Interaction picture

Let's write $\tilde{b}_n(t) = e^{iH_E t} b_n e^{-iH_E t}$

where $\tilde{b}_n(t)$ is an environment annihilation operator in the interaction picture

If we differentiate with respect to time, we have

$$\frac{d}{dt}\tilde{b}_n(t) = iH_E e^{iH_E t} b_n e^{-iH_E t} - i e^{iH_E t} b_n e^{-iH_E t} H_E$$

$[H_E, e^{-iH_E t}] = 0$ so we can rearrange

$$\Rightarrow \frac{d}{dt}\tilde{b}_n(t) = i e^{iH_E t}(H_E b_n - b_n H_E) e^{-iH_E t}$$

$$= i e^{iH_E t}[H_E, b_n] e^{-iH_E t}$$

This is a Heisenberg equation of motion for b_k under evolution governed by H_E

from $H_E = \sum_k \omega_k b_k^\dagger b_k$

we have $[H_E, b_k] = \sum_{k'} \omega_{k'} [b_{k'}^\dagger b_{k'}, b_k]$

$$= \sum_{k'} \omega_{k'} (b_{k'}^\dagger b_{k'} b_k - b_k b_{k'}^\dagger b_{k'})$$

$$= \sum_{k'} \omega_{k'} (b_{k'}^\dagger b_k b_{k'} - b_k b_{k'}^\dagger b_{k'})$$

$$= \sum_{k'} \omega_{k'} [b_{k'}^\dagger, b_k] b_{k'}$$

$$= \sum_{k'} \omega_{k'} (-\delta_{kk'}) b_{k'}$$

$$= -\omega_k b_k$$

$$\therefore \frac{d}{dt} \hat{b}_k(t) = i e^{iH_E t} (-\omega_k b_k) e^{-iH_E t}$$

$$\Rightarrow \frac{d}{dt}\tilde{b}_k(t) = -i\omega_k \tilde{b}_k(t)$$

$$\Rightarrow \tilde{b}_k(t) = e^{-i\omega_k t}\,\tilde{b}_k(0)$$

but $\tilde{b}_k(0) = b_k$ by definition

$$\Rightarrow \tilde{b}_k(t) = e^{-i\omega_k t}\, b_k$$

Taking the Hermitian conjugate

$$\Rightarrow \tilde{b}_k^{+}(t) = e^{i\omega_k t}\, b_k^{+}$$

An alternative way to get the same result is to use the operator identity (based on the Baker-Campbell-Hausdorff formula):

$$e^{\hat{A}}\hat{B}e^{-\hat{A}} = \hat{B} + [\hat{A},\hat{B}] + \frac{1}{2!}[\hat{A},[\hat{A},\hat{B}]] + \dots$$

Occupation numbers

Consider $\langle b^\dagger b \rangle = \mathrm{tr}(b^\dagger b\, \rho_E)$

$$= \frac{\mathrm{tr}\left(b^\dagger b\, e^{-H_E/k_BT}\right)}{\mathrm{tr}\left(e^{-H_E/k_BT}\right)}$$

For a single mode, $H_E = \omega b^\dagger b$

Cons. $\mathrm{tr}\left(e^{-H_E/k_BT}\right) = \sum_{n=0}^{\infty} \langle n | e^{-\omega b^\dagger b/k_BT} | n \rangle$

$$= \sum_{n=0}^{\infty} \langle n | e^{-\omega n/k_BT} | n \rangle$$

$$= \sum_{n=0}^{\infty} e^{-\omega n/k_BT}$$

$$= \frac{e^{\omega/k_BT}}{e^{\omega/k_BT} - 1}$$

likewise,

$$\mathrm{tr}\left(b^\dagger b\, e^{-\omega b^\dagger b/k_BT}\right)$$

$$= \sum_{n=0}^{\infty} \langle n | b^\dagger b\, e^{-\omega b^\dagger b/k_BT} | n \rangle$$

$$= \sum_{n=0}^{\infty} \langle n | b^\dagger b\, e^{-\omega n/k_BT} | n \rangle$$

$$= \sum_{n=0}^{\infty} \langle n | b^\dagger b | n \rangle\, e^{-\omega n/k_BT}$$

$$= \sum_{n=0}^{\infty} n\, e^{-\omega n/k_BT} = \frac{e^{\omega/k_BT}}{\left(e^{\omega/k_BT}-1\right)^2}$$

