3. Quantum Master Equation I.

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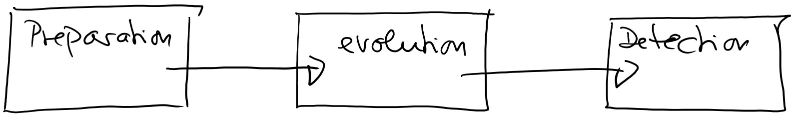
<u>Motivation</u>: complete description of the system's dynamics



$|\psi(0)\rangle$ $\qquad U(t,t_0)|\psi(t_0)\rangle = |\psi(t)\rangle \qquad |a^+|\psi(t)\rangle|^2 = \langle a^+ a\rangle$

$\rho(0) = \sum_n c_n |\psi(0)\rangle\langle\psi(0)| \qquad U(t,t_0)\rho(0)U^+(t,t_0) = \rho(t) \qquad tr(a^+ a \rho(t)) = \langle a^+ a\rangle$

conserved quantities

$\dot\rho = -\frac{i}{\hbar}[H,\rho]$ (i) Heisenberg picture $[a(t), a(t')] = \delta(t-t')\mathbb{1}$

(ii) Schrödinger picture $\langle\psi(t)|\psi(t)\rangle = 1$

(iii) Density matrix $tr(\rho(t)) = 1$

a nice and convenient way to prove consistency is via the trace $tr(\rho(t)) = 1$, $tr(\dot\rho) = 0$
$= tr(-\frac{i}{\hbar}[H,\rho]) = 0$

a very general open quantum formulation is Lindblad

$$\dot\rho_{system} = -\frac{i}{\hbar}[H_s, \rho_s] + D[J]\rho_s$$

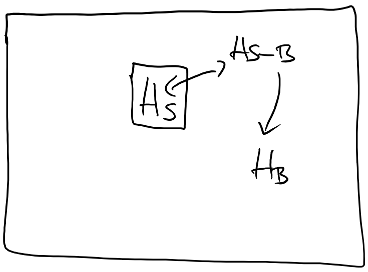
$\leftarrow$ arbitrary system operator

$$= -\frac{i}{\hbar}[H_s, \rho_s] + 2J\rho_s J^+ - J^+J\rho - \rho J^+ J$$

$$tr(\dot\rho_s) = -\frac{i}{\hbar}\underbrace{tr(H_s\rho_s - \rho_s H_s)}_{\substack{= tr(H_s\rho_s) - tr(H_s\rho_s) \\ = 0}} + \underbrace{2\underbrace{tr(J\rho_s J^+)}_{= tr(\rho_s J^+ J)} - \underbrace{tr(J^+J\rho) - tr(\rho J^+ J)}_{= 2\, tr(\rho_s J^+ J)}}_{= 0}$$

$= 0$ with initial condition $tr(\rho_s(0)) = 1$.

how to derive the Lindblad form?
and which assumptions are necessary?
let's start with a generic model



$H = H_S + H_B + \underline{H_{S+B}}$
interaction between system and bath

<u>given</u>: system and the bath are prepared in an initially <u>uncorrelated</u> state
$\rho(0) = \rho_S \otimes \rho_B$ (this assumption is almost always fulfilled, e.g.

excitons in semiconductors, or ions in traps)

Dynamics given via $\dot{\rho} = -\frac{i}{\hbar}[H, \rho]$

go to the interaction picture [important to discuss time-scales]

choose: $U(t,0) = \exp[-\frac{i}{\hbar}(H_S + H_B)t]$

remember: $i\hbar\frac{d}{dt}(\underbrace{U^+U}_{=\mathbb{1}}|\psi(t)\rangle) = i\hbar(\frac{d}{dt}U^+)\underbrace{U|\psi(t)\rangle}_{=|\psi\rangle_I} = HU^+U|\psi(t)\rangle$

$$\Rightarrow i\hbar\frac{d}{dt}|\psi(t)\rangle_I = [UHU^+ - i\hbar U\frac{d}{dt}U^+]|\psi(t)\rangle_I = H_I(t)|\psi(t)\rangle_I$$

with $|\psi(t)\rangle_I = U(t,0)|\psi(0)\rangle$

$$\dot{\rho} = \frac{d}{dt}(U^+U\rho U^+U) = \{\frac{d}{dt}U^+\}\rho_I + U^+\dot{\rho}_I U + U^+\rho_I\{\frac{d}{dt}U\}$$

$$= -\frac{i}{\hbar}HU^+U\rho U^+U + \frac{i}{\hbar}U^+U\rho U^+UH \quad |\cdot U^+, |U.$$

