Dynamics of Open Systems

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closed system $H=H_A+V+H_B$

$$\langle O \rangle_t = \langle \psi(t) | O | \psi(t) \rangle$$

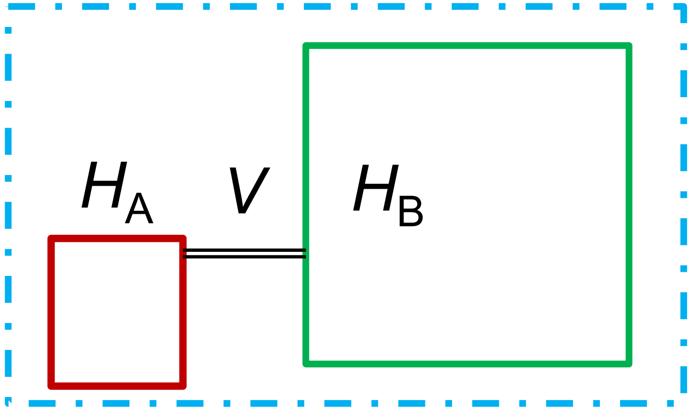
$$| \psi(t) \rangle = U_{t,t_0} | \psi_0 \rangle$$

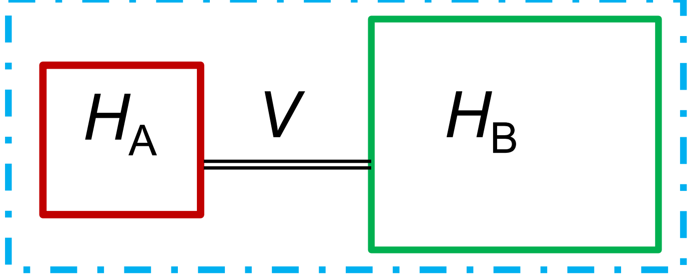
$$U_{t,t_0} = \Omega_{t_0}^{t} \left[\frac{1}{i\hbar} H\right] \longrightarrow \exp\left[-\frac{i}{\hbar}(t-t_0)H\right]$$

open system

Is there a state vector $|\psi\rangle^{\text{o.s.}}$??

a self–adjoint $H^{\text{o.s.}}$ and unitary $U_{t,t_0}^{\text{o.s.}}$??





Concept of "state vector" and "evolution operator" must be generalized

closed system $H=H_A+V+H_B$

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$$\langle O \rangle_t = \mathrm{Tr}\,\{O\rho_t\}$$

$$|\psi(t)\rangle \longrightarrow \rho_t = |\psi(t)\rangle\langle\psi(t)| \quad \text{pure}$$

$$U_{t,t_0} \longrightarrow \mathcal{U}_{t,t_0} = \Omega^t_{t_0}\left[\tfrac{1}{\mathrm{i}\hbar}\widehat{H}\right] \equiv \underline{U_{t,t_0}}\ \overline{U^\dagger_{t,t_0}}$$

$$\widehat{H}\,O = [H\,,\,O]$$

open system

Is there a state vector $|\psi\rangle^{\text{o.s.}}$??

a self–adjoint $H^{\text{o.s.}}$ and unitary $U^{\text{o.s.}}_{t,t_0}$?

"open–system state" $\left|\rho^A_t\right) = \mathcal{E}_{t,t_0}\left|\rho^A_0\right)$

