Clarifications from previous lecture

Recall that the reduced density matrix (No Born and No Markov approximation yet) was $\boxed{\text{Eq. 8}}$ in $\boxed{\text{previous lecture.}}$

$$\dot{\hat{\rho}} = -\frac{1}{\hbar^2}\int_0^t dt'\, tr_R\left\{\left[\hat{H}_{SR}(t), \left[\hat{H}_{SR}(t'), \tilde{\chi}(t')\right]\right]\right\}$$

$\hookrightarrow \boxed{\text{Eq. 8}}$ previous lecture

Now for the Born approximation we need to do some approximation on $\tilde{\chi}(t')$

We had written

$$\tilde{\chi}(t) = \hat{\rho}(t) R_0 + O(H_{SR}) \rightarrow \boxed{\text{Eq. 10}} \text{ of previous lecture}$$

where recall that

$$\hat{\chi}(t) \equiv e^{i/\hbar\,(H_S + H_R)t}\,\chi(t)\, e^{-i/\hbar\,(H_S + H_R)t}$$

$\hat{\chi}(t)$ ↓ Interaction picture

$\chi(t)$ ↓ Schrodinger picture

and $$\tilde{\rho}(t) \equiv e^{i/\hbar \, H_S t} \rho(t) \, e^{-i/\hbar \, H_S t}$$

To arrive at $\boxed{\text{Eq } 10}$ let us make the decoupling assumption in Schrodinger Picture

$$\chi(t) = \rho(t) R(t) + O(H_{SR}) \rightarrow \boxed{\text{Eq C1}}$$

Now we act both sides of above equation $\boxed{(\text{Eq C1})}$ with $e^{i/\hbar (H_S + H_R)t}$ on left and $e^{-i/\hbar (H_S+H_R)t}$ on right respectively.

schrodinger picture

This gives

$$e^{i/\hbar (H_S+H_R)t} \chi(t) \, e^{-\frac{i}{\hbar}(H_S+H_R)}$$

$$= \underbrace{e^{i/\hbar \, H_S t} \rho(t) \, e^{-i/\hbar \, H_S t}}_{\tilde{\rho}(t)} \, e^{i/\hbar \, H_R t} R(t) \, e^{-i/\hbar \, H_R t}$$

$$+ \, e^{i/\hbar (H_S+H_R)t} O(H_{SR}) \, e^{-i/\hbar (H_S+H_R)t}$$

$$\rightarrow \boxed{\text{Eq C2}}$$

Simplifying Eq C2 further we get

$$\hat{x}(t) = \hat{\rho}(t)\, e^{i/\hbar H_R t} \underbrace{R(t)}_{\text{schrodinger picture}} e^{-i/\hbar H_R t} + O(\hat{H}_{SR}) \quad \boxed{\text{Eq C3}}$$

We will now assume that $R(t)$ evolves with its own dynamics as if there was no H_{SR}. This is OK since anyway the corrections are higher order in H_{SR} which we anyway neglect.

Therefore Eq C3 becomes

$$\hat{x}(t) = \hat{\rho}(t)\, \underbrace{e^{i/\hbar H_R t} e^{-i/\hbar H_R t}}_{I} \underbrace{R(0)}_{\text{Initial } t=0 \text{ density operator}} \underbrace{e^{+i/\hbar H_R t} e^{-i/\hbar H_R t}}_{I} + O(\hat{H}_{SR}) \quad \boxed{\text{Eq C4}}$$

(these cancel)

Above Eq C4 becomes

$$\hat{x}(t) = \hat{\rho}(t)\, R_0 + O(\hat{H}_{SR})$$

which is what we wrote in previous lecture.

Some additional comments about Born-Markov approximation

i) Under Born approximation (no Markov yet)
the bath density matrix is evolving
(in Schrodinger picture) by its own dynamics
as if it is completely decoupled from
the system. The effect of the interecation
between bath and system (H_{SR}) on the
bath evolution is neglected in the leading
order. This is because we anyway have
$[\tilde{H}_{SR}, [\tilde{H}_{SR} \ldots]]$ in Eq. 8 of previous lecture
and we are not interested in additional
orders. We want only upto quadradic
order in system-bath coupling.
In the interaction picture, the bath
doesnot evolve under the
Born approximation.

