent equation, to which some second-order perturbation theory approximations are made, which is then solved "exactly". This exact equation is written by integrating Eq. (2) to obtain:

$$\widetilde{\chi}(t) = \widetilde{\chi}(0) - \frac{i}{\hbar}\int_0^t dt' \left[\widetilde{H}_{SR}(t'), \widetilde{\chi}(t')\right] \tag{3}$$

and then substituting that equation back into Eq. (2):

$$\dot{\widetilde{\chi}}(t) = \left[\widetilde{H}_{SR}(t), \widetilde{\chi}(0)\right] - \frac{1}{\hbar}\left[\widetilde{H}_{SR}(t), \int_0^t dt' \left[\widetilde{H}_{SR}(t'), \widetilde{\chi}(t')\right]\right]. \tag{4}$$

This equation is then simplified to an equation for the reduced density matrix $\rho(t) = \mathrm{Tr}_R\{\chi(t)\}$.

$$\dot{\widetilde{\rho}}(t) = \mathrm{Tr}_R\left[\widetilde{H}_{SR}(t), \widetilde{\chi}(0)\right] - \frac{1}{\hbar^2}\mathrm{Tr}_R\left\{\int_0^t dt' \left[\widetilde{H}_{SR}(t), \left[\widetilde{H}_{SR}(t'), \widetilde{\chi}(t')\right]\right]\right\}. \tag{5}$$

Before simplyfying Eq. (5) further we demonstrate that two possible interpretations of $\widetilde{\rho}(t)$ define the same operator. We start with a formula expressing $\widetilde{\rho}$ as the trace over reservoirvariables of $\widetilde{\chi}$ and show that the result agrees with the transformation to the interaction picture of the Schrodinger representation of $\rho(r) = \mathrm{Tr}_R\{\chi\}$:

$$\mathrm{Tr}_R\{\widetilde{\chi}(t)\}_{s,s'} = \mathrm{Tr}_R\left\{e^{+iH_0t/\hbar}\chi e^{-iH_0t/\hbar}\right\}_{s,s'} \tag{6}$$

$$= \sum_r \left\{e^{+iH_0t/\hbar}\chi e^{-iH_0t/\hbar}\right\}_{sr,s'r} \tag{7}$$

$$= \sum_{rr_1r_1'}\sum_{s_1s_1'} \left(e^{+iH_St/\hbar}\right)_{ss_1}\left(e^{+iH_Rt/\hbar}\right)_{rr_1}\chi_{s_1r_1;s_1'r_1'}\left(e^{-iH_Rt/\hbar}\right)_{r_1'r}\left(e^{-iH_St/\hbar}\right)_{s_1's'} \tag{8}$$

$$= \sum_r\sum_{s_1s_1'} \left(e^{+iH_St/\hbar}\right)_{s,s_1}\chi_{s_1r;s_1'r}\left(e^{-iH_St/\hbar}\right)_{s_1',s'} \tag{9}$$

$$= \sum_r\sum_{s_1s_1'} \left(e^{+iH_St/\hbar}\right)_{s,s_1}\rho_{s_1;s_1'}\left(e^{-iH_St/\hbar}\right)_{s_1',s'}, \tag{10}$$

where the transition from Eq. (8) to Eq. (9) depends on the unitarity of the transition of the operator transforming the reservoirindicies from the Schrodinger to the interaction picture:

$$\sum_r \left(e^{+iH_Rt/\hbar}\right)_{rr_1}\left(e^{-iH_Rt/\hbar}\right)_{r_1'r} = \left(e^{-iH_Rt/\hbar}\,e^{+iH_Rt/\hbar}\right)_{r_1',r_1}\delta_{r_1,r_1'}. \tag{11}$$

Equation (5) is exact but not easy to work with because it expresses the derivative of $\widetilde{\rho}(t)$ in terms of $\widetilde{\rho}(t')$ at *all* earlier t', so some approximations need to be made.

