PHYS 414: 4-29-20

$$\hat{\rho}(t+\delta t) \simeq \sum_{\gamma=1}^{N^2} \hat{M}_\gamma \, \hat{\rho}(t) \, \hat{M}_\gamma^\dagger$$

GOAL: $\hat{\rho}(t+\delta t) = \hat{\rho}(t) + \sim\sim\sim \; \delta t$ keep track of low. order in δt

$\Rightarrow \dfrac{\partial}{\partial t} \hat{\rho}(t) = \sim\sim\sim$ Qu. master. equ.

special limiting case: turn off interact. b/t sys + env. $\Rightarrow$ isolated qu. sys

$$\hat{\rho}(t+\delta t) = \hat{U}_s \, \hat{\rho}(t) \, \hat{U}_s^\dagger$$

sys. Hamilt. $\hat{H}_s$ (time-ind. for simp.)

$$\Rightarrow \hat{U}_s = e^{-i\hat{H}_s \delta t/\hbar}$$

in this limit $\hat{M}_1 = \hat{U}_s$, $\hat{M}_\gamma = 0 \quad \gamma > 1$

$$\hat{\rho}(t+\delta t) = \left(\mathbb{1} - i\hat{H}_s \delta t/\hbar + \ldots\right) \hat{\rho}(t) \cdot \left(\mathbb{1} + i\hat{H}_s \delta t/\hbar + \ldots\right)$$

$$= \hat{\rho}(t) - \frac{i}{\hbar}\left[\hat{H}_s, \hat{\rho}(t)\right] \delta t + \ldots$$

$$\Rightarrow \frac{\partial \hat{\rho}}{\partial t} = -\frac{i}{\hbar}\left[\hat{H}_s, \hat{\rho}\right]$$

qu. master equ. for an isolated sys.
(von Neumann equation)

Put interact. w/ env. back on:

$$\hat{M}_1 \approx \mathbb{1} - \frac{i\hat{H}_s \delta t}{\hbar} + \underbrace{\hat{K}\,\delta t}$$

correction due to env. interactions at order δt

$\gamma > 1: \quad \hat{M}_\gamma = \sqrt{\delta t}\, \hat{L}_\gamma$

note: when env. is turned off $\hat{L}_\gamma, \hat{K} \to 0$

demand (to order δt):

$$\hat{\mathbb{1}} = \sum_\gamma \hat{M}_\gamma^\dagger \hat{M}_\gamma$$

$$= \hat{\mathbb{1}} + \delta t \underbrace{\left[2\hat{K} + \sum_{\gamma>1} \hat{L}_\gamma^\dagger \hat{L}_\gamma \right]}_{=0} + \cdots$$

$$\Rightarrow \hat{K} = -\frac{1}{2} \sum_{\gamma>1} \hat{L}_\gamma^\dagger \hat{L}_\gamma$$

Plug back into Kraus form for $\hat{\rho}(t+\delta t)$:

end-result:

$$\boxed{\frac{\partial \hat{\rho}}{\partial t} = -\frac{i}{\hbar}[\hat{H}_s, \hat{\rho}] + \underbrace{\sum_{\gamma>1} \left(\hat{L}_\gamma \hat{\rho} \hat{L}_\gamma^\dagger - \frac{1}{2} \hat{L}_\gamma^\dagger L_\gamma \hat{\rho} - \frac{1}{2} \hat{\rho} \hat{L}_\gamma^\dagger L_\gamma \right)}_{\text{effects of env. interactions on time evol. of } \hat{\rho}}}$$

Lindblad equation (1976): general quantum master equation

N^2-1 operators $\hat{L}_\gamma \Rightarrow$ Lindblad operators

Want: intuitive physical interpretation of $\hat{L}_\gamma$

To get there note the following:

Lindblad equ. structure is invariant under these transformations:

i) $\hat{L}_\gamma \to \hat{L}'_\gamma = \sum_\alpha U_{\gamma\alpha} \hat{L}_\alpha$ where U is a $(N^2-1)\times(N^2-1)$ unitary matrix

ii) $\hat{L}_\gamma \to \hat{L}'_\gamma = L_\gamma + c_\gamma$ where c_γ = complex number

$$\hat{\mathcal{H}}_s \to \hat{\mathcal{H}}'_s = \hat{\mathcal{H}}_s - \underbrace{\frac{i\hbar}{2} \sum_{\gamma > 1}' \left(c_\gamma^* \hat{L}_\gamma - c_\gamma \hat{L}_\gamma^\dagger \right)}_{\text{Hermitian}}$$