2) Using the above Born approximation we get an evolution equation for the reduced density matrix of the system. This is still non-local in time (Non-Markovian). Then to make the equation local, we use the assumption of time-scale separations. We say that the bath correlation decay time is much much shorter that typical time scale of system evolution. We then finally get local equation for reduced density matrix. It is to be noted that in our definition bath-bath correlation not only depends on

bath properties but also depends on system-bath coupling details. Hence correlation decay time for bath depends on nature of system-bath coupling in addition to bath-alone properties (such as temperature, chemical potential, energy density of states)

3) One can, in principle, do only a Born approximation without doing further Markov approximation.

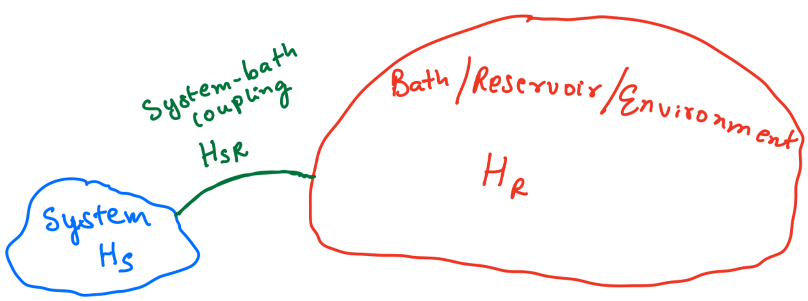
In other words, Born approximation doesnot rely on bath correlation time scales or reservoir memory and we could have a Born non-Markovian description. Ofcourse, in traditional literature Born and Markov approximation is done together.

Lecture-2

→ Quantum Master Equation (QME) : General setup

→ Application to damped quantum harmonic oscillator.

In lecture-1, we gave a motivation and general construction for open Quantum Systems and we outlined the system-reservoir approach. We will now make our construction of H_{SR} a little more specific.



$$H_{SR} = \hbar \sum_i s_i \Gamma_i$$

where s_i are operators that act in the Hibert space of S and Γ_i are reservoir operators that act in the Hibert space of R.

Note that we have expressed many quantities in interaction picture-

$$\hat{H}_{SR}(t) = \hbar \sum_i e^{i/\hbar (H_S + H_R)t} \, s_i \Gamma_i \, e^{-i/\hbar (H_S + H_R)t} = \hbar \sum_i \hat{s}_i(t) \hat{\Gamma}_i(t) \quad \boxed{Eq.1}$$

The master equation only in Born approximation, i.e, Eq. 11 of lecture-1 (not Markov) becomes

$$\dot{\hat{\rho}} = -\sum_{ij} \int_0^t dt' \Big\{ \left[\hat{s}_i(t) \hat{s}_j(t') \hat{\rho}(t') - \hat{s}_j(t') \hat{\rho}(t') \hat{s}_i(t) \right] \langle \hat{\Gamma}_i(t) \hat{\Gamma}_j(t') \rangle_R$$
$$+ \left[\hat{\rho}(t') \hat{s}_j(t') \hat{s}_i(t) - \hat{s}_i(t) \hat{\rho}(t') \hat{s}_j(t') \right] \langle \hat{\Gamma}_j(t') \hat{\Gamma}_i(t) \rangle_R \Big\} \quad \boxed{Eq.2}$$

where
$$\langle \hat{\Gamma}_i(t) \hat{\Gamma}_j(t') \rangle_R = tr_R \left[R_0 \hat{\Gamma}_i(t) \hat{\Gamma}_j(t') \right]$$
$$\langle \hat{\Gamma}_j(t') \hat{\Gamma}_i(t) \rangle_R = tr_R \left[R_0 \hat{\Gamma}_j(t') \hat{\Gamma}_i(t) \right] \quad \boxed{Eq.3}$$

The information of the reservoirs (Eq.3) enters via correlations into Eq.2. We can justify the replacement $\hat{\rho}(t')$ by $\hat{\rho}(t)$ if correlations decay very rapidly on the system time-scales on which $\tilde{\rho}(t)$ varies. Obviously the ideal situation is $\langle \tilde{\Gamma}_i(t) \tilde{\Gamma}_j(t') \rangle_R \propto \delta(t-t')$.