2 Born and Markov approximations

Equation (5) is simplied by two important approximations. The first, referred to by Carmichael as the Born approximation, replaces the complete density matrix $\widetilde{\chi}(t')$ appearing at the right in Eq. (5) by the product $\widetilde{\rho}(t')R_0$ where R_0 is the equilibrium distribution of the reserverior. This replacement is justify by the fact the in this expression which already contains two factors of H_{SSR}, the terms beinng neglected are of third order in H_{SR} and the expectation that the long-term effects of the interaction will not cause these third-order effects to grow. One expects that they will continue have a small effect on the very large reservoireven as the time increases.

With this approximation one then specializes the system-reservoirinteraction to be the sum of products system operators S_i and reservoiroperators Γ_i:

$$H_{RS} = \sum_{i=1}^{N} S_i \Gamma_i. \tag{12}$$

This product description covers a sufficient number of interesting cases to make the subsequent discussion of value. The combination of the Born approximation and this product-form specialization allows Eq. (5) to be written in clarifying form:

$$\begin{aligned}
\dot{\widetilde{\rho}}(t) &= \sum_{i=1}^{N} \mathrm{Tr}_R \left[\widetilde{S}_i(t)\widetilde{\Gamma}_i(t), \rho(0)R_0\right] \qquad (13)\\
&\qquad -\frac{1}{\hbar^2}\sum_{ij}\int_0^t dt' \mathrm{Tr}_R \left\{\left[\widetilde{S}_i(t)\widetilde{\Gamma}_i(t), \left[\widetilde{S}_j(t')\widetilde{\Gamma}_j(t'), \widetilde{\rho}(t')R_0\right]\right]\right\}. \\
&= -\frac{1}{\hbar^2}\sum_{ij}\int_0^t dt' \Big\{ \widetilde{S}_i(t)\widetilde{S}_j(t')\widetilde{\rho}(t')\,\mathrm{Tr}_R\left(\widetilde{\Gamma}_i(t')\widetilde{\Gamma}_j(t)R_0\right) \qquad (14)\\
&\qquad -\widetilde{S}_i(t)\widetilde{\rho}(t')\widetilde{S}_j(t')\,\mathrm{Tr}_R\left(\widetilde{\Gamma}_i(t')R_0\widetilde{\Gamma}_j(t)\right)\\
&\qquad -\widetilde{S}_j('t)\widetilde{\rho}(t')\widetilde{S}_i(t)\,\mathrm{Tr}_R\left(\widetilde{\Gamma}_j(t')R_0\widetilde{\Gamma}_i(t)\right)\\
&\qquad +\widetilde{\rho}(t')\widetilde{S}_j('t)\widetilde{S}_i(t)\,\mathrm{Tr}_R\left(R_0\widetilde{\Gamma}_j(t')\widetilde{\Gamma}_i(t)\right).
\end{aligned}$$

To obtain Eq. (14) we have removed the commuator in the first line of Eq. (13) because it is proportional to averages over the initial thermal reservoirof the interaction factor Γ_i which will typically vanish. It is only at second order in such factors that a thermal average will be non-zero. The remaining four terms are simply the four terms in the double commutator in Eq. (13) written in a way to separate the system oprators from the independent reservoiraverages.

Equation (14) now allows the second "Markov" approximation to be made. Here we argue for reservoiraverages such as $\mathrm{Tr}_R\left(\widetilde{\Gamma}_i(t')\widetilde{\Gamma}_j(t)R_0\right)$ the to interation terms will be correlated and their product non-zero only when the time $\tau = t - t'$ is on the order of the time scale of the reservoirwhich is at the temperature T, typically $\hbar/kT$. If this time scale is small compared to the time scale over which $\widetilde{\rho}(t)$varies then we can replace the corresponding factor, *e.g.* $\widetilde{S}_i(t)\widetilde{S}_j(t')\widetilde{\rho}(t')$ by its value at $t = t'$. If such a substitution is made then only $\rho(t)$ appears on the right-hand side of Eq. (14) and we have a simple differential equiation without an integration over earlier values of $\rho(t')$ once the reservoiraverages such as $\mathrm{Tr}_R\left(\widetilde{\Gamma}_i(t')\widetilde{\Gamma}_j(t)R_0\right)$ have been performed.