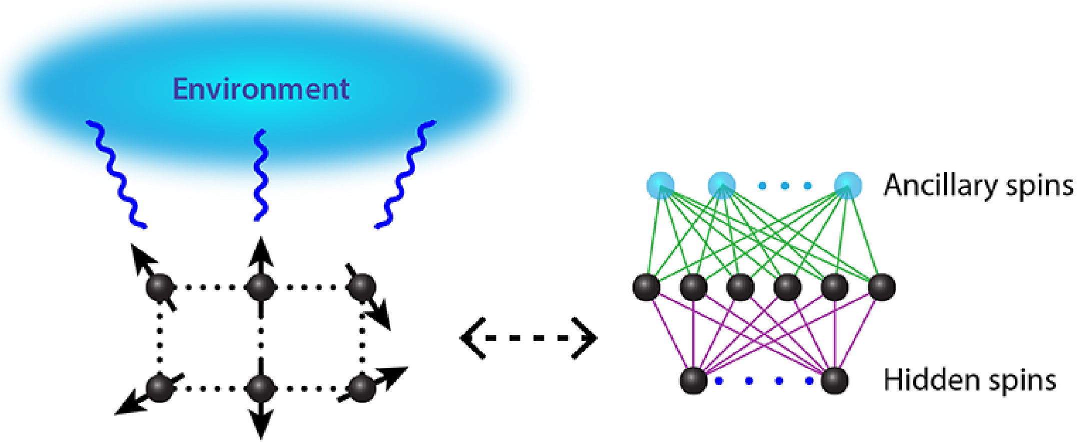
closed-system state $\left|\rho_t\right) = \mathcal{U}_{t,t_0}\left|\rho_0\right)$

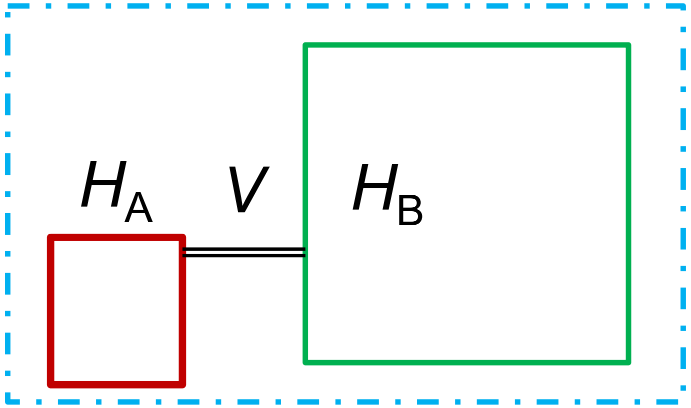
non-unitary ``evolutor´´

unitary ``evolutor´´

- represented by $(d_A^2 \times d_A^2)$ - matrix

Physics **VIEWPOINT**





$$\rho^{A}_{\text{steady}} = \lim_{t\to\infty} \rho^{A}_{t}$$

Figure 1: Four teams have designed a neural network (right) that can find the stationary steady states for an ``open'' quantum system (left). Their approach is built on neural network models for closed systems, where the wave function was represented by a statistical distribution over ``visible spins'' connected to a number of ``hidden spins.'' To extend the idea to an open system, three of the teams [35] added in a third set of ``ancillary spins,'' which capture correlations between the system and environment.
(APS/Alan Stonebraker)

by Maria Schuld, Ilya Sinayskiy, and Francesco Petruccione

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$$|i;\mu\rangle = |i\rangle \otimes |\mu\rangle$$

$$W_{i\to f}(t) = \sum_\nu \sum_\mu |\langle f;\nu | U_{t,t_0} | i,\mu\rangle|^2 p_\mu$$

probability to find A-system in $|f>$ at time t, provided it was in $|i>$ initially

$$W_f(t) = \sum_i p_i W_{i\to f}(t)$$

$$= \sum_\nu \sum_i p_i \sum_\mu p_\mu \langle f;\nu | U_{t,t_0} | i;\mu\rangle\langle i;\mu | U^\dagger_{t,t_0} | f;\nu\rangle$$

$$= \langle f | \underbrace{\mathrm{Tr}_B\left\{U_{t,t_0}\left(\rho_0^A \otimes \rho^B\right) U^\dagger_{t,t_0}\right\}} | f\rangle$$

open-system statistical operator

$$\rho^B = \sum_\nu |\mu\rangle p_\mu \langle\mu|$$

$$\rho_0^A = \sum_i |i\rangle p_i \langle i|$$

$$W_f(t) = \langle f | \rho_t^A | f\rangle = \mathrm{Tr}_A\left\{P_f\, \rho_t^A\right\}$$

probability to find A-system in $|f>$ at time t

$$P_f = |f\rangle\langle f|$$

$$A = \sum_f a_f P_f$$

$$\langle A\rangle_t = \sum_f a_f W_f(t) \quad = \mathrm{Tr}_A\left\{A\, \rho_t^A\right\}$$

