Lindblad equ.
qu. master equ:

Sys. Hamiltonian

$\hat{M}_\gamma = \sqrt{\delta t}\,\hat{L}_\gamma$

Kraus op.

Lindblad eq.

$$\frac{d\hat{\rho}}{dt} = -\frac{i}{\hbar}[\hat{H}_s, \hat{\rho}] + \sum_{\gamma > 1} \left(\hat{L}_\gamma \hat{\rho} \hat{L}_\gamma^\dagger - \frac{1}{2}\hat{L}_\gamma^\dagger \hat{L}_\gamma \hat{\rho} - \frac{1}{2}\hat{\rho}\hat{L}_\gamma^\dagger \hat{L}_\gamma \right)$$

up to N^2-1 terms in sum (env. interactions)

this eq. is invariant (structure preserved) when:

i) $\hat{L}_\gamma \to \hat{L}_\gamma' = \sum_\alpha U_{\gamma\alpha} L_\alpha$ where $U_{\gamma\alpha}$ are comp's of unitary $(N^2-1)\times(N^2-1)$ matrix

ii) $\hat{L}_\gamma \to \hat{L}_\gamma' = L_\gamma + c_\gamma$ (complex # const.)

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

Using these freedoms, we choose a set of $\hat{L}_\gamma$ w/ following properties:

$$\mathrm{tr}(\hat{L}_\gamma) = 0 \quad \text{for } \gamma > 1$$ [use ii choose c_γ]

$$\mathrm{tr}(\hat{L}_\gamma \hat{L}_\alpha^\dagger) = \alpha_\gamma \delta_{\gamma\alpha}$$ [using i, choosing U]

Hilbert-Schmidt inner product

Some number $a_\gamma \geq 0$

Kronecker delta

$$\hat{A}, \hat{B} \Rightarrow \mathrm{tr}(\hat{A}\hat{B}^\dagger)$$

$\Rightarrow$ these properties give a unique set of $\hat{L}_\gamma$

Write: $\hat{L}_\gamma = \sqrt{a_\gamma}\, \hat{\Lambda}_\gamma$ $\qquad \mathrm{tr}(\hat{\Lambda}_\gamma \hat{\Lambda}_\alpha^\dagger) = \delta_{\gamma\alpha}$

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

two types of $\hat{\Lambda}_\gamma$, write in a Hilbert space w/ basis elements $\{|i\rangle\}$ N-dim.

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

$$\begin{array}{c|cccc} & & & j & \\ \hline & 0 & 0 & 0 & 0 \\ i & 0 & 0 & 1 & 0 \\ & 0 & 0 & 0 & 0 \\ & 0 & 0 & 0 & 0 \end{array}$$

"jump" $j \to i$; $\hat{\Lambda}_\gamma |j\rangle = |i\rangle$

$N(N-1)$ distinct jump op's labeled by i, j

coeffs: $a_\gamma \Rightarrow \Omega_{ij}$

$$\hat{L}_\gamma = \sqrt{\Omega_{ij}}\, |i\rangle\langle j|$$ "jump" operators

$|i\rangle\langle j|$

$(|k\rangle\langle l|)^\dagger = |l\rangle\langle k|$

$$|i\rangle \underbrace{\langle j | l\rangle}_{\delta_{jl}} \langle k| = |i\rangle\langle k|\, \delta_{jl}$$

b) $\hat{\Lambda}_\gamma = \frac{\hat{I} - N|i\rangle\langle i|}{\sqrt{N}}$ $\quad i = 2, 3, \ldots, N$

$$\frac{1}{\sqrt{N}} \begin{array}{cc} & i \\ & \begin{pmatrix} 1 & & & & \\ & 1 & & & \\ & & -N & & \\ & & & 1 & \\ & & & & 1 \end{pmatrix} \end{array} i$$

N-1 operators

act on superimposition of basis states $|i\rangle$

$\Rightarrow$ change phases b/t the $|i\rangle$ states

$\Rightarrow$ "dephasing" operators

coeffs: $\alpha_\gamma \Rightarrow \Gamma_i$

$$\hat{L}_\gamma = \sqrt{\Gamma_i} \left(\frac{\hat{I} - N|i\rangle\langle i|}{\sqrt{N}} \right)$$

plug these op's into Lindblad.