Delaying the introduction of the Markov approximation until a specific example is being considered and recognizing that:

$$\mathrm{Tr}_R\left(\widetilde{\Gamma}_i(t')\widetilde{\Gamma}_j(t)R_0\right) = \mathrm{Tr}_R\left(\widetilde{\Gamma}_j(t')R_0\widetilde{\Gamma}_i(t)\right) \tag{15}$$

$$\mathrm{Tr}_R\left(\widetilde{\Gamma}_i(t')R_0\widetilde{\Gamma}_j(t)\right) = \mathrm{Tr}_R\left(R_0\widetilde{\Gamma}_j(t')\widetilde{\Gamma}_i(t)\right) \tag{16}$$

Eq. (14) can be written:

$$\begin{aligned}\dot{\widetilde{\rho}}(t) &= \qquad\qquad (17)\\ -\frac{1}{\hbar^2}\sum_{ij}\int_0^t dt' \Big\{ &\left(\widetilde{S}_i(t)\widetilde{S}_j(t')\widetilde{\rho}(t') - \widetilde{S}_j(t')\widetilde{\rho}(t')\widetilde{S}_i(t)\right)\mathrm{Tr}_R\left(\widetilde{\Gamma}_i(t)\widetilde{\Gamma}_j(t')R_0\right)\\ &+\left(\widetilde{\rho}(t')\widetilde{S}_j(t')\widetilde{S}_i(t) - \widetilde{S}_j(t')\widetilde{\rho}(t')\widetilde{S}_i(t)\right)\mathrm{Tr}_R\left(\widetilde{\Gamma}_j(t')\widetilde{\Gamma}_i(t)R_0\right)\Big\}.\end{aligned}$$

we now work out the specific case of a damped simple harmonic oscillator.

3 Damped simple harmonic oscillator

We now consider the case where the system is a single simple harmonic oscillator, the reservoiris a large collection of harmonic oscillators with varying masses and frequencies and their interaction is a sum of simple products of the lowering operator in the system and the raising operators in the reservoir(and their hermitian conjugates):

$$\begin{aligned}
H_S &= \hbar\omega_0 a^\dagger a && (18)\\
H_R &= \sum_k \hbar\omega_k r_k^\dagger r_k && (19)\\
H_{SR} &= \sum_k \left\{ a\,\kappa_k^* r_k^\dagger + a^\dagger\,\kappa_k r_k \right\} && (20)\\
&= a\Gamma^\dagger + a^\dagger\Gamma, && (21)
\end{aligned}$$

where $\Gamma = \sum_k \kappa_k$.

This coupling between raising and lowering operators is unusual on a classical level involving both the momenta and positions of the coupled degrees of freedom. Carmichael describes this as the "rotating waver" approximation to a more common interaction between the position operators of the form xy_k approximated according to:

$$\begin{aligned}
xy_k &= \sqrt{\frac{\hbar}{2m\omega_0}}\sqrt{\frac{\hbar}{2m_k\omega_k}}(a + a^\dagger))(r_k + r_k^\dagger) && (22)\\
&\approx \sqrt{\frac{\hbar}{2m\omega_0}}\sqrt{\frac{\hbar}{2m_k\omega_k}}\left(ar_k^\dagger + a^\dagger r_k\right) && (23)
\end{aligned}$$

where the terms that are dropped, ar and $a^\dagger r_k^\dagger$ oscillate classically with the sum of the frequenice ω and ω_k and hence might be viewed as far from resonant and therefore less important.