expectation value of open-system observable A closed system

$$\langle A \rangle_t = \langle \psi(t) \,|\, A \,|\, \psi(t) \rangle$$

$$|\, \psi(t) \rangle = U_{t,t_0} \,|\, \psi_0 \rangle$$

$$U_{t,t_0} = \Omega^t_{t_0}\left[\tfrac{1}{\mathrm{i}\hbar} H\right] \longrightarrow \exp\left[-\tfrac{\mathrm{i}}{\hbar}(t - t_0) H\right]$$

open system

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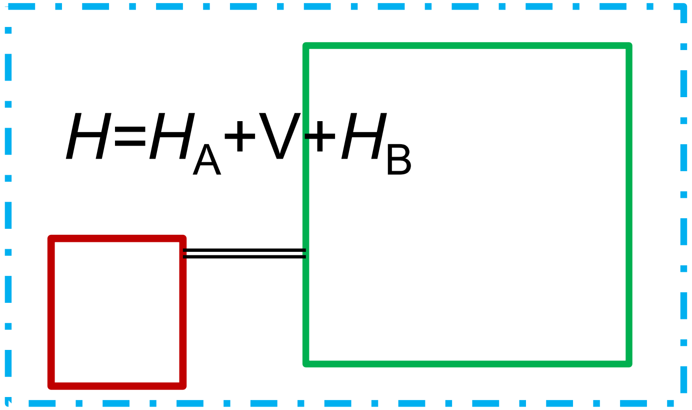
"open–system state" $\left|\, \rho^{\mathrm{A}}_t \right) = \mathcal{E}_{t,t_0} \left|\, \rho^{\mathrm{A}}_0 \right)$

non-unitary ``evolutor´´



$$\mathrm{i}\hbar \frac{\mathrm{d}}{\mathrm{d}t} \rho_t = [H_t \,,\, \rho_t] = \widehat{H}_t \rho_t \Longleftrightarrow \rho_t = \Omega^t_{t_0}\left[\frac{1}{\mathrm{i}\hbar} \widehat{H}\right] \rho_0$$

$$\rho^{\mathrm{A}}_t = \mathrm{Tr}_{\mathrm{B}} \left\{ \overbrace{U_{t,t_0} \left(\rho^{\mathrm{A}}_0 \otimes \rho^{\mathrm{B}} \right) U^{\dagger}_{t,t_0}} \right\}$$

$$\left|\, \rho^{\mathrm{A}}_t \right) = \left\langle \Omega^t_{t_0}\left[\frac{1}{\mathrm{i}\hbar} \widehat{H}\right] \right\rangle_{\mathrm{B}} \left|\, \rho^{\mathrm{A}}_0 \right)$$

Derivation: master equation

Idempotents

$\mathcal{P} = \mathcal{I}^{\mathsf{A}} \otimes \rho^{\mathsf{B}}\} \mathrm{Tr}_{\mathsf{B}}\{\mathcal{I}^{\mathsf{B}} = \mathcal{P}^2$ and $\mathcal{Q} = \mathcal{I} - \mathcal{P}$

imply decomposition of any $\mathcal{X}$

$$\begin{aligned} \mathcal{X} &= (\mathcal{P}+\mathcal{Q})\mathcal{X}(\mathcal{P}+\mathcal{Q}) \\ &= \underbrace{\mathcal{P}\mathcal{X}\mathcal{P}+\mathcal{Q}\mathcal{X}\mathcal{Q}}_{\mathcal{X}'}+\underbrace{\mathcal{P}\mathcal{X}\mathcal{Q}+\mathcal{Q}\mathcal{X}\mathcal{P}}_{\mathcal{X}''} \end{aligned}$$

with properties

$$\mathcal{P}\mathcal{X}' = \mathcal{P}\mathcal{X}'\mathcal{P} = \mathcal{X}'\mathcal{P}\,, \qquad \mathcal{Q}\mathcal{X}' = \mathcal{Q}\mathcal{X}'\mathcal{Q} = \mathcal{X}'\mathcal{Q}$$
$$\mathcal{P}\mathcal{X}'' = \mathcal{P}\mathcal{X}\mathcal{Q} = \mathcal{X}''\mathcal{Q}\,, \qquad \mathcal{Q}\mathcal{X}'' = \mathcal{Q}\mathcal{X}\mathcal{P} = \mathcal{X}''\mathcal{P}$$