Turns out that because of these freedoms, we can transform to a set of $\hat{L}_\gamma$ w/ following properties:

$$\mathrm{tr}(\hat{L}_\gamma) = 0 \quad \text{for } \gamma > 1 \quad [\text{by choosing } c_\gamma]$$

$$\mathrm{tr}(\hat{L}_\gamma \hat{L}_\alpha^\dagger) = a_\gamma \delta_{\gamma\alpha} \quad [\text{by choosing } U]$$

where $a_\gamma \geq 0$ orthog. under Hilbert-Schmidt

$\mathrm{tr}(\hat{A} \hat{B}^\dagger)$
= Hilbert-Schmidt inner product b/t operators

Let's write $\hat{L}_\gamma = \sqrt{a_\gamma}\, \hat{\Lambda}_\gamma$ $\quad$ $\mathrm{tr}(\hat{\Lambda}_\gamma \hat{\Lambda}_\alpha^\dagger) = \delta_{\gamma\alpha}$

$\mathrm{tr}(\hat{\Lambda}_\gamma) = 0$

there is a unique set of $\hat{\Lambda}_\gamma$ satisfying this:

N-dim basis : $\{ |i\rangle \}$

two types of $\hat{\Lambda}_\gamma$

i) $\hat{\Lambda}_\gamma = |i\rangle\langle j|$ $\quad i \neq j$

"jump" operators $j \to i$

$N(N-1)$ diff. kinds

ii) $\hat{\Lambda}_\gamma = \dfrac{\hat{\mathbb{1}} - 2|i\rangle\langle i|}{\sqrt{N}}$ $\quad i = 2, 3, \ldots, N$

"dephasing" operators

$N-1$ diff. kinds

prefactors

encode the details of inter. w/ env.

$a_\gamma \equiv W_{ij}$

$a_\gamma = \Gamma_i$

concrete example: spin $\frac{1}{2}$ particle interacting w/ env.

$$N = 2 \qquad |\uparrow\rangle = |1\rangle$$
$$|\downarrow\rangle = |2\rangle$$

$N^2 - 1 = 3$ Lindblad operators:

$$\hat{\Lambda}_1 = |1\rangle\langle 2| = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}$$

$$\hat{\Lambda}_2 = |2\rangle\langle 1| = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}$$

$$\hat{\Lambda}_3 = \frac{1}{\sqrt{2}}\left(\hat{\mathbb{1}} - 2|2\rangle\langle 2|\right) = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

Let's denote $a_1 \equiv W_{12} \quad a_2 = W_{21} \quad a_3 = \Gamma_2$

$$\hat{L}_1 = \sqrt{W_{12}}\,\hat{\Lambda}_1 \qquad \hat{L}_2 = \sqrt{W_{21}}\,\hat{\Lambda}_2 \qquad \hat{L}_3 = \sqrt{\Gamma_2}\,\hat{\Lambda}_3$$

Choose our basis $\{|i\rangle\}$ to be basis where $\hat{H}_s$ is diagonal: $\hat{H}_s = \begin{pmatrix} E_1 & 0 \\ 0 & E_2 \end{pmatrix}$ for $N = 2$

a) take $\langle i| \frac{\partial \hat{\rho}}{\partial t} |i\rangle = \langle i|$ Lindblad equ. $|i\rangle$

algebra $\Rightarrow$ $$\frac{\partial \rho_{ii}}{\partial t} = \sum_j \left(\overbrace{W_{ij}\,\rho_{jj}}^{\text{gain}} - \overbrace{W_{ji}\,\rho_{ii}}^{\text{loss}} \right)$$

$$\hat{\rho} = \begin{pmatrix} \ddots & & \\ & \rho_{ii} & \\ & & \ddots \end{pmatrix}$$

diag. components of $\hat{\rho}$ obey a classical master equ w/ p_i replaced by ρ_{ii}

$N=2$: $$\frac{\partial}{\partial t}\begin{pmatrix}\rho_{11}\\ \rho_{22}\end{pmatrix} = \underbrace{\begin{pmatrix}-W_{21} & W_{12}\\ +W_{21} & -W_{12}\end{pmatrix}}_{\Omega \text{ matrix}}\begin{pmatrix}\rho_{11}\\ \rho_{22}\end{pmatrix}$$

vector of diag comp. $\begin{pmatrix}\rho_{11}\\ \rho_{22}\end{pmatrix}$ behaves like classical prob.