$$\Rightarrow \langle b^\dagger b \rangle = \frac{\cancel{e^{\omega/k_BT}}}{\left(e^{\omega/k_BT}-1\right)^{\cancel{2}}} \frac{\cancel{\left(e^{\omega/k_BT}-1\right)}}{\cancel{e^{\omega/k_BT}}}$$

$$\therefore \langle b^{+} b \rangle = \frac{1}{e^{\omega/k_B T} - 1} = N(\omega)$$

$$\sum_{n=0}^{\infty} n e^{-wn/k_BT}$$

let $x = w/k_BT \Rightarrow \displaystyle\sum_{n=0}^{\infty} n e^{-xn}$

$$= -\frac{d}{dx} \sum_{n=0}^{\infty} e^{-xn}$$

$$= -\frac{d}{dx} \left(\frac{e^x}{e^x - 1} \right)$$

$$= \frac{e^x}{(e^x - 1)^2}$$

$$= \frac{e^{w/k_BT}}{(e^{w/k_BT} - 1)^2}$$

Spin-boson master equation

Let us consider the following model of a dissipative two-level system, known as the spin-boson model

$$H = \frac{\epsilon}{2}\sigma_z + \frac{\Delta}{2}\sigma_x + \sum_k \omega_k b_k^\dagger b_k + \sigma_z \sum_k g_k (b_k + b_k^\dagger)$$

Here, $\sigma_z = |e\rangle\langle e| - |g\rangle\langle g|$, $\sigma_x = |e\rangle\langle g| + |g\rangle\langle e|$ for a two-level system with ground state $|g\rangle$ and excited state $|e\rangle$ in the basis set by σ_z

We let $H = H_S + H_B + H_I$

where $H_S = \frac{\epsilon}{2}\sigma_z + \frac{\Delta}{2}\sigma_x$, $H_B = \sum_k \omega_k b_k^\dagger b_k$

and $H_I = \sigma_z \sum_k g_k (b_k^\dagger + b_k)$

Moving into the interaction picture, we have

$$\tilde{H}_I(t) = e^{iH_s t}\sigma_z e^{-iH_s t}\sum_k g_k\left(b_k^\dagger e^{i\omega_k t} + b_k e^{-i\omega_k t}\right)$$

It is convenient to work in the eigenbasis of H_s, which can be expressed as

$$|+\rangle = \sin(\theta/2)|g\rangle + \cos(\theta/2)|e\rangle$$
$$|-\rangle = \cos(\theta/2)|g\rangle - \sin(\theta/2)|e\rangle$$

Here $\theta = \tan^{-1}(\Delta/\varepsilon)$

$$\Rightarrow \cos\theta = \frac{\varepsilon}{\eta}, \quad \sin\theta = \frac{\Delta}{\eta} \quad \text{where } \eta = \sqrt{\varepsilon^2+\Delta^2}$$

Recall that $H_s = \frac{\varepsilon}{2}\sigma_z + \frac{\Delta}{2}\sigma_x$

In terms of $|\pm\rangle$ we then have

$$H_s = \frac{\eta}{2}\left(|+\rangle\langle+| - |-\rangle\langle-|\right)$$

Such that $H_S |\pm\rangle = \pm(\eta/2)|\pm\rangle$

likewise, $\sigma_z = |e\rangle\langle e| - |g\rangle\langle g| = \cos\theta\,(|+\rangle\langle +| - |-\rangle\langle -|)$
$- \sin\theta\,(|+\rangle\langle -| + |-\rangle\langle +|)$

Moving into the interaction picture is now straight forward, since $e^{\pm iH_S t} = e^{\pm i(\eta/2)(|+\rangle\langle+| - |-\rangle\langle-|)t}$

$$= |+\rangle\langle+| e^{\pm i\eta t/2} + |-\rangle\langle-| e^{\mp i\eta t/2}$$

$$\Rightarrow e^{iH_S t}\sigma_z e^{-iH_S t} = \cos\theta\,(|+\rangle\langle+| - |-\rangle\langle-|) - \sin\theta\,(|+\rangle\langle-| e^{i\eta t} + |-\rangle\langle+| e^{-i\eta t})$$

$$= P_0 - (P_\eta^\dagger e^{i\eta t} + P_\eta e^{-i\eta t})$$

Here, $P_0 = \cos\theta\,(|+\rangle\langle+| - |-\rangle\langle-|) = (\varepsilon/\eta)(|+\rangle\langle+| - |-\rangle\langle-|)$