$$U\dot{U}^+\rho_I + \dot{\rho}_I + \rho_I\dot{U}U^+ = -\frac{i}{\hbar}UHU^+\rho_I + \frac{i}{\hbar}UHU^+$$

$$\dot{\rho}_I = -\frac{i}{\hbar}[H_I(t), \rho_I(t)] \quad , \quad \dot{U}^+ = \frac{i}{\hbar}(H_S + H_B)U^+$$

integrate formally $\rho_I(t) - \rho_I(0) = -\frac{i}{\hbar}\int_0^t dt'[H_I(t'), \rho_I(t')]$

$$\dot{\rho}_I = -\frac{i}{\hbar}[H_I(t), \rho_I(0) - \frac{i}{\hbar}\int_0^t dt'[H(t'), \rho_I(t')]]$$

$$= -\frac{i}{\hbar}[H_I(t), \rho_I(0)] - \frac{1}{\hbar^2}\int_0^t dt'[H_I(t), [H_I(t'), \rho_I(t')]]$$

$\Rightarrow t' = t - \tau, \; dt' = -d\tau$

$\tau = t - t'|_{t'=0} = t, \; \tau = t - t'|_{t'=t} = 0$

$$\dot{\rho}_I = -\frac{i}{\hbar}[H_I(t), \rho_I(0)] - \frac{1}{\hbar^2}\int_0^t d\tau[H_I(t), [H_I(t-\tau), \rho_I(t-\tau)]]$$

until now we are exact <u>but</u> $\rho_I(t-\tau)$ not known!!

for a large bath, equilibrium can be assumed, i.e. the bath stays constant in time $\Rightarrow$ system does not perturb the reservoir

$\Rightarrow$ Born factorization is justified

(i) $\rho_I(t-\tau) \approx \rho_S^I(t-\tau) \otimes \rho_B(t-\tau) \approx \rho_S^I(t-\tau)\rho_B(0)$

furthermore we assume that the system's dynamics is mainly affected by its present state while interacting with the reservoir (strong assumption, and is in general wrong but often all we can do)

$\Longrightarrow$ Markovian approximation

(ii) $\rho_I(t-\tau) \overset{\text{Born}}{\approx} \rho_S^I(t-\tau) \otimes \rho_B \approx \rho_S^I(t) \otimes \rho_B$

$$\dot{\rho}_I \approx -\frac{1}{\hbar^2}\int_0^t d\tau \left[H_I(t), \left[H_I(t-\tau), \rho_S^I(t) \otimes \rho_B \right]\right] - \frac{i}{\hbar}\left[H_I(t), \rho_I(0)\right]$$

transform back into the Schrödinger picture. $\quad \left| \cdot U(t,0) \right.$ $\quad U^\dagger(t,0)\cdot$

$$\dot{\rho} = -\frac{i}{\hbar}\left[H_S + H_B, \rho(t)\right] - \frac{i}{\hbar}\left[H_{SB}, \underbrace{\rho(-t)}\right] - \frac{1}{\hbar^2}\int_0^t d\tau \left[H_I, \left[H_I(-\tau), \rho_S(t) \otimes \rho_B\right]\right]$$

(Breuer / Petruccione, chap. 3)

$\rightarrow U^\dagger(t,0)\rho(0)U(t,0) = \rho(-t)$, $\quad U(t,0)\rho(0)U^\dagger(t,0) = \rho(t)$

$$H_I(t) = U H U^\dagger - i\hbar U \frac{d}{dt} U^\dagger = H_{SB}(t)$$

as we are only interested in the system, we trace out the bath's degrees of freedom

$$\mathrm{tr}_B(\dot{\rho}) = \dot{\rho}_S = -\frac{i}{\hbar}\left[H_S, \rho_S(t)\right] \underbrace{\mathrm{tr}_B(\rho_B)}_{=1}$$

$$-\frac{i}{\hbar}\underbrace{\mathrm{tr}_B\left\{\left[H_B, \rho_S(t) \otimes \rho_B\right]\right\}}_{=0}$$

$$-\frac{i}{\hbar}\underbrace{\mathrm{tr}_B\left\{\left[H_I, \rho(-t) \otimes \rho_B\right]\right\}}$$

