Open quantum systems

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Closed quantum systems

Hilbert space of states $\mathcal{H}$

- pure state: $\psi \in \mathcal{H}$, $\|\psi\| = 1$
- mixed state: density matrix $\rho \in \mathcal{B}(\mathcal{H})$

Observables: $A \in \mathcal{B}(\mathcal{H}) \qquad (A = A^*)$

Hamiltonia

Dynamics: • Schrödinger
$$\begin{cases} \psi_t = e^{-itH}\psi_0 \\ \rho_t = e^{-itH}\rho_0 e^{itH} \end{cases}$$

• Heisenberg $\quad A_t = e^{itH} A e^{-itH}$

Average of observable in state:

$$\langle A \rangle_t = \mathrm{Tr}(\rho_t A) = \mathrm{Tr}(\rho A_t)$$

Dynamics is generated by Hamiltonian —
a group — energy is conserved $\quad H_t = H, \ \forall t.$

Physics determines Hilbert space

* **Particle in a potential**

$$\mathcal{H} = L^2(\mathbb{R}^3, d^3x) \;, \quad H = -\Delta + V$$

$\psi_t \in \mathcal{H}$: $\quad |\psi_t(x)|^2$ probability density for location of particle

* **A spin $\frac{1}{2}$; a qubit**

$$\mathcal{H} = \mathbb{C}^2 \;, \quad H = \frac{1}{2}\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \;, \quad \psi_{up} = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \quad \psi_{down} = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$$

$\psi_t \in \mathbb{C}^2$: $\quad \psi_t = a_t \psi_{up} + b_t \psi_{down}$

$|a_t|^2$ probability of being in state 'up'

* **Photons**

$$\mathcal{H} = \bigoplus_{n=0}^{\infty} L^2_{sym}(\mathbb{R}^{3n}, d^{3n}k) \;, \quad H = d\Gamma(|k|)$$

$\psi_t \in \mathcal{H}$: $\quad \psi_t = \{ [\psi_t]_n \}$

$|[\psi_t]_n(k_1, \dots, k_n)|^2$ probability density for n particles in momentum space

Composite systems

$$\left.\begin{array}{ll}\mathcal{H}_1, & H_1 \\ \mathcal{H}_2, & H_2\end{array}\right\}$$ two quantum systems

- composite system Hilbert space $\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2$
- composite system Hamiltonian $H = H_1 \otimes \mathbb{1} + \mathbb{1} \otimes H_2 + V$

interaction

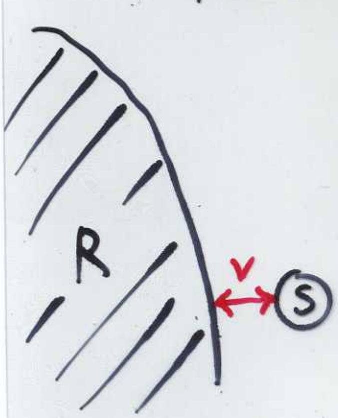
An open quantum system is

- a system in contact with another one
- the reduction of a composite system to one of its subsystems

Most often: system - reservoir models

- few degrees of freedom

- infinitely extended
- characterized by thermodyn. parameters
- source of 'noise'



Dynamics of open system $\quad (\underline{\mathcal{H}_S} \otimes \mathcal{H}_R)$

A observable of S only

$$\langle A \rangle_t = \mathrm{Tr}_{R+S}\left(\rho_t\,(A \otimes \mathbb{1}_R)\right) = \mathrm{Tr}_S\left(\left(\mathrm{Tr}_R\,\rho_t\right) A\right)$$

$$=: \mathrm{Tr}_S\left(\bar{\rho}_t\, A\right) \qquad \bar{\rho}_t := \mathrm{Tr}_R\,\rho_t \quad \text{reduced density matrix.}$$

Evolution of reduced density matrix: restriction to open system S destroys hamiltonian nature of dynamics!