$P_\eta = \sin\theta\,|-\rangle\langle+| = (\Delta/\eta)\,|-\rangle\langle+|$

So, our interaction picture interaction Hamiltonian can be written

$$\tilde{H}_I(t) = \tilde{A}(t)\,\tilde{B}(t)$$

where $\tilde{A}(t) = P_0 - (P_q^\dagger e^{iqt} + P_q e^{-iqt})$

$$\tilde{B}(t) = \sum_k g_k (b_k^\dagger e^{i\omega_k t} + b_k e^{-i\omega_k t})$$

From the lecture notes, our interaction picture master equation is then

$$\dot{\tilde{\rho}}_S(t) = -\int_0^\infty d\tau \Big([\tilde{A}(t), \tilde{A}(t-\tau)\tilde{\rho}_S(t)]\, C(\tau) \qquad ①$$
$$+ [\tilde{\rho}_S(t)\hat{A}(t-\tau), \tilde{A}(t)]\, C(-\tau) \Big)$$

The correlation function $C(\tau) = \langle \tilde{B}(\tau) B(0) \rangle$ where $\langle \dots \rangle = \mathrm{tr}(\dots \rho_B)$ assuming bath in thermal equilibrium

$$\Rightarrow C(\tau) = \sum_{k,k'} g_k g_{k'} \Big(\langle b_k^\dagger b_{k'}^\dagger \rangle e^{i\omega_k \tau} + \langle b_k^\dagger b_{k'} \rangle e^{i\omega_k \tau}$$
$$+ \langle b_k b_{k'}^\dagger \rangle e^{-i\omega_k \tau} + \langle b_k b_{k'} \rangle e^{-i\omega_k \tau} \Big)$$

Using $\langle b_k^+ b_{k'}^+ \rangle = 0 = \langle b_k b_{k'} \rangle$

and $\langle b_k b_{k'}^+ \rangle = \delta_{kk'} (1 + N(\omega_{k'}))$

$\langle b_k^+ b_{k'} \rangle = \delta_{kk'} N(\omega_{k'})$

with $N(\omega) = (e^{\omega/k_BT} - 1)^{-1}$ the bath occupation number

$$\Rightarrow C(\pm\tau) = \int_0^\infty d\omega\, J(\omega) \left(N(\omega) e^{\pm i\omega\tau} + (1 + N(\omega)) e^{\mp i\omega\tau} \right)$$

where we have taken the continuum limit and defined the spectral density $J(\omega) = \sum_k g_k^2 \delta(\omega - \omega_k)$

So, we know the form of the bath correlation function that goes into the master equation ①

Let's now consider the system part

for example, expanding out $[\tilde{A}(t), \tilde{A}(t-\tau) \tilde{\rho}_S(t)]$

$\Rightarrow \tilde{A}(t) \tilde{A}(t-\tau) \tilde{\rho}_S(t) - \tilde{A}(t-\tau) \tilde{\rho}_S(t) \tilde{A}(t)$

Considering the first term:

$$\hat{A}(t)\hat{A}(t-\tau)\tilde{\rho}_s(t) = \left(P_0 - (P_\eta^+ e^{i\eta t} + P_\eta e^{-i\eta t})\right)$$
$$\times\left(P_0 - (P_\eta^+ e^{i\eta(t-\tau)} + P_\eta e^{-i\eta(t-\tau)})\right)$$
$$\times\, \tilde{\rho}_s(t)$$
$$= \Big(P_0^2 - P_0(P_\eta^+ e^{i\eta(t-\tau)} + P_\eta e^{-i\eta(t-\tau)})$$
$$- (P_\eta^+ e^{i\eta t} + P_\eta e^{-i\eta t})P_0$$
$$+ P_\eta^{+2} e^{i\eta(2t-\tau)} + P_\eta^+ P_\eta e^{i\eta\tau}$$
$$+ P_\eta P_\eta^+ e^{-i\eta\tau} + P_\eta^2 e^{-i\eta(2t-\tau)}\Big)\hat{\rho}_s(t)$$

The secular approximation now consists of neglecting all "fast" oscillating terms at frequencies $\pm\eta t$ and $\pm 2\eta t$ under the assumption that their contributions are small on the system relaxation timescale, which governs the dynamics in the interaction picture.