The Markov approximation as mentioned previously relies on two widely separated time scales, a slow time scale for the dynamics of the system and a fast time scale characterizing the decay of reservoir correlation functions.

A deeper understanding of this can be achieved when we proceed to our first example - The Damped Quantum Harmonic Oscillator.

The Damped Quantum Harmonic Oscillator

The microscopic/explicit model for a damped quantum harmonic oscillator is given by the composite system $S \otimes R$,

$$H_S = \hbar \omega_c a^\dagger a \rightarrow \boxed{\text{Eq.4}}$$

$$H_R = \hbar \sum_j \omega_j r_j^\dagger r_j$$

$$H_{SR} = \sum_j \hbar \left(\kappa_j^* a r_j^\dagger + \kappa_j a^\dagger r_j \right) \equiv \hbar \left(a\Gamma^\dagger + a^\dagger \Gamma \right)$$

system-reservoir coupling constant

The system S is a harmonic oscillator with frequency ω_0 and creation/anhillation operators $a^\dagger$ and a respectively. The reservoir R is modelled as a collection of Harmonic oscillators with frequencies ω_j and corresponding creation and anhillation operators $r_j^\dagger$ and r_j respectively. The oscillator "a" couples to j-th reservoir oscillator via coupling constant κ_j.

As emphasized before note that the total Hamiltonian $H = H_S + H_R + H_{SR}$ is still Hermitian. Therefore we start with a microscopic Hermitian setup and end with a non-Hermitian formalism for the reduced situation which we will call as the system.

We take the reservoir to be in thermal equilibrium at temperature T with density operator

$$R_0 = \prod_j e^{-\frac{\hbar\omega_j r_j^\dagger r_j}{k_B T}} \left(1 - e^{-\hbar\omega_j/k_B T}\right) \rightarrow \boxed{Eq.5}$$

where k_B is the Boltzman constant. Note that it is not necessary to be so specific about reservoir models (Eq.5). The oscillators playing the role of reservoirs is physically reasonable in many circumstances.

→ Many modes of vacuum radiation field into which an optical cavity mode decays through partially transmitting mirrors (Leaky cavities)

→ Many modes of vacuum radiation field into which an excited atom decays via spontaneous emission.

→ The reservoir oscillators might represent phonon modes in a solid.

Note that our general notation was $H_{SR} = \hbar \sum_i s_i \Gamma_i$ and Eq. 4 results in the identification

$s_1 \equiv a$, $s_2 = a^+$, $\Gamma_1 = \Gamma^+ = \sum_j K_j^* r_j^+$

$\Gamma_2 = \Gamma \equiv \sum_j K_j r_j$. Using this identification after some algebra, we arrive at,

$$
\begin{aligned}
\dot{\tilde{\hat{\rho}}} = \int_0^t dt' \Big\{ & \left[a a \tilde{\hat{\rho}}(t') - a \tilde{\hat{\rho}}(t') a \right] e^{-i\omega_e(t+t')} \langle \tilde{\hat{\Gamma}}^+(t) \tilde{\hat{\Gamma}}^+(t') \rangle_R \\
& + h.c \\
& + \left[a^+ a^+ \tilde{\hat{\rho}}(t') - a^+ \tilde{\hat{\rho}}(t') a^+ \right] e^{i\omega_e(t+t')} \langle \tilde{\hat{\Gamma}}(t) \tilde{\hat{\Gamma}}(t') \rangle_R \\
& + h.c \\
& + \left[a a^+ \tilde{\hat{\rho}}(t') - a^+ \tilde{\hat{\rho}}(t') a \right] e^{-i\omega_e(t-t')} \langle \tilde{\hat{\Gamma}}^+(t) \tilde{\hat{\Gamma}}(t') \rangle_R \\
& + h.c \\
& + \left[a^+ a \tilde{\hat{\rho}}(t') - a \tilde{\hat{\rho}}(t') a^+ \right] e^{i\omega_e(t-t')} \langle \tilde{\hat{\Gamma}}(t) \tilde{\hat{\Gamma}}^+(t') \rangle_R \\
& + h.c \Big\}
\end{aligned}
$$