$\rightarrow$ choose ρ_B in a way, this term vanishes, e.g. thermal state

$$-\frac{1}{\hbar^2}\int_0^t d\tau \; \mathrm{tr}_B\left\{\left[H_I, \left[H_I(-\tau), \rho_S(t) \otimes \rho_B\right]\right]\right\}$$

$$\boxed{\dot{\rho}_S = -\frac{i}{\hbar}[H_S, \rho_S(t)] - \frac{1}{\hbar^2}\int_0^t d\tau \, \mathrm{tr}_B \{ H_I H_I(-\tau)\rho_S(t)\rho_B - H_I \rho_S(t)\rho_B H_I(-\tau) - H_I(-\tau)\rho_S(t)\rho_B H_I + \rho_S(t)\rho_B H_I(-\tau) H_I \}}$$

final form. to evaluate further, we have to specify the system and the bath

let's choose a thermal bath $\rho_B = \frac{1}{Z}\exp[\beta \underbrace{\sum_k \hbar\omega_k r_k^+ r_k}_{=:H_B}]$

but we let the system operator very general

$$H_{S-B}(t) = H_I(t) = \hbar\sum_k [\, g_k \; r_k^+(t) J(t) + \hbar g_k^* \, r_k(t) \, J^+(t) \,]$$

$$J(t) = J^+(t) \quad [\ \sigma_z(t) = \sigma_z^+(t), \ J(t) = e^{i\omega_0 t}\sigma^+ + e^{-i\omega_0 t}\sigma^- \ \text{e.g.}\ ]$$

$$J(t) \neq J^+(t) \quad [\ J^+(t) = a^+ e^{i\omega_0 t}, \ J(t) = a e^{-i\omega_0 t} \ ]$$

define commutation for reservoir operators $[r_k, r_{k'}^+] = \delta(k-k')$

$$\langle r_k r_{k'} \rangle = \mathrm{tr}_B(\rho_B r_k r_{k'}) = 0 = \langle r_k^+ r_{k'}^+ \rangle$$

therefore, the memory kernel simplifies

$$R(t) = \sum_k g_k e^{-i\omega_k t} r_k, \quad R^+(t) = [R(t)]^+ = \sum_k g_k^* e^{i\omega_k t} r_k^+$$

$$\dot{\rho}_S = -\frac{i}{\hbar}[H_S, \rho_S] - \int_0^t d\tau \Big(\langle R^+ R(-\tau)\rangle J J^+(-\tau)\rho_S + \langle R R^+(-\tau)\rangle J^+ J(-\tau)\rho_S$$
$$+ \rho_S J^+(-\tau) J \langle R(-\tau) R^+\rangle + \rho_S J(-\tau) J^+ \langle R^+(-\tau) R\rangle$$
$$- \langle R^+(-\tau) R\rangle J^+ \rho_S J(-\tau) - \langle R(-\tau) R^+\rangle J \rho_S J^+(-\tau)$$
$$- \langle R^+ R(-\tau)\rangle J^+(-\tau)\rho_S J - \langle R R^+(-\tau)\rangle J(-\tau)\rho_S J^+ \Big)$$

$$\dot{\rho}_S = -\frac{i}{\hbar}[H_S, \rho_S] - \int_0^t d\tau \Big\{ \langle R^+ R(-\tau)\rangle \big(J J^+(-\tau)\rho_S - J^+(-\tau)\rho_S J \big)$$
$$+ \langle R^+(-\tau) R\rangle \big(\rho_S J(-\tau) J^+ - J^+ \rho_S J(-\tau) \big)$$
$$+ \langle R R^+(-\tau)\rangle \big(J^+ J(-\tau)\rho_S - J(-\tau)\rho_S J^+ \big)$$
$$+ \langle R(-\tau) R^+\rangle \big(\rho_S J^+(-\tau) J - J \rho_S J^+(-\tau) \big) \Big\}$$

<u>1. example</u>: assume $T = 0$ $\quad \rho_B \longrightarrow |vac\rangle\langle vac|$

$$\langle R^+ R\rangle = 0$$

$$\langle R R^+(-\tau)\rangle = \sum_{k,k'} g_k g_{k'}^* e^{-i\omega_{k'}\tau} \langle \underbrace{r_k r_{k'}^+}_{} \rangle \qquad +$$

$$= \delta(z-z') + r_{z'} r_z$$

$$= \sum_z |g_z|^2 e^{-i\omega_z \tau} = \sum_z \frac{\Delta z}{\Delta z} |g_z|^2 e^{-i\omega_z \tau} = \frac{1}{\Delta z} \int_0^\infty dz\, |g_z|^2 e^{-i\omega_z \tau}$$