This implies a condition of the form $\eta \gg \Gamma$ where the rate Γ will be defined later

Implementing the secular approximation, we find

$$\tilde{A}(t)\hat{A}(t-\tau)\hat{\rho}_S(t) \to (P_0^2 + P_\eta^\dagger P_\eta e^{i\eta\tau} + P_\eta P_\eta^\dagger e^{-i\eta\tau})\hat{\rho}_S(t)$$

likewise, expanding out the commutators in ① and performing the secular approximation on the other terms, we find

$$\hat{A}(t-\tau)\hat{\rho}_S(t)\hat{A}(t) \to P_0\hat{\rho}_S(t)P_0 + P_\eta^\dagger\hat{\rho}_S(t)P_\eta e^{-i\eta\tau} + P_\eta\hat{\rho}_S(t)P_\eta^\dagger e^{i\eta\tau}$$

$$\hat{\rho}_S(t)\hat{A}(t-\tau)\hat{A}(t) \to \hat{\rho}_S(t)(P_0^2 + P_\eta^\dagger P_\eta e^{-i\eta\tau} + P_\eta P_\eta^\dagger e^{i\eta\tau})$$

$$\hat{A}(t)\hat{\rho}_S(t)\hat{A}(t-\tau) \to P_0\hat{\rho}_S(t)P_0 + P_\eta^\dagger\hat{\rho}_S(t)P_\eta e^{i\eta\tau} + P_\eta\hat{\rho}_S(t)P_\eta^\dagger e^{-i\eta\tau}$$

Now, we substitute these expressions into ① along with $C(\pm\tau)$ to get our secular-Born-Markov master equation. We can perform the integrals over time using

$$\int_0^\infty d\tau\, e^{\pm i\nu t} = \pi\delta(\nu) \pm iP\left(\frac{1}{\nu}\right)$$

where P denotes the Principal value of the subsequent frequency integral we then perform the integral over frequency with the help of the Dirac delta function (leaving the Principal value integrals unevaluated), which gives after some algebra

$$\dot{\hat{\rho}}_S(t) = -i\left[H_{LS}, \hat{\rho}_S(t)\right] + \Gamma_0\left(P_0 \hat{\rho}_S(t) P_0 - \tfrac{1}{2}\{P_0^2, \hat{\rho}_S(t)\}\right)$$
$$+ \Gamma(q)(1+N(q))\left(P_q \hat{\rho}_S(t) P_q^+ - \tfrac{1}{2}\{P_q^+ P_q, \hat{\rho}_S(t)\}\right)$$
$$+ \Gamma(q) N(q)\left(P_q^+ \hat{\rho}_S(t) P_q - \tfrac{1}{2}\{P_q P_q^+, \hat{\rho}_S(t)\}\right)$$

Here, $\Gamma_0 = 2\pi \lim_{\omega \to 0} J(\omega)(1 + 2N(\omega))$

$$\Gamma(q) = 2\pi J(q), \quad \{\hat{X}, \hat{Y}\} = \hat{X}\hat{Y} + \hat{Y}\hat{X}$$

and $H_{LS} = -\Lambda_0 P_0^2 + \Lambda_1 (P_q^+ P_q - P_q P_q^+) + \Lambda_2 (P_q^+ P_q + P_q P_q^+)$

with Principal value integrals

$$\Lambda_0 = P\int_0^\infty d\omega \frac{J(\omega)}{\omega}, \quad \Lambda_1 = P\int_0^\infty d\omega \frac{J(\omega)(1+2N(\omega))q}{q^2 - \omega^2}$$

$$\Lambda_2 = P\int_0^\infty d\omega \frac{\omega J(\omega)}{q^2 - \omega^2}$$

H_{LS} is sometimes called the Lamb-shift as it gives a Hamiltonian-like renormalisation of the system energy scales, whereas the other terms in the secular master equation cause dissipation and dephasing (loss of coherence)