↳ $\boxed{\text{Eq. 6}}$

where the reservoir correlation functions are explicitly,

$$\langle \hat{\Gamma}^{+}(t)\hat{\Gamma}^{+}(t')\rangle_R = \sum_{jk} \kappa_j^{*}\kappa_k^{*} e^{i\omega_j t} e^{i\omega_k t'} \underbrace{tr_R[R_0 r_j^{+} r_k^{+}]}_{=0}$$

$$\langle \hat{\Gamma}(t)\hat{\Gamma}(t')\rangle_R = \sum_{jk} \kappa_j \kappa_k e^{-i\omega_j t} e^{-i\omega_k t'} \underbrace{tr_R[R_0 r_j r_k]}_{=0}$$

$$\langle \hat{\Gamma}^{+}(t)\hat{\Gamma}(t')\rangle_R = \sum_{jk} \kappa_j^{*}\kappa_k e^{i\omega_j t} e^{-i\omega_k t'} tr_R[R_0 r_j^{+} r_k]$$

$$= \sum_j |\kappa_j|^2 e^{i\omega_j (t-t')} \bar{n}(\omega_j, T)$$

$$\langle \hat{\Gamma}(t)\hat{\Gamma}^{+}(t')\rangle_R = \sum_{jk} \kappa_j \kappa_k^{*} e^{-i\omega_j t} e^{i\omega_k t'} tr_R[R_0 r_j r_k^{+}]$$

$$= \sum_j |\kappa_j|^2 e^{-i\omega_j (t-t')} [\bar{n}(\omega_j, T)+1]$$

$\rightarrow \boxed{\text{Eq. 7}}$

with $\bar{n}(\omega_j, T) = tr_R[R_0 r_j^{+} r_j] = \dfrac{e^{-\hbar\omega_j/k_B T}}{1-e^{-\hbar\omega_j/k_B T}}$ $\rightarrow \boxed{\text{Eq. 8}}$

The correlation functions in Eq. 7 can be derived by evaluating the trace using multi-mode fock states as the basis.

$\bar{n}(\omega_j, T)$ is mean photon number or bosonic occupation number of an oscillator with frequency ω_j in thermal equilibrium at temperature T.

The non-vanishing reservoir correlations in Eq. 7 involve a summation over reservoir oscillators.

We will change the summation to integration by introducing density of states (DOS) $g(\omega)$ such that $g(\omega)d\omega$ gives the number of oscillators with frequencies in the interval ω to $\omega + d\omega$. In other words, we transform $\sum_j \Rightarrow \int d\omega\, g(\omega)$. By making suitable change of variables $\tau = t - t'$, Eq. 6 can be written compactly as

$$\dot{\tilde{\rho}} = -\int_0^t d\tau \Big\{ \left[a a^{\dagger} \tilde{\rho}(t-\tau) - a^{\dagger} \tilde{\rho}(t-\tau) a\right] e^{-i\omega_c \tau} \langle \tilde{\Gamma}^{\dagger}(t) \tilde{\Gamma}(t-\tau)\rangle_R + h.c$$
$$+ \left[a^{\dagger} a \tilde{\rho}(t-\tau) - a \tilde{\rho}(t-\tau) a^{\dagger}\right] e^{i\omega_c \tau} \langle \tilde{\Gamma}(t) \tilde{\Gamma}^{\dagger}(t-\tau)\rangle_R + h.c \Big\}$$

$\boxed{\text{Eq. 9}}$

The non-zero reservoir correlations are given below.

$$\langle \tilde{\Gamma}^{\dagger}(t)\tilde{\Gamma}(t-\tau)\rangle_R = \int_0^{\infty} d\omega\, e^{i\omega\tau}\, \overbrace{g(\omega)\,|K(\omega)|^2}^{J(\omega)\ \text{is called bath spectral density}}\, \bar{n}(\omega,T) \quad \rightarrow \boxed{\text{Eq.10}}$$

$$\langle \tilde{\Gamma}(t)\tilde{\Gamma}^{\dagger}(t-\tau)\rangle_R = \int_0^{\infty} d\omega\, e^{-i\omega\tau}\, g(\omega)\,|K(\omega)|^2 \left(\bar{n}(\omega,T)+1\right)$$

with $$\bar{n}(\omega,T) = \frac{e^{-\hbar\omega/k_BT}}{1-e^{-\hbar\omega/k_BT}} \quad \rightarrow \boxed{\text{Eq.11}}$$

We now revisit the issue of Markov approximation.