Equation (17) can now be specialized to this system. Here the system-reservoir coupling contains two terms where we identify:

$$S_1\Gamma_1 = a\,\Gamma^\dagger \quad \text{and} \quad S_2\Gamma_2 = a^\dagger\,\Gamma. \tag{24}$$

Which can be substitued into Eq. (17). This substitution is simplied by noting that equilibrium reservoir density matirx in a basis of energy eigenstates has no off-diiagonal terms connecting states with different occupation numbers so the terms:

$$\langle\Gamma(t)\Gamma(t')\rangle_R = \langle\Gamma(t)^\dagger\Gamma(t')^\dagger\rangle_R = 0 \tag{25}$$

and only the two choices $i = 1$, $j = 2$ and $j = 1$, $i = 2$ are non-zero. In addition, the term on the second line of Eq. (17) with $i = 2$ and $j = 1$ is the hermitian conjugate of the term on the first line with $i = 1$ and $j = 2$ and vice-versa. The becomes:

$$
\begin{aligned}
\dot{\widetilde{\rho}}(t) \quad = \quad - \int_0^t d\tau \Bigg\{ & \Big(\widetilde{a}(t)\widetilde{a}^\dagger(t-\tau)\widetilde{\rho}(t-\tau) - \widetilde{a}^\dagger(t-\tau)\widetilde{\rho}(t-\tau)\widetilde{a}(t) \Big) \\
& \qquad \times \mathrm{Tr}_R \left(\widetilde{\Gamma}^\dagger(t)\widetilde{\Gamma}(t-\tau)R_0 \right) + h.c \\
& + \Big(\widetilde{a}^\dagger(t)\widetilde{a}(t-\tau)\widetilde{\rho}(t-\tau) - \widetilde{a}(t-\tau)\widetilde{\rho}(t-\tau)\widetilde{a}^\dagger(t) \Big) \\
& \qquad \times \mathrm{Tr}_R \left(\widetilde{\Gamma}(t)\widetilde{\Gamma}^\dagger(t-\tau)R_0 \right) + h.c. \Bigg\},
\end{aligned}
\tag{26}
$$

where we have introduced $\tau = t - t'$ and changed the integration variable from t' to τ. Note the first two lines in Eq. (26), including the "+ h.c.", correspond to both lines of Eq. (17) for the case $i = 1$ and $j = 2$ while the secon d two lines in Eq. (26) correpond to both lines of Eq. (17) for the case $i = 2$ and $j = 1$.

Next, referring to the discussion in Carmichael, we will assume that the functions $\mathrm{Tr}_R \left(\widetilde{\Gamma}^\dagger(t)\widetilde{\Gamma}(t-\tau) \right)$ and $\mathrm{Tr}_R \left(\widetilde{\Gamma}(t)\widetilde{\Gamma}^\dagger(t-\tau) \right)$ appearing in Eq. (26) vanish rapidly with increasing τ on a much shorter time scale than the time scale over which $\rho(t-\tau)$ varies. This allows us to set $\tau = 0$ whenever it appears in an argument of ρ. The remaining dependence on τ outside of the reservoir averages is in the system raising and lowering operators where it can be extracted by using the definition of the interaction picture:

$$
\widetilde{a}(t-\tau) = \widetilde{a}(t)e^{i\omega_0\tau} \quad \text{and} \quad \widetilde{a}^\dagger(t-\tau) = \widetilde{a}^\dagger(t)e^{-i\omega_0\tau}. \tag{27}
$$

Thus, we need to evaluate two time-integrated reservoir averages that are represented by linear combinations of two complex constants. Following Carmichae we definel:

$$
\beta = \int_0^\infty d\tau e^{i\omega_0\tau} \mathrm{Tr}_R \left(\widetilde{\Gamma}^\dagger(t-\tau)\widetilde{\Gamma}(t)R_0 \right) \tag{28}
$$

$$
\alpha + \beta = \int_0^\infty d\tau e^{i\omega_0\tau} \mathrm{Tr}_R \left(\widetilde{\Gamma}(t)\widetilde{\Gamma}^\dagger(t-\tau)R_0 \right) \tag{29}
$$

where Eq. (29) directly evaluates the integral whose integrand appears on the fourth line of Eq. (26) while Eq. (28) defines the complex conjugate of the integral whose integrand appears on the second line of Eq. (26). Since the integrands in Eqs. (28) and eq:alpha-def1 are assumed to fall rapidly with increasing τ we have extended the range of the τ integration to infinity.