Moving back to the Schrödinger picture is straightforward when working with a secular master equation in the system eigenbasis, and gives

$$
\begin{aligned}
\dot{\rho}_S(t) = & -i[H_S + H_{LS}, \rho_S(t)] \\
& + \Gamma_0 \left(P_0 \rho_S(t) P_0 - \tfrac{1}{2}\{P_0^2, \rho_S(t)\} \right) \\
& + \Gamma(\eta)(1+N(\eta)) \left(P_\eta \rho_S(t) P_\eta^{+} - \tfrac{1}{2}\{P_\eta^{+} P_\eta, \rho_S(t)\} \right) \\
& + \Gamma(\eta) N(\eta) \left(P_\eta^{+} \rho_S(t) P_\eta - \tfrac{1}{2}\{P_\eta P_\eta^{+}, \rho_S(t)\} \right)
\end{aligned}
$$

Secular master equation in the Schrödinger picture

Usually, the Lamb shift is ignored, under the assumption that it is small, and can anyway be absorbed into the original Hamiltonian parameters ε and Δ.

To specify Γ_0 and $\Gamma(\eta)$ we need to consider a particular spectral density

A simple choice is $J(\omega) = \alpha\,\omega$ (known as Ohmic)

where α is a dimensionless coupling strength

$$\Rightarrow \Gamma_0 = 2\pi \lim_{\omega \to 0} \left(\alpha\omega(1+2N(\omega)) \right) = 4\pi\alpha k_B T$$

$$\Gamma(\eta) = 2\pi\alpha\eta$$

Hence, ignoring H_{LS} $\Rightarrow$

$$\begin{aligned}\dot{\rho}_s(t) = -i[H_s, \rho_s(t)] &+ \Gamma_0 \left(P_0 \rho_s(t) P_0 - \tfrac{1}{2}\{P_0^2, \rho_s(t)\} \right) \\ &+ \Gamma(\eta)(1+N(\eta)) \left(P_\eta \rho_s(t) P_\eta^\dagger - \tfrac{1}{2}\{P_\eta^\dagger P_\eta, \rho_s(t)\} \right) \\ &+ \Gamma(\eta) N(\eta) \left(P_\eta^\dagger \rho_s(t) P_\eta - \tfrac{1}{2}\{P_\eta P_\eta^\dagger, \rho_s(t)\} \right)\end{aligned}$$

Remember that $H_S = \eta/2 \left(|+\rangle\langle+| - |-\rangle\langle-| \right)$

$$P_\eta = \sin\theta |-\rangle\langle+| = (\Delta/\eta)|-\rangle\langle+|$$

$$P_\eta^+ = \sin\theta |+\rangle\langle-| = (\Delta/\eta)|+\rangle\langle-|$$

where $\eta = \sqrt{\varepsilon^2 + \Delta^2}$

and $P_0 = \cos\theta \left(|+\rangle\langle+| - |-\rangle\langle-| \right) = (\varepsilon/\eta)\left(|+\rangle\langle+| - |-\rangle\langle-| \right)$

we also stated that we require

$$\eta \gg \Gamma$$

for $\Gamma_0 \Rightarrow \quad \eta \gg 4\pi\alpha k_B T$

$$\Rightarrow \alpha \ll \frac{\eta}{4 k_B T}$$

for $\Gamma(\eta) \Rightarrow \quad \eta \gg 2\pi\alpha\eta \quad \Rightarrow \alpha \ll \frac{1}{2\pi}$

Actually, more generally, we should have

$$\eta \gg \Gamma(\eta)(1+N(\eta)) \Rightarrow \eta \gg 2\pi\alpha\eta(1+N(\eta))$$

$$\Rightarrow \alpha \ll 1/(2\pi(1+N(\eta)))$$

Note that if we consider similar conditions to Daley, i.e. $\varepsilon = 0$, then $\eta = \Delta$

and $\cos\theta = \frac{\varepsilon}{\eta} = 0$

$\sin\theta = \frac{\Delta}{\eta} = 1$

$\Rightarrow P_0 = 0 \quad , P_\eta = 1 - X + 1 \quad , P_\eta^+ = 1 + X - 1$

$$\Gamma(\eta) = \Gamma(\Delta) = 2\pi\alpha\Delta$$

$\therefore \Gamma(\Delta) = \frac{\Delta}{6}$ implies $2\pi\alpha\cancel{\Delta} = \frac{\cancel{\Delta}}{6}$

$$\Rightarrow \alpha = \frac{1}{12\pi}$$