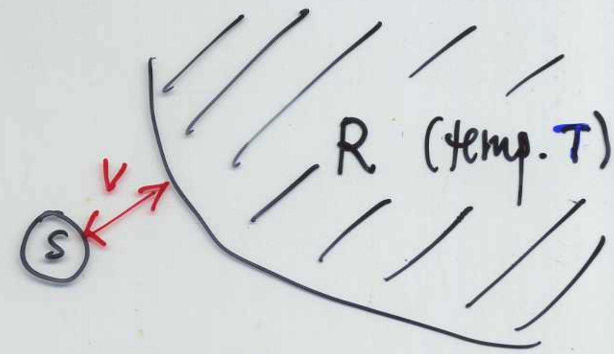
$$\bar{\rho}_t = \mathrm{Tr}_R\left(e^{-itH}\rho_0\, e^{+itH}\right) \neq e^{-itH_{red}}\, \underbrace{\mathrm{Tr}_R(\rho)}_{\bar{\rho}_0}\, e^{+itH_{red}}$$

E.g. $t \mapsto \bar{\rho}_t$ does not even have group property.

Dynamics of $\bar{\rho}_t$ is complicated $\rightarrow$ approximations, simplifications

Open systems models

- **Close to equilibrium**

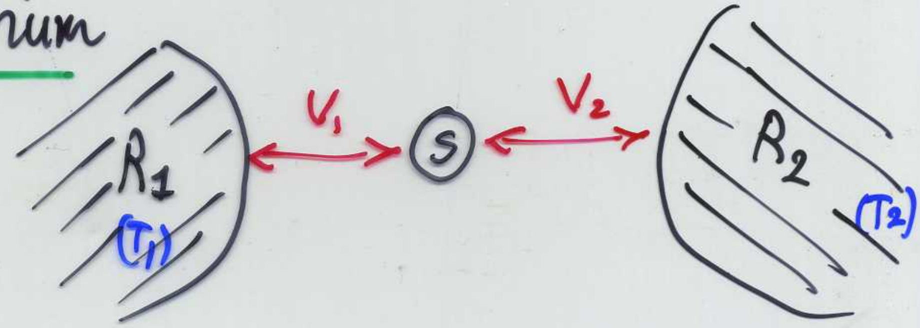


S: collection of spins — N-level system

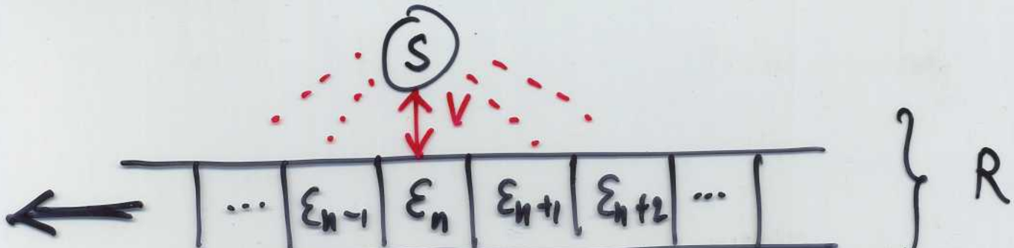
R: thermal quantum field (Bosons/Fermions, ∞ extended

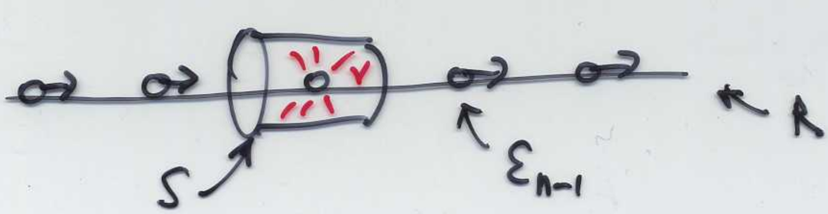
- **Far from equilibrium**

temp. gradient
$T_1 \neq T_2$



- **Repeated interaction systems**





Large time asymptotics

- Return to equilibrium
- Convergence to Non Equilibrium Stationary State (NESS)
- convergence to periodic repeated interaction state

Basic tasks

- prove convergence of dynamics ($t \to \infty$)
- construct asymptotic states (perturbatively)
- find physical (thermodyn.) properties
- find speed of convergence
- → describe dynamics effectively <u>for all times</u>
- → derive open systems phenomena

Rigorous approach to open system dynamics: Dynamical quantum resonance method (S+R)

$$\bar{\rho}_t = \mathrm{Tr}_R\left(e^{-itH}\rho_0\, e^{itH}\right)$$ reduced dmat