In other words, one can ask if Eq.10 can be approximated to a Dirac delta function $\delta(\tau)$?

In Eq.10 note that for large enough τ the oscillating exponential function $e^{\pm i\omega\tau}$ will average out the slowly varying functions $g(\omega), |K(\omega)|^2, \bar{n}(\omega,T)$ basically to zero.

Can we get some estimate for the width of these reservoir correlations?

Let us see Eq.10 and take $g(\omega)|K(\omega)|^2 = c\,\omega$ where c is a constant.

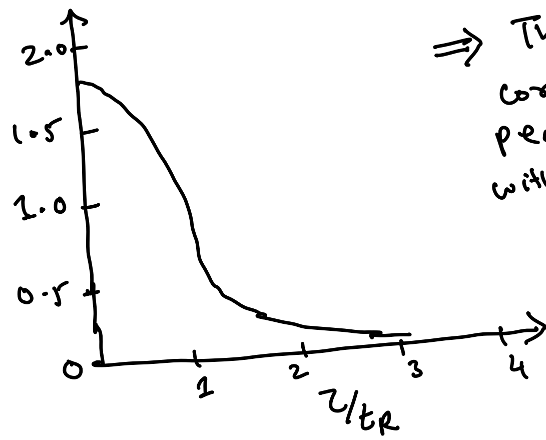
Using this, we get

$$\langle \tilde{\Gamma}^{+}(t)\Gamma(t-\tau)\rangle_R = \frac{c}{t_R^2}\,\psi'\left(1-\frac{i\tau}{t_R}\right) \rightarrow \text{trigamma function} \quad \boxed{\text{Eq. 12}}$$

where reservoir correlation time is $t_R = \frac{\hbar}{k_B T}$

Below is a sketch of the plot for $\mathrm{Re}\left[\psi'(1-i\tau/t_R)\right]$

See book [1] for more details and discussions.



$\Rightarrow$ This plot shows that correlation function is peaked about $\tau=0$ with a width $\sim t_R = \frac{\hbar}{k_B T}$

The reservoir correlations are integrated against two time dependent terms $\hat{\rho}(t-\tau)$ and $e^{\pm i\omega_c \tau}$

We can have situations when system time scales is far greater than reservoir time scales $(t_s \gg t_R)$ which can justify the Markov approximation replacement $\tilde{\rho}(t-\tau) \rightarrow \hat{\rho}(t)$.

Also integrating the reservoir correlation functions against oscillatory terms $e^{\pm i\omega_c \tau}$ will extract their ω_0 frequency components (just like a fourier transform)

By applying the Markov approximation Eq. 9 becomes

$$\dot{\tilde{\rho}} = \alpha\left(a\tilde{\rho}a^{+} - a^{+}a\tilde{\rho}\right) + \beta\left(a\tilde{\rho}a^{+} + a^{+}\tilde{\rho}a - a^{+}a\tilde{\rho} - \tilde{\rho}aa^{+}\right) + h.c$$

$\hookrightarrow$ $\boxed{\text{Eq. 13}}$

where $\alpha = \int_0^t d\tau \int_0^\infty d\omega \, e^{-i(\omega-\omega_c)\tau} g(\omega)|K(\omega)|^2$

$\beta = \int_0^t d\tau \int_0^\infty d\omega \, e^{-i(\omega-\omega_c)\tau} g(\omega)|K(\omega)|^2 \bar{n}(\omega, T)$ $\hookrightarrow$ $\boxed{\text{Eq. 14}}$