Sol'n to $N=2$: $$\rho_{ii}(t) = \rho_{ii}^{s} + (\rho_{ii}(0) - \rho_{ii}^{s})\, e^{-t/T_1} \qquad i=1,2$$

$$① \underset{W_{12}}{\overset{W_{21}}{\rightleftarrows}} ②$$

$$\rho_{11}^{s} = \frac{W_{12}}{W_{12}+W_{21}} \qquad \rho_{22}^{s} = \frac{W_{21}}{W_{12}+W_{21}}$$

related to Bloch eqn's in NMR or MRI famous T_1 time

$$T_1 = \frac{1}{W_{12}+W_{21}}$$ relaxation time to "equilibrium"

as $t \to \infty$, $t \gg T_1$ $\quad \rho_{ii}(t) \to \rho_{ii}^{s}$ stationary probabilities

$i \neq j$

analogously $$\langle i | \frac{\partial \hat{\rho}}{\partial t} | j \rangle = \langle i | \sim\sim\sim | j \rangle$$

$$\Rightarrow \frac{\partial \rho_{ij}}{\partial t} = (-i\omega_{ij} - \gamma_{ij})\, \rho_{ij}$$

$$\omega_{ij} = \frac{E_i - E_j}{\hbar} \qquad \gamma_{ij} = \frac{1}{2}\sum_k (W_{kj} + W_{ki}) + 2(\Gamma_i + \Gamma_j) \geq 0$$

$$\rho_{ij}(t) = e^{-i\omega_{ij}t}\, e^{-\gamma_{ij}t}\, \rho_{ij}(0)$$

for no env. interactions $W_{ij}, \Gamma_i \to 0 \Rightarrow \gamma_{ij} = 0$ | w/ env. interact. $\gamma_{ij} > 0 \Rightarrow \rho_{ij}(t) \to 0$ as $t \to \infty$

⇒ Decoherence under env. interactions

$$N=2: \quad \rho_{12}(t) = e^{-\frac{i}{\hbar}(E_1-E_2)t}\, e^{-t/T_2} \longrightarrow 0 \quad \text{for } t \gg T_2$$

$$T_2 = \frac{1}{\gamma_{12}} = \left(2\Gamma_2 + \frac{W_{12}+W_{21}}{2}\right)^{-1}$$

decoherence time

typically $T_2 \ll T_1$: for H^+ in protein

$T_1 \sim 250$ ms

$T_2 \sim 0.1-1$ ms

for timescales $t \gg T_2$ we have class. master equ. dynamics

in NMR we can use ext. field to initialize ensemble

$$\hat{\rho}(0) = |1\rangle\langle 1| = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \quad \text{all spins } \uparrow \text{ in ensemble}$$

time $\gg T_1, T_2$

$$\hat{\rho}(t) = \rho_{11}^s |1\rangle\langle 1| + \rho_{22}^s |2\rangle\langle 2| = \begin{pmatrix} \rho_{11}^s & 0 \\ 0 & \rho_{22}^s \end{pmatrix}$$

$$S(\hat{\rho}(0)) = 0 \rightsquigarrow S(\hat{\rho}(t))$$
$$= -\rho_{11}^s \ln \rho_{11}^s - \rho_{22}^s \ln \rho_{22}^s > 0$$

Missing links: MR relation $\quad \dfrac{W_{12}}{W_{21}} = e^{-\beta(E_1-E_2)}$

coupled to ext. degrees of freedom for work $\quad = e^{-\beta(E_1-E_2 + \dots)}$

no known purely quantum derivation of the MR & its generalizations

(recall that classically we derived these using ergodicity & mixing of total = sys + env.)

Duct tape sol'n: describe total = sys + env classically get MR

$$\Rightarrow \rho^s_{11} = \frac{e^{-\beta E_1}}{Z} \qquad \rho^s_{22} = \frac{e^{-\beta E_2}}{Z}$$

recover classical Boltzmann prob. for diag. elements of $\hat{\rho}$