$g_z = \sqrt{\Delta z}\, g_0 =$ const., therefore $\langle R R^+(-\tau)\rangle = g_0^2 \int_0^\infty dz\, e^{-i\omega_z \tau}$

$$\langle R R^+(-\tau)\rangle = g_0^2 \left(\pi \delta(\tau c) + i P \frac{\Lambda}{\omega} \right) = \frac{g_0^2 \pi}{c} \delta(\tau) + \text{shift}$$

and we yield a Lindblad version

$$\dot{\rho}_S = -\frac{i}{\hbar}[H_S, \rho_S] - \int_0^t d\tau\, \frac{\pi g_0^2}{c} \delta(\tau) \{ J^+ J(-\tau) \rho_S - J(-\tau) \rho_S J^+ + \rho_S J^+(-\tau) J - J \rho_S J^+(-\tau) \}$$

$$= -\frac{i}{\hbar}[H_S, \rho_S] + \underbrace{\frac{\pi g_0^2}{2c}}_{=:\Gamma} (2 J \rho_S J^+ - J^+ J \rho - \rho J^+ J)$$

$$= -\frac{i}{\hbar}[H_S, \rho_S] + D[\sqrt{\Gamma} J] \rho_S \quad \text{(Lindblad equation)}$$

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2. example: $T > 0$, $J(t) = J^+(t)$, $\rho(0) = \rho_S(0) \otimes \rho_B$, $\rho_B = \frac{1}{Z} e^{-\beta H_B}$

let's assume that the time evolution of our system operator is mainly governed by its free evolution

$$J(t) = \sigma^- e^{-i\omega_0 t} + \sigma^+ e^{i\omega_0 t}$$

(or in other words, the interaction with the reservoir does not change within the interaction of the system itself – dressed states do not matter)

then, $\langle R R^+(-\tau)\rangle = \sum_z |g_z|^2 e^{-i\omega_z \tau} (\bar{n}_z + 1)$

$\langle R^+(-\tau) R\rangle = \sum_z |g_z|^2 e^{-i\omega_z \tau}\, \bar{n}_z$, $\bar{n}_z = [\exp[\hbar\omega_z / k_B T] - 1]^{-1}$

$$\dot{\rho}_S = -\frac{i}{\hbar}[H_S, \rho_S] - \sum_z |g_z|^2 \int_0^t d\tau \Big\{ \bar{n}_z e^{i\omega_z \tau} \big(J (e^{-i\omega_0 \tau} \sigma^+ + e^{i\omega_0 \tau} \sigma^-) - (e^{-i\omega_0 \tau} \sigma^+ + e^{i\omega_0 \tau} \sigma^-) \rho_S J \big)$$
$$+ \bar{n}_z e^{-i\omega_z \tau} (\rho_S J(-\tau) J - J \rho_S J(-\tau))$$
$$+ (\bar{n}_z + 1) e^{-i\omega_z \tau} (J J(-\tau) \rho_S - J(-\tau) \rho_S J)$$
$$+ (\bar{n}_z + 1) e^{i\omega_z \tau} (\rho_S J(-\tau) J - J \rho_S J(-\tau)) \Big\}$$

now, we need the second Markovian approximation

$$\int_0^t d\tau \longrightarrow \int_0^\infty d\tau \,, \quad \int_0^\infty d\tau\, e^{i\Delta\tau} = \pi\,\delta(\Delta) - \underbrace{i\,P\frac{1}{\Delta}}_{\to \text{ shift}}$$

we yield two contributions $\int_0^\infty d\tau\, e^{i(\omega_0-\omega_k)\tau} = \pi\,\delta(\omega_k-\omega_0) + i\,P\frac{1}{\omega_k-\omega_0}$

and $\int_0^\infty d\tau\, e^{i(\omega_0+\omega_k)\tau} = \pi\,\underbrace{\delta(\omega_k+\omega_0)}_{\omega_0>0,\,\omega_k\geq 0} + i\,\underbrace{P\frac{1}{\omega_k+\omega_0}}_{\to 0}$

(effectively consistent with rotating wave approximation, post trace RWA)

$$\dot{\varrho}_S = -\frac{i}{\hbar}[H_S,\varrho_S] - \underbrace{\sum_k |g_k|^2\,\delta(\omega_0-\omega_k)}_{=\int d\omega\, J(\omega)}\Big[\bar{n}_k\big(J\sigma^+\varrho_S - \sigma^+\varrho_S J + \varrho_S\sigma^- J - J\varrho_S\sigma^-\big)$$
$$+(\bar{n}_k+1)\big(J\sigma^-\varrho_S - \sigma^-\varrho_S J + \varrho_S\sigma^+ \underbrace{J}_{J=\sigma^++\sigma^-} - J\varrho_S\sigma^+\big)\Big]$$

$$\dot{\varrho}_S = -\frac{i}{\hbar}[H_S,\varrho_S] + \int d\omega\, J(\omega)\,\bar{n}(\omega)\,D[\sigma^+]\varrho_S$$
$$+\int d\omega\, J(\omega)\,(\bar{n}(\omega)+1)\,D[\sigma^-]\varrho_S$$
$$+2\int d\omega\, J(\omega)\,(\sigma^+\varrho_S\sigma^+ + \sigma^-\varrho_S\sigma^-)$$