Note that t is of the order of t_s and τ integration is dominated by much shorter times t_R. Hence we can extend τ integration to ∞ and evaluate α and β. After some algebra and going back to Schrodinger picture, we get

$$\dot{\rho} = -i\omega_c'\left[a^{+}a, \rho\right] + \gamma(\bar{n}+1)L[a](\rho) + \gamma\bar{n}L[a^{+}](\rho)$$ $\hookrightarrow$ $\boxed{\text{Eq. 15}}$

where $L[\hat{F}](\rho) \equiv F\rho F^{+} - \frac{1}{2}\left(F^{+}F\rho - \rho F^{+}F\right)$ $\hookrightarrow$ $\boxed{\text{Eq. 16}}$

$\hookrightarrow$ Lindblad Super-operator

(Lindblad Master Equation)

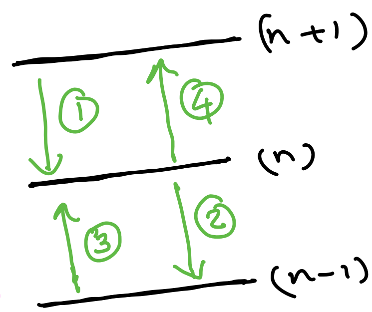
Some definitions used in Eq. 15 are given below.

$$\gamma = 2\pi\, g(\omega_c)\,|K(\omega_c)|^2 \;, \quad \bar{n} = \bar{n}(\omega_c, T) \quad \rightarrow \boxed{\text{Eq 17}}$$

$$\omega_c' = \omega_c + \Delta \quad \text{where} \quad \Delta = P\int_0^\infty d\omega\, \frac{g(\omega)|K(\omega)|^2}{\omega_c - \omega} \quad \rightarrow \boxed{\text{Eq. 18}}$$

Eq. 16 is the Lindblad Master Equation for the damped harmonic oscillator. From Eq. 16 one can get important information. For e.g one can get rate equation for probabilities $P_n = \langle n|\rho|n\rangle$ for the oscillator to be found in the n-th energy eigenstate.

$$\dot{P}_n = \overset{1}{\gamma(\bar{n}+1)(n+1)P_{n+1}} - \overset{2}{\gamma(\bar{n}+1)\,n P_n} + \underset{3}{\gamma\,\bar{n}\, n\, P_{n-1}} - \underset{4}{\gamma\,\bar{n}\,(n+1)P_n} \quad \hookrightarrow \boxed{\text{Eq 19}}$$



Expectation Values

Our theory is written in the Schrodinger picture. From there we want to calculate solutions for expectation values of operators.

For example,

Eq 15 is plugsed in here

$$\langle \dot{a} \rangle = tr[a \; \dot{\rho}] \rightarrow \boxed{Eq\ 20}$$

After some algebra Eq 20 becomes

$$\langle \dot{a} \rangle = -\left(\gamma/_2 + i\omega_c'\right)\langle a \rangle \rightarrow \boxed{Eq\ 21}$$

which gives the solution

$$\langle a(t) \rangle = e^{-(\gamma/_2 + i\omega_c')t} \langle a(0) \rangle \rightarrow \boxed{Eq\ 22}$$

Similarly, the bosonic occupation number

$\hat{n} = a^{+}a$ satisfies,

$$\langle \dot{\hat{n}} \rangle = -\gamma\left(\langle \hat{n} \rangle - \bar{n}\right) \rightarrow \boxed{Eq\ 23}$$

which gives the solution

$$\langle \hat{n}(t) \rangle = \langle \hat{n}(0) \rangle e^{-\gamma t} + \bar{n}\left(1 - e^{-\gamma t}\right) \rightarrow \boxed{Eq\ 24}$$

In above Eq 24, note that thermal fluctuations (thermal noise) is fed into the oscillator from the reservoirs.

As a consequence of this the mean energy doesnot decay to zero. In fact in the steady state the mean energy becomes that for a quantum harmonic oscillator with frequency ω_c in thermal equilibrium at temperature T. The oscillator acquires the environment temperature.

Note that Eq 15 and subsequent consequences such as Eq 22 and Eq 24 essentially involved a system-bath perturbative approach and a Markov approximation. This is the main essence of Born-Markov Quantum Master Equation. This is an important approach to deal with open Quantum Systems. To benchmark these results it is worthwhile to discuss a non-perturbative approach known as Quantum Langevin approach which is the topic of next lecture (lecture 3).