The reservoir averages which appear in Eqs. (28) and (29) can be compactly expressed by replacing the sum over modes in these averages by a continuum integration using $g(\omega)$ as the density of modes per unit frequency:

$$\begin{aligned}
\beta &= \int_0^\infty d\tau e^{i\omega_0\tau} \sum_{k,k'} \mathrm{Tr}_R \left\{ \kappa_k^* \widetilde{r}_k^\dagger(t-\tau) \kappa_{k'} \widetilde{r}_{k'}(t) R_0 \right\} &(30)\\
&= \int_0^\infty d\tau \int_0^\infty d\omega g(\omega) |\kappa(\omega)|^2 \overline{n}_R(\omega, T)) e^{-i(\omega-\omega_0)\tau} &(31)\\
\alpha + \beta &= \int_0^\infty d\tau e^{i\omega_0\tau} \sum_{k,k'} \mathrm{Tr}_R \left\{ \kappa_k^* \widetilde{r}_k(t) \kappa_{k'} \widetilde{r}_{k'}^\dagger(t-\tau) R_0 \right\} &(32)\\
&= \int_0^\infty d\tau \int_0^\infty d\omega g(\omega) |\kappa(\omega)|^2 \big(\overline{n}_R(\omega, T) + 1\big) e^{-i(\omega-\omega_0)\tau}. &(33)
\end{aligned}$$

Here $\overline{n}_R(\omega, T)$ is the average occupation number for a single harmonic oscillator of requency ω in equilibrium at the temperature T:

$$\overline{n}_R(\omega, T) = \frac{e^{-\frac{\hbar\omega}{kT}}}{1 - e^{-\frac{\hbar\omega}{kT}}} \tag{34}$$

Equations (31) and (33) can be further evaluated if we exchange the integrals over τ and ω. This can be permitted if we first add a small positive imaginary part to the variable ω_0. Removing β from Eq. (33) we find:

$$\begin{aligned}
\beta &= \int_0^\infty d\omega g(\omega) |\kappa(\omega)|^2 \overline{n}_R(\omega, T)) \int_0^\infty d\tau e^{-i(\omega-\omega_0-i\epsilon)\tau} &(35)\\
\alpha &= \int_0^\infty d\omega g(\omega) |\kappa(\omega)|^2 \overline{n}_R(\omega, T) \int_0^\infty d\tau e^{-i(\omega-\omega_0-i\epsilon)\tau}. &(36)
\end{aligned}$$

These equation can be further simplified by performing the integral over τ and a standard formula from complex analysis:

$$\int_0^\infty d\tau e^{-i(\omega-\omega_0-i\epsilon)\tau} = -i\frac{1}{\omega - \omega_0 - i\epsilon} = \pi\delta(\omega - \omega_0) + i\mathcal{P}\frac{1}{\omega_0 - \omega}. \tag{37}$$

Introducing Carmichael's parameters γ, Δ and Δ' we obtain:

$$\begin{aligned} \frac{\gamma}{2}\overline{n}_R + i\Delta' &\equiv \beta = \pi g(\omega_0)|\kappa(\omega_0)|^2\overline{n}_R(\omega_0,T)) \\ &\qquad + i\mathcal{P}\!\!\int_0^\infty d\omega g(\omega)\frac{|\kappa(\omega)|^2\overline{n}_R(\omega,T))}{\omega_0-\omega} \end{aligned} \tag{38}$$

$$\frac{\gamma}{2} + i\Delta \equiv \alpha = \pi g(\omega_0)|\kappa(\omega_0)|^2 + i\mathcal{P}\!\!\int_0^\infty d\omega g(\omega)\frac{|\kappa(\omega)|^2}{\omega_0-\omega}. \tag{39}$$