employed in finding open–system 'evolutor'

$$\mathcal{E}_{t,t_0} = \left\langle \Omega^t_{t_0}[\mathcal{X}] \right\rangle_{\mathsf{B}} \qquad \mathcal{X}_t = \frac{1}{\mathrm{i}\hbar}\widehat{H}_t$$

$$\mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}t}\rho_t = [H_t\,,\,\rho_t] \equiv \widehat{H}_t\rho_t \iff \rho_t = \Omega^t_{t_0}[\mathcal{X}]\,\rho_0$$

$$\begin{aligned} \frac{\partial}{\partial t}\mathcal{E}_{t,t_0} &= \left\langle \mathcal{X}_t\, \Omega^t_{t_0}[\mathcal{X}] \right\rangle_{\mathsf{B}} \\ &= \left\langle \mathcal{X}_t\,(\mathcal{P}+\mathcal{Q})\,\Omega^t_{t_0}[\mathcal{X}] \right\rangle_{\mathsf{B}} \\ &= \langle \mathcal{X}_t \rangle_{\mathsf{B}}\,\mathcal{E}_{t,t_0} + \left\langle \mathcal{X}_t\mathcal{Q}\,\Omega^t_{t_0}[\mathcal{X}]\mathcal{P} \right\rangle_{\mathsf{B}} \end{aligned}$$

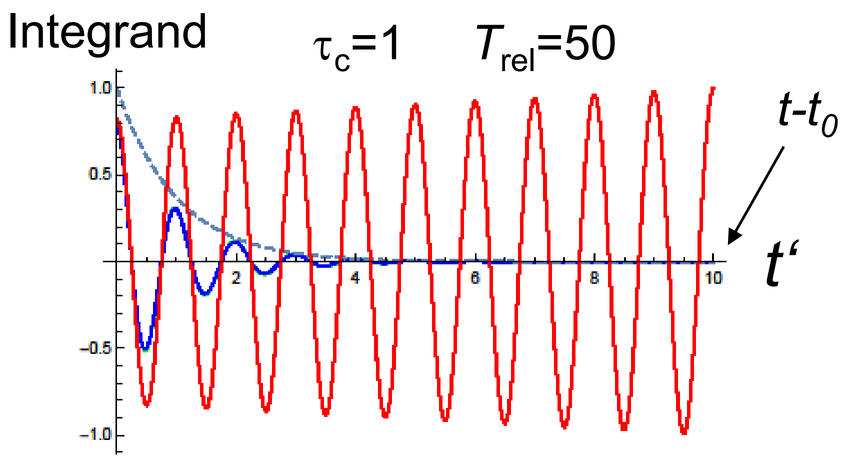
$$\Omega^t_{t_0}[\mathcal{X}] = \Omega^t_{t_0}[\mathcal{X}'] + \int_{t_0}^{t}\mathrm{d}\tau\;\Omega^t_\tau[\mathcal{X}']\,\mathcal{X}''_\tau\,\Omega^\tau_{t_0}[\mathcal{X}]$$

$[\mathcal{Q}\,,\,\mathcal{X}'] = 0$ and $\mathcal{Q}\mathcal{X}'' = \mathcal{Q}\mathcal{X}\mathcal{P}$ imply

$$\mathcal{Q}\,\Omega^t_{t_0}[\mathcal{X}]\mathcal{P} = \int_{t_0}^{t}\mathrm{d}\tau\;\Omega^t_\tau[\mathcal{Q}\mathcal{X}\mathcal{Q}]\,\mathcal{Q}\mathcal{X}_\tau\,\mathcal{P}\Omega^\tau_{t_0}[\mathcal{X}]\mathcal{P}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\rho^{\mathsf{A}}_t = \langle \mathcal{X}_t \rangle_{\mathsf{B}}\,\rho^{\mathsf{A}}_t - \int_0^{t-t_0}\mathrm{d}t'\;\mathcal{M}(t;t-t')\rho^{\mathsf{A}}_{t-t'}$$

$$\mathcal{M}(t;\tau) = \mathrm{i}^2\left\langle \mathcal{X}_t\mathcal{Q}\;\Omega^t_\tau[\mathcal{Q}\mathcal{X}\mathcal{Q}]\,\mathcal{Q}\mathcal{X}_\tau \right\rangle_{\mathsf{B}}$$