Choose a basis $\{|i\rangle\}$ where $\mathcal{H}_s = \begin{pmatrix} E_1 & & 0 \\ & \ddots & \\ 0 & & E_N \end{pmatrix}$

diag.

$\langle i |$ Lindblad $| i \rangle$

$$\langle i | \frac{\partial \hat{\rho}}{\partial t} | i \rangle = \langle i | \text{RHS} | i \rangle$$

algebra $\Rightarrow$ $\frac{\partial \rho_{ii}}{\partial t} = \sum_{j=1}^{N} (\underbrace{\Omega_{ij} \rho_{jj}}_{\text{prob. into } |i\rangle} - \underbrace{\Omega_{ji} \rho_{ii}}_{\text{prob. out of } |i\rangle})$

conserv. of probability

$$\sum_i \rho_{ii} = 1$$

prob. to jump $|j\rangle \to |i\rangle$ | prob. of $|j\rangle$ | prob. to jump $|i\rangle \to |j\rangle$ | prob. of $|i\rangle$

ρ_{ii} ~ "classical prob."

~ prob. to measure $|i\rangle$ in ensemble

define Ω matrix:

off-diag. Ω_{ij} coeff's

diag: $\Omega_{ii} = -\sum_j \Omega_{ji}$

$$\Rightarrow \frac{\partial \rho_{ii}}{\partial t} = \sum_j \Omega_{ij} \rho_{jj}$$

derived a version of classical master equ.

classical master equ: $\vec{p}(t+\delta t) = W \vec{p}(t)$

$$\Rightarrow \frac{d\vec{p}}{dt} = \Omega \vec{p}$$

$$\Omega = \frac{(W - I)}{\delta t}$$

matrix of prob. rates

$$\langle i | \frac{\partial \hat{\rho}}{\partial t} | j \rangle = \langle i | \mathrm{RHS} | j \rangle$$

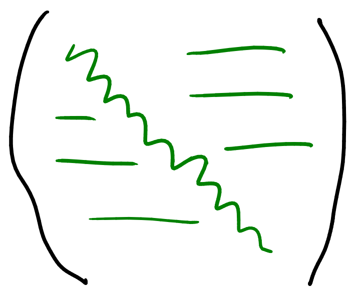
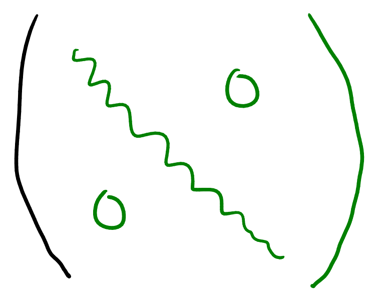
algebra: $$\frac{\partial \rho_{ij}}{\partial t} = (-i\omega_{ij} - \gamma_{ij}) \rho_{ij}$$

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

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

as $t \to \infty$, $\rho_{ij}(t) \to 0$

decoherence

$\hat{\rho}(0) =$  $\xrightarrow[t \to \infty]{}$ $\hat{\rho}(t) =$ 

decoherence time scale for H^+ in a protein under MRI : $T_2 \approx 0.1 - 1$ ms

decoh. time $\rho_{ij} \to 0$ $i \neq j$

diag. elements

$\rho_{ii} \longrightarrow$ stationary state ρ_{ii}^{s}

timescale : $T_1 \approx 250$ ms

missing element: $\Omega = \dfrac{(W - I)}{\delta t}$

class. matrix satisfied LDB:

$$\frac{W_{ij}}{W_{ji}} = e^{-\beta(E_i - E_j)}$$