We can now return to Eq. (26) and replace the two reservoir averages withthe parameters α and β. Returning to the Schrodinger picture we find:

$$\begin{aligned} \dot{\rho}(t) &= -i\omega_0[a^\dagger a,\rho(t)] - \Big(aa^\dagger\rho(t) - a^\dagger\rho(t)a(t)\Big)\beta^* - \Big(\rho(t)aa^\dagger - a^\dagger\rho(t)a(t)\Big)\beta \\ &\quad - \Big(a^\dagger a\rho(t) - a\rho(t)a^\dagger\Big)(\alpha+\beta) - \Big(\rho(t)a^\dagger a - a\rho(t)a^\dagger\Big)(\alpha+\beta)^* \end{aligned} \tag{40}$$

$$\begin{aligned} &= -i\omega_0[a^\dagger a,\rho(t)] \\ &\quad - \Big(a^\dagger a\rho(t) - a\rho(t)a^\dagger\Big)(\frac{\gamma}{2}+i\Delta) - \Big(\rho(t)a^\dagger a - a\rho(t)a^\dagger\Big)(\frac{\gamma}{2}-i\Delta) \\ &\quad - \Big(\rho(t)aa^\dagger - a^\dagger\rho(t)a(t)\Big)(\frac{\gamma}{2}\overline{n}_R + i\Delta') - \Big(a^\dagger a\rho(t) - a\rho(t)a^\dagger\Big)(\frac{\gamma}{2}\overline{n}_R + i\Delta') \\ &\quad - \Big(aa^\dagger\rho(t) - a^\dagger\rho(t)a(t)\Big)(\frac{\gamma}{2}\overline{n}_R - i\Delta') - \Big(\rho(t)a^\dagger a - a\rho(t)a^\dagger\Big)(\frac{\gamma}{2}\overline{n}_R - i\Delta') \end{aligned} \tag{41}$$

$$\begin{aligned} &= -i(\omega_0+\Delta)[a^\dagger a,\rho(t)] - \Big(a^\dagger a\rho(t) + \rho(t)a^\dagger a - 2a\rho(t)a^\dagger\Big)\frac{\gamma}{2} \\ &\quad - \Big(\rho(t)(aa^\dagger + a^\dagger a) + -2a^\dagger\rho(t)a(t) + (a^\dagger a + aa^\dagger)\rho(t) - 2a\rho(t)a^\dagger\Big)\frac{\gamma}{2}\overline{n}_R \\ &\quad - \Big(\rho(t)(aa^\dagger - a^\dagger a) + (a^\dagger a - aa^\dagger)\rho(t)\Big)(i\Delta') \end{aligned} \tag{42}$$

$$\begin{aligned} &= -i(\omega_0+\Delta)[a^\dagger a,\rho(t)] + \frac{\gamma}{2}\Big(2a\rho(t)a^\dagger - a^\dagger a\rho(t) - \rho(t)a^\dagger a\Big) \\ &\quad \gamma\overline{n}_R\Big(a^\dagger\rho a + a\rho(t)a^\dagger - \rho(t)aa^\dagger - a^\dagger a\rho\Big). \end{aligned} \tag{43}$$

While this result appears unusually complex, it is indeed remarkable. As we showed in class, Eq. (43) can be readily used to compute

$$\langle\dot{n}(t)\rangle = \mathrm{Tr}\{a^\dagger a\dot{\rho}(t)\} = -\gamma\left(\langle n(t)\rangle - \overline{n}_R(\omega_0,T)\right). \tag{44}$$

which implies that $\langle n(t)\rangle$ relaxes exponentially to the average occupation number of the reservoir. Similarly, a homework problem demonstrates that the thermal distribution for the system SHO,

$$\rho = \exp\{-H_S/(kT)\}/\mathrm{Tr}\exp\{-H_S/(kT)\} \tag{45}$$

is time independent provided T is the temperature of the reservior.