GME (non–Markovian) $\qquad \mathcal{X}_t \to -\frac{i}{\hbar}\widehat{H}_t$

$$\frac{d}{dt}\rho_t^A = -\frac{i}{\hbar}\left\langle \widehat{H}_t \right\rangle_B \rho_t^A - \int_0^{t-t_0} dt' \ \mathcal{M}(t;t-t')\rho_{t-t'}^A$$

$$\mathcal{M}(t;\tau) = \frac{1}{\hbar^2}\left\langle \widehat{H}_t \mathcal{Q} \ \Omega_\tau^t \left[-\frac{i}{\hbar}\mathcal{Q}\widehat{H}\mathcal{Q}\right] \mathcal{Q}\widehat{H}_\tau \right\rangle_B$$

$$\rho_{t-t'}^A \ \longrightarrow \ \Omega_t^{t-t'}\left[-\frac{i}{\hbar}\left\langle \widehat{H}\right\rangle_B\right]\rho_t^A$$

$$t_0 = -\infty \quad \Longrightarrow \quad \mathrm{Min}(t-t_0) \gg \tau_c,$$

ME (Markovian)

$$\frac{d}{dt}\rho_t^A = \left\{-\frac{i}{\hbar}\left\langle \widehat{H}_t \right\rangle_B - \mathcal{R}_t\right\}\rho_t^A$$

$$\mathcal{R}_t = \int_0^\infty dt' \ e^{-ot'}\mathcal{M}(t;t-t') \ \Omega_t^{t-t'}\left[-\frac{i}{\hbar}\left\langle \widehat{H}\right\rangle_B\right]$$

ME (time–homogeneous Markovian)

$$H_t \to H_A' + \Delta V + H_B$$

$$\left\langle \widehat{H}_t \right\rangle_B \to \hbar\mathcal{L}_A' , \qquad \widehat{\Delta V}_t \to \hbar\mathcal{V}$$

$$\mathcal{R}_t \to \int_0^\infty d\tau \ e^{-o\tau}\left\langle \mathcal{V}e^{-i\tau(\mathcal{L}_A'+\mathcal{L}_B+\mathcal{Q}\mathcal{V}\mathcal{Q})}\mathcal{V}\right\rangle_B e^{i\tau\mathcal{L}_A'}$$

$$\frac{d}{dt}\rho_t^A = \left(-i\mathcal{L}_A' - \mathcal{R}\right)\rho_t^A \Longleftrightarrow \rho_t^A = e^{t(-i\mathcal{L}_A'-\mathcal{R})}\rho_0^A$$

Born–Markov

$$\mathcal{R} = \int_0^\infty d\tau \ e^{-o\tau}\left\langle \mathcal{V}\mathcal{V}(-\tau)\right\rangle_B$$

Steady state:

$$\left(-i\mathcal{L}_A' - \mathcal{R}\right)\rho_{\mathrm{steady}}^A = 0$$

$$\left(m\,n\middle|\mathcal{R}\middle|k\,l\right) = \delta_{mk}\delta_{ln}\left[\Gamma_{k\,l} + \frac{\mathrm{i}}{\hbar}(\Delta E_k - \Delta E_l)\right] + (1-\delta_{km})\delta_{mn}\delta_{kl}\,[-w_{k\to m}]$$

$$\Gamma_{k\,l} = \Gamma^{\mathrm{ine}}_{k\,l} + \Gamma^{\mathrm{ela}}_{k\,l}\,, \qquad \Delta E_n = \sum_s \Delta\varepsilon_{n\to s}$$

$$\Gamma^{\mathrm{ine}}_{k\,l} = \frac{\gamma_k+\gamma_l}{2}\,, \qquad \Gamma^{\mathrm{ine}}_{k\,k} = \gamma_k \equiv \sum_{s(\neq k)}{}' w_{k\to s}$$