S+R

$$H = H_S + H_R + \lambda V$$ λ: coupling constant

- Absence of interaction, $\lambda=0$: $\bar{\rho}_t = e^{-itH_S}\,\bar{\rho}_0\, e^{itH_S}$

  ↳ matrix elements in energy basis $\left(H_S\varphi_E = E\varphi_E\right)$

$$[\bar{\rho}_t]_{E,E'} = e^{-it(E-E')}[\bar{\rho}_0]_{E,E'}$$

- Effects of interaction with reservoir:

  1. Bohr energies $e = E-E'$ become complex resonance energies ε

  $$e^{-it(E-E')} \xrightarrow{\lambda\neq 0} e^{-it\,\varepsilon_{E-E'}(\lambda)}, \quad \varepsilon \in \mathbb{C}$$

  (IRREVERSIBILITY!)

  2. Matrix elements do not evolve independently (but in groups)

Theorem There is a $\lambda_0 > 0$ s.t. if $\lambda < \lambda_0$ then we have for all $t \geq 0$:

$$[\bar{\rho}_t]_{mn} = \sum_{(k,l) \in C(E_m - E_n)} A_t(m,n;k,l) [\bar{\rho}_0]_{kl} + O(\lambda^2$$

uniform in

- $C(E_m - E_n) = \{ (k,\ell) : E_k - E_\ell = E_m - E_n \}$ (clusters

- A_t satisfy Chapman-Kolmogorov eq$^{\underline{n}}$

$$A_{t+r}(m,n;k,\ell) = \sum_{(p,q) \in C(E_m - E_n)} A_t(m,n;p,q) A_r(p,q;k,\ell)$$

(with IC $A_0(m,n;k,\ell) = \delta_{m=k} \delta_{n=\ell}$)

- A_t given by resonance data (eigenvalues & vectors)

$$A_t(m,n;k,\ell) = \sum_{s=1}^{\mathrm{mult}(E_n - E_m)} e^{it\varepsilon^{(s)}_{E_n - E_m}} C_{k,\ell;m,n}$$

accessible by analytic perturbation theory (λ)

Coherence & decoherence

Classical dynamical system:

Φ phase space coordinate $\quad\quad (\Phi = (\vec{x}, \vec{p}))$

μ state: measure on phase space $d\mu(\Phi)$

A observable: $A(\Phi) \in \mathbb{R}$

System with probability p in state μ_1, with proba. $1-p$ in state μ_2.

Average of A: $\langle A \rangle = p \langle A \rangle_{\mu_1} + (1-p) \langle A \rangle_{\mu_2}$

$\left(\langle A \rangle_{\mu_j} = \int A(\Phi)\, d\mu_j(\Phi) \right)$

statistical uncertainty.

Quantum analogue:

ψ: state (vector in Hilbert space)

A: observable

statistical uncertainty encoded in structure of mixed state given by density matrix

$$\rho = p\,|\psi_1\rangle\langle\psi_1| + (1-p)\,|\psi_2\rangle\langle\psi_2|$$

$$\cong \begin{bmatrix} p & 0 \\ 0 & 1-p \end{bmatrix} \quad \text{in orthonormal basis } \{\psi_1, \psi_2\}$$

$$\langle A\rangle := \mathrm{Tr}(\rho A) = p\,\langle A\rangle_{\psi_1} + (1-p)\,\langle A\rangle_{\psi_2}$$

$$\left(\langle A\rangle_{\psi_j} = \langle \psi_j, A\psi_j\rangle \right)$$

Additional, purely quantum "uncertainty"

Pure state: $\psi = \alpha\psi_1 + \beta\psi_2$

$$\langle A\rangle_\psi = \langle \psi, A\psi\rangle = |\alpha|^2 \langle A\rangle_{\psi_1} + |\beta|^2 \langle A\rangle_{\psi_2} + 2\,\mathrm{Re}\left(\bar{\alpha}\beta\, \langle \psi_1, A\psi_2\rangle\right)$$

"interference term"

$$\rho = |\psi\rangle\langle\psi| \cong \begin{bmatrix} |\alpha|^2 & \bar{\alpha}\beta \\ \alpha\bar{\beta} & |\beta|^2 \end{bmatrix} \quad \text{in ONB } \{\psi_1, \psi_2\}$$

ψ is said to be a <u>coherent</u> <u>superposition</u> of ψ_1, ψ_2.

$(\alpha\beta \neq 0)$

Presence of off-diagonal matrix elements indicates coherence (in fixed basis)

$$\rho = \begin{bmatrix} p & c \\ \bar{c} & 1-p \end{bmatrix} \quad \text{in basis} \quad \{\psi_1, \psi_2\}$$

① $c=0$: the system is in one of the two states, either ψ_1 or ψ_2. We do not know in which, but we have corresponding probabilities. Same as in classical situation.

② $c \neq 0$: each of the states ψ_1 and ψ_2 are simultaneously present in the state of the system. There is COHERENCE between ψ_1 and ψ_2.

Example: $\rho = |\psi\rangle\langle\psi|$ pure state, $\psi = \alpha\psi_1 + \beta\psi_2$

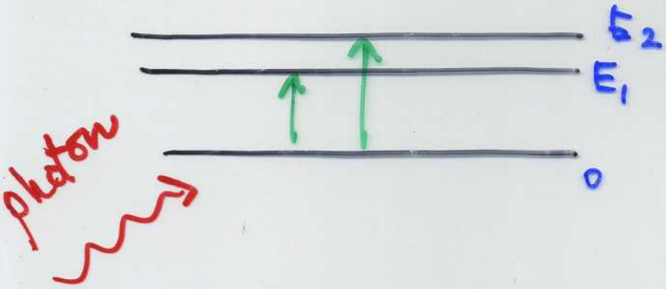
Has no classical analogue.

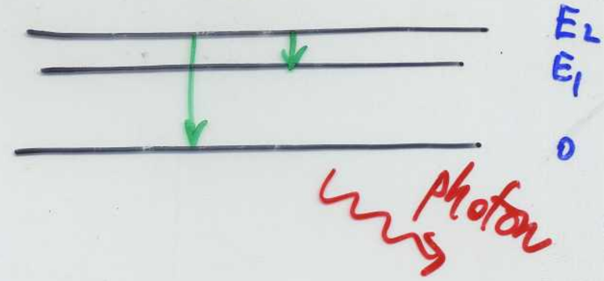
Example: Quantum beats

Atom: ground state energy $E_0 = 0$
excited energies $0 < E_1 < E_2$

at $t=0$, atom gets excited by photon absorption (light pulse) $\Rightarrow$ state $\rho(0)$ (2x2 density matrix describing excitation distribution).

at $t>0$, excited atom relaxes to ground state (photon emission), with life-times γ_1, γ_2

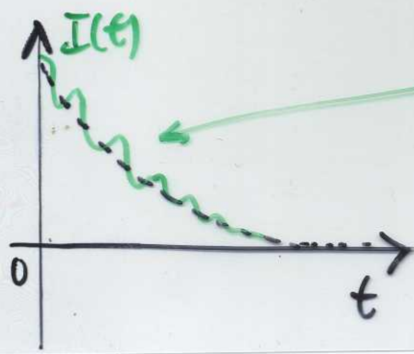




Intensity of emitted light:

$$I(t) \sim \left|\rho_{11}(0) A_1\right|^2 e^{-\gamma t} + \left|\rho_{22}(0) A_2\right| e^{-\gamma t} + 2\mathrm{Re}\left[\rho_{12}(0)\, e^{-\frac{i}{\hbar}(E_1-E_2)t}\right] e^{-\gamma t}$$

$\left(\gamma = \frac{\gamma_1+\gamma_2}{2}\right)$



coherence induces quantum beats (energy basis)

Decoherence is the dynamical process of losing coherence.

$$\rho(0) = \sum_{ij} c_{ij} \, |\psi_i\rangle\langle\psi_j|$$

$$\xrightarrow{t \gg 1} \qquad \rho(t) = \sum_i p_i(t) \, |\psi_i\rangle\langle\psi_i|$$

Loss of coherence; approach of classical probabilistic theory; disappearence of off-diagonal density matrix elements

Origin: exterior noise, "openness", randomness, complexity

Qn: In which basis does the system decohere (become diagonal)?

This depends on interaction with reservoir.

Pure initial state $\psi(0) = \sum_{n\geq 0} a_n |n\rangle \otimes \psi_{R,\beta}$

$\begin{cases} \psi_{R,\beta} : & \text{thermal state of reservoir} \\ \{|n\rangle\} & \text{ONB of } \mathcal{H}_S \end{cases}$

interacting dynamics $\Rightarrow$ $\psi(t) = \sum_{n\geq 0} |n\rangle \otimes \mathcal{E}_n(t)$

If the $\mathcal{E}_n(t)$ are orthogonal then by measuring R we know state of S;

$$r_{m,n}(t) := \langle \mathcal{E}_m(t), \mathcal{E}_n(t) \rangle_R$$

The closer $r_{m,n}(t)$ is to $\delta_{m,n}$, the better R resolves the states $|n\rangle$ of S.

$$\begin{aligned} r_{m,n}(t) &= \langle \psi(t), \left(|m\rangle\langle n| \otimes \mathbb{1}_R \right) \psi(t) \rangle \\ &= \mathrm{tr}\left(\bar{\rho}_t \; |m\rangle\langle n| \right) \\ &= \langle n | \bar{\rho}_t \, m \rangle \end{aligned}$$

dmat elements of $\bar{\rho}_t$ in basis $\{|n\rangle\}$

$\Rightarrow$ <u>Decoherence happens in the basis of S which is well resolved by measurements on R.</u>

Preferred basis is selected by interaction $S \leftrightarrow R$.

Illustration: decoherence of a qubit

- $H_S = \begin{bmatrix} E_1 & 0 \\ 0 & E_2 \end{bmatrix}$, $\Delta = E_2 - E_1 > 0$ "spin, qubit"
- $H_R = \int_{\mathbb{R}^3} |k|\, a^*(k)\, a(k)\, d^3k$ $\left(\text{"} \sum_k \omega_k a_k^\dagger a_k \text{"} \right)$

  free Bose field, spatially ∞ extended, at temperature $1/\beta > 0$.
- $V = \begin{bmatrix} a & c \\ \bar{c} & b \end{bmatrix} \otimes \frac{1}{\sqrt{2}} \left(a^*(g) + a(g) \right)$ coupling with constant λ
- Initial condition: $\bar{\rho}_0 = \frac{1}{2} \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}$

Result:

$$[\bar{\rho}_t]_{1,1} = \left(\tfrac{1}{2} - p_\infty\right) e^{it\varepsilon_0} + p_\infty + O(\lambda^2)$$

$$p_\infty = \frac{e^{-\beta E_1}}{e^{-\beta E_1} + e^{-\beta E_2}}$$

$$[\bar{\rho}_t]_{1,2} = \tfrac{1}{2} e^{it\varepsilon_1} + O(\lambda^2)$$

$$\varepsilon_0 = i \lambda^2 |c|^2 \coth\left(\frac{\beta\Delta}{2}\right) + O(\lambda^4)$$

$$\varepsilon_1 = \Delta + \lambda^2 \underbrace{r}_{\in\mathbb{R}} + \tfrac{1}{2}\varepsilon_0 + \tfrac{i}{2}\lambda^2 (b-a)^2 \underbrace{c_1}_{\geq 0} + O(\lambda^4)$$

(AB) entanglement

ρ: density matrix

Von Neumann entropy: $S(\rho) = -\mathrm{Tr}(\rho \ln \rho) \geq 0$

Entanglement: Bipartite system $A+B$, measures 'how much a state is of product form'.

Def.: • $\psi \in \mathcal{H}_A \otimes \mathcal{H}_B$, $\mathcal{E}(\psi) := S\left(\mathrm{Tr}_B |\psi\rangle\langle\psi|\right)$

• ρ dmat on $\mathcal{H}_A \otimes \mathcal{H}_B$

$$\mathcal{R}(\rho) = \left\{ (\psi_j, p_j) : \psi_j \in \mathcal{H}_A \otimes \mathcal{H}_B,\ \|\psi_j\| = 1,\ 0 \leq p_j \leq 1,\ \text{s.t. } \rho = \sum_j p_j |\psi_j\rangle\langle\psi_j| \right\}$$

$$\mathcal{E}(\rho) := \inf_{\mathcal{R}(\rho)} \sum_j p_j\, \mathcal{E}(\psi_j)$$

Properties: • $\mathcal{E}(\rho) \geq 0$

• $\mathcal{E}(\rho) = 0 \Leftrightarrow \rho$ is separable

$$\left(\rho = \sum_j p_j\, |\psi_j^A\rangle\langle\psi_j^A| \otimes |\psi_j^B\rangle\langle\psi_j^B| \right)$$

Disentanglement: Due to coupling to "noise" (reservoir), initially entangled state becomes disentangled. (t large)

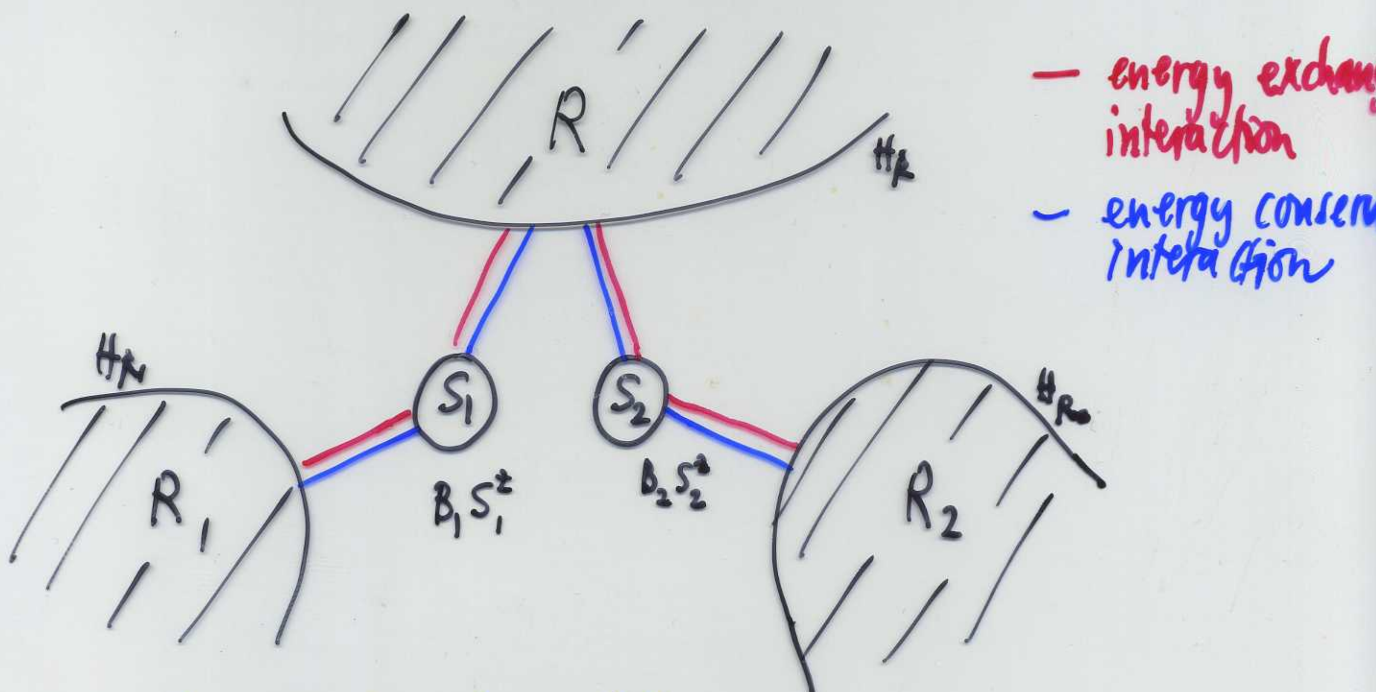
However, there can also be

Creation of entanglement: Two initially not entangled systems can become entangled due to interaction to a common reservoir (at intermediate times)

Problem: definition of $\mathcal{E}(\rho)$ very complicated!

But: for two spins ($\mathcal{H}_A = \mathcal{H}_B = \mathbb{C}^2$), Wootters found 'easy' expression equivalent to $\mathcal{E}(\rho)$: the Concurrence. (Amenable to analytic and numerical analysis.)

Illustration: dynamics of entanglement



Family of (pure) initial states

$$\psi_0 = \alpha\,|++\rangle + \beta\,|--\rangle$$

$$\rho_0 = |\psi_0\rangle\langle\psi_0| = \begin{bmatrix} |\alpha|^2 & 0 & 0 & \alpha\bar{\beta} \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ \bar{\alpha}\beta & 0 & 0 & |\beta|^2 \end{bmatrix}$$

$\mathcal{E}(\rho_0)$ varies from 0 to 1 (depending on α, β).

'Cluster evolution' $\Rightarrow$

$$\rho_t \approx \begin{bmatrix} p_1(t) & 0 & 0 & a(t) \\ 0 & p_2(t) & 0 & 0 \\ 0 & 0 & p_3(t) & 0 \\ \bar{a}(t) & 0 & 0 & p_4(t) \end{bmatrix} + O(\lambda^2)$$

coupling strength

ρ_t is rather sparse (many zeros)

$\to$ can calculate (estimate) entanglement $\mathcal{E}(\rho_t)$

Theorem. Suppose $\mathcal{E}(\rho_0) > 0$ $\quad (|\alpha|^2 \neq 0, 1)$.

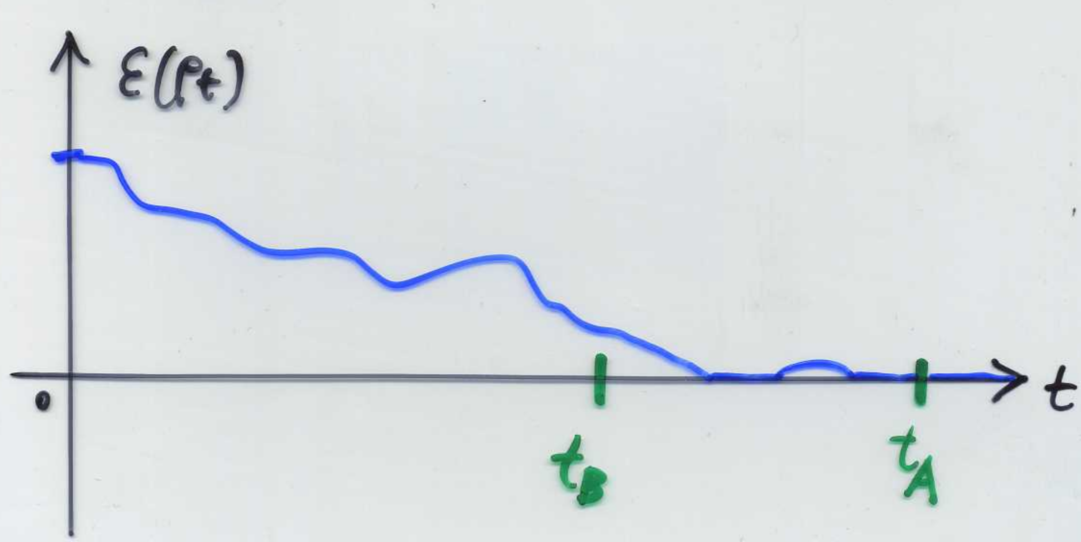
For $0 \neq |\lambda| < \lambda_0 \cdot \mathcal{E}(\rho_0)$ we have:

A (Entanglement death)

- $\exists\, t_A > 0$ s.t. for $t \geq t_A$, we have $\mathcal{E}(\rho_t) = 0$
- t_A is given explicitly in terms of resonance data

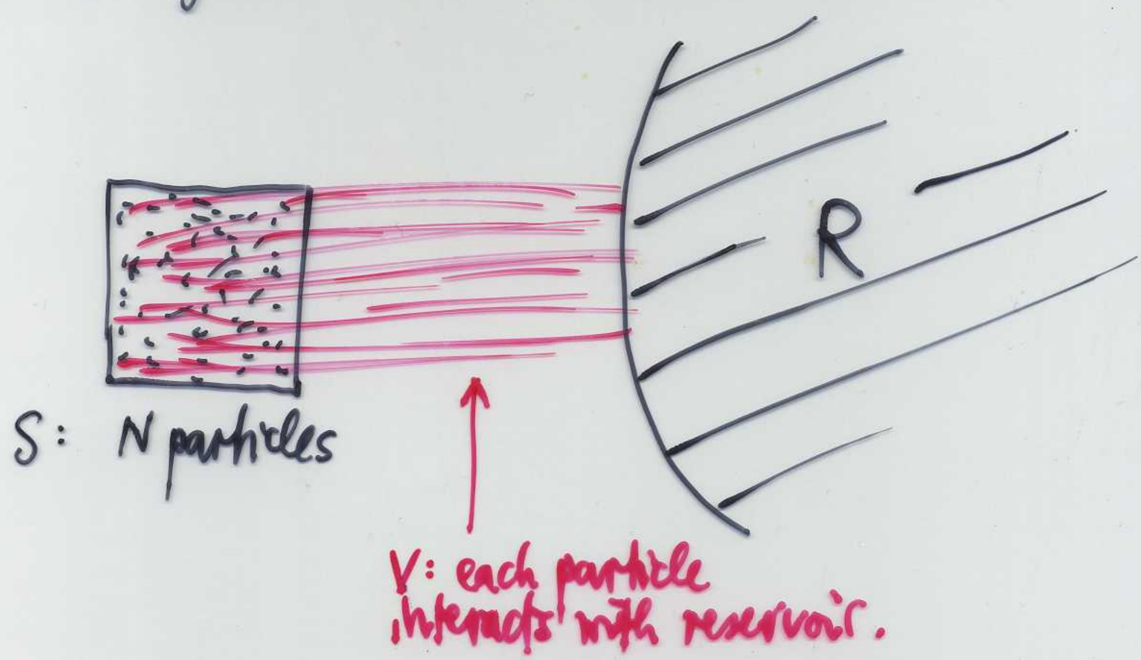
B (Entanglement survival)

- $\exists\, t_B > 0$ s.t. for $t < t_B$, we have $\mathcal{E}(\rho_t) > 0$
- t_B explicit in terms of resonance data.



Complexity & factorization

What if system S is 'not so small'?



- $H_S = \sum_{j=1}^{N} h_j \qquad V = \underbrace{\frac{1}{\sqrt{N}}}_{\text{mean field scaling}} \sum_{j=1}^{N} v_j \otimes \varphi$

- Initial condition: factorised

  $\rho_{n,N}(t)$ = reduced density matrix of particles $1, \dots, n$

  $\rho_{n,N}(0) = \rho_1 \otimes \rho_1 \otimes \cdots \otimes \rho_1$ (n factors)

QN Dynamics of $\rho_{n,N}$ as $N \to \infty$?

Answer :

$$\rho_{n,N}(t) \xrightarrow{N\to\infty} \rho_1(t)\otimes\cdots\otimes\rho_1(t)$$

single-particle density matrix satisfies

$$i\,\dot{\rho}_1(t) = \big[h,\ \rho_1(t)\big] + \mathrm{Tr}_2\big[W_{\mathrm{eff}}(t),\ \rho_1(t)\otimes\rho_1(t)\big]$$

free dynamics

effective time-dep. two body interaction

→ time-dependent nonlinear Hartree - Lindblad equation.

→ COMPLEXITY DISABLES CREATION OF ENTANGLE-MENT

Example: N spins $1/2$

Each spin:

$$h = \frac{\omega}{2}\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} = \omega S^z \qquad (\omega > 0)$$

interaction with common reservoir: $\quad S^z \otimes \frac{1}{\sqrt{2}}\left(a^*(f) + a(f)\right)$

→ Hartree-Lindblad eq$^{\underline{n}}$ for single spin:

$$i\dot{\rho}_t = \omega\left[S^z, \rho_t\right] + 2\dot{s}(t)\,\mathrm{Tr}_2\left[S^z \otimes S^z, \rho_t \otimes \rho_t\right]$$

where $s(t)$ is explicit real function

Exact solution:

$$\begin{cases} [\rho_t]_{jj} = [\rho_0]_{jj}, & j = 1,2 \\ [\rho_t]_{12} = e^{-i\omega t}\, e^{-\frac{i}{2}(2p-1)s(t)}\,[\rho_0]_{12} \end{cases}$$

where $p = [\rho_0]_{11}$ (initial condition)

Cumulative effect of all spins on a single, fixed one DOES NOT CREATE DECOHERENCE.