Dynamics of open quantum systems via resonances

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Open quantum systems

- System + Environment models Hamiltonian

$$H = H_{\mathrm{S}} + H_{\mathrm{R}} + \lambda V$$

– $H_{\mathrm{S}} = \mathrm{diag}(E_1, \ldots, E_N)$ system Hamiltonian (finite-dimensional)
– Environment a 'heat bath' of non-interacting Bosons (Fermions) at thermal equilibrium ($T = 1/\beta > 0$) w.r.t. Hamiltonian

$$H_{\mathrm{R}} = \sum_k \omega_k a_k^\dagger a_k$$

ω_k dispersion relation

– Interaction constant λ, interaction operator

$$V = G \otimes \sum_k \left(g_k a_k^\dagger + h.c. \right)$$

$G = G^\dagger$ acts on the system, $g_k \in \mathbb{C}$ is a *form factor*.

• Schrödinger dynamics

$$\rho_{\rm tot}(t) = {\rm e}^{-{\rm i}tH} \rho_{\rm S} \otimes \rho_{\rm R} \, {\rm e}^{{\rm i}tH}$$

$\rho_{\rm S}$ arbitrary system inital state, $\rho_{\rm R}$ thermal reservoir state

• Irreversible dynamical effects (in S or R) are visible in the limit of *continuous bath modes* (*e.g.* thermodynamic limit: ∞ volume)

Examples: convergence to a final state, decoherence, loss of entanglement, dissipation of energy into the bath

• The limits of: continuous modes, large time, small coupling,.... are *not* independent

• Our approach starts off with infinite-volume (true) reservoirs; *first* we perform continuous mode limit, then we consider $t \to \infty$, $\lambda \to 0$,....

The coupled infinite system

- Liouville representation (purification, GNS representation): view density matrix as a *vector* in 'larger space' (ancilla)
  - system state $\rho = \sum_j p_j |\psi_j\rangle\langle\psi_j| \quad \rightarrow \quad \Psi_{\rm S} = \sum_j \sqrt{p_j}\, \psi_j \otimes \psi_j$
  - ∞-volume reservoir equilibrium state $\quad \rightarrow \quad \Psi_{\rm R}$
  - Initial system-reservoir state: $\Psi_0 = \Psi_{\rm S} \otimes \Psi_{\rm R}$
- Dynamics generated by self-adjoint *Liouville (super-)operator L*

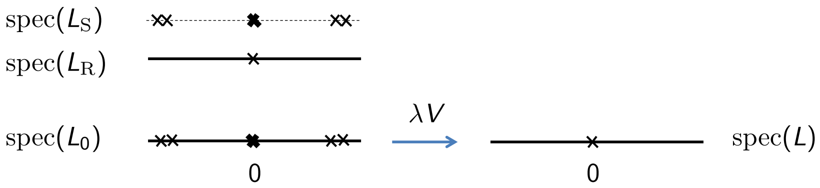
$$\Psi_t = \mathrm{e}^{-\mathrm{i}tL}\Psi_0,$$

with

$$L = L_0 + \lambda V, \qquad L_0 = L_{\rm S} + L_{\rm R}$$

Dynamics and spectrum of $L = L_0 + \lambda V$

- Guiding principle: spectral decomposition " $\mathrm{e}^{-\mathrm{i}tL} = \sum_j \mathrm{e}^{-\mathrm{i}te_j} P_j$ "