$$\Gamma^{\mathrm{ela}}_{k\,l} = \frac{w_{k\,k}+w_{l\,l}-w_{k\,l}-w_{l\,k}}{2}\,, \qquad \Gamma^{\mathrm{ela}}_{kk} = 0\,.$$

inelastic

$\hbar = 1$

$$w_{n\to s} = \left\langle \delta V^{\dagger}_{n\to s} 2\pi\delta(\omega_{ns}-\mathcal{L}_{\mathrm{B}})\delta V_{n\to s}\right\rangle_{\mathrm{B}} \geq 0$$

$$\Delta\varepsilon_{n\to s} = \left\langle \delta V^{\dagger}_{n\to s}\frac{\mathrm{PP}}{\omega_{ns}-\mathcal{L}_{\mathrm{B}}}\delta V_{n\to s}\right\rangle_{\mathrm{B}} = \Delta\varepsilon^{*}_{n\to s}$$

$$w_{n\,s} = \left\langle \delta V^{\dagger}_{n\to n} 2\pi\delta(\mathcal{L}_{\mathrm{B}})\delta V_{s\to s}\right\rangle_{\mathrm{B}} = w^{*}_{n\,s} = w_{s\,n}$$

$$\Delta\varepsilon_{n\,s} = \left\langle \delta V^{\dagger}_{n\to n}\frac{\mathrm{PP}}{-\mathcal{L}_{\mathrm{B}}}\delta V_{s\to s}\right\rangle_{\mathrm{B}} = -\Delta\varepsilon^{*}_{n\,s} = -\Delta\varepsilon_{s\,n}$$

elastic

Open two–state system (qubit)

'Evolutor' $\mathcal{E}_t$ is represented by (4×4) Matrix $\mathcal{E}_t = \mathrm{e}^{t(-\mathrm{i}\mathcal{L}'_{\mathrm{A}}-\mathcal{R})}$ is easily evaluated analytically (thanks to MATHEMATICA's built-in function 'MatrixExponent')

$$\rho^{\mathrm{A}}_{\mathrm{steady}} = \frac{\begin{bmatrix} w_{1\to0} & 0 \\ 0 & w_{0\to1} \end{bmatrix}}{w_{0\to1} + w_{1\to0}} = \frac{\begin{bmatrix} 1 & 0 \\ 0 & \mathrm{e}^{-\frac{\Delta}{kT}} \end{bmatrix}}{1 + \mathrm{e}^{-\frac{\Delta}{kT}}}$$

Gorini-Kossakowski-Sudarshan-Lindblad equation (GKSL)

$$\begin{aligned}\frac{\mathrm{d}\rho_t^{\mathsf{A}}}{\mathrm{d}t} &= (-\mathrm{i}\mathcal{L}'_{\mathsf{A}} - \mathcal{R})\rho_t^{\mathsf{A}} \\ &= \sum_{i,j} d_{ij}\left\{2F_i\rho_t^{\mathsf{A}}F_j^\dagger - \left[F_j^\dagger F_i\,,\,\rho_t^{\mathsf{A}}\right]_+\right\} \\ &\quad -\frac{\mathrm{i}}{\hbar}\left[H'_{\mathsf{A}} + \sum_{i,j} h_{ij}F_j^\dagger F_i\,,\,\rho_t^{\mathsf{A}}\right]\end{aligned}$$

$$\begin{aligned}F_i \rightarrow \quad P_{ss'} &= |\,s\,\rangle\langle\,s'\,| \\ d_{ij} \rightarrow d_{ss'\,\bar{s}\bar{s}'} &= \delta_{s\bar{s}}\delta_{s'\bar{s}'}\left[\frac{w_{s'\to s}}{2}\right] \\ &\quad +\delta_{ss'}\delta_{\bar{s}\bar{s}'}(1-\delta_{s\bar{s}})\left[\frac{w_{\bar{s}\,s}}{2}\right] \\ h_{ij} \rightarrow h_{ss'\,\bar{s}\bar{s}'} &= \delta_{s\bar{s}}\delta_{s'\bar{s}'}\;\Delta\varepsilon_{s'\to s}\end{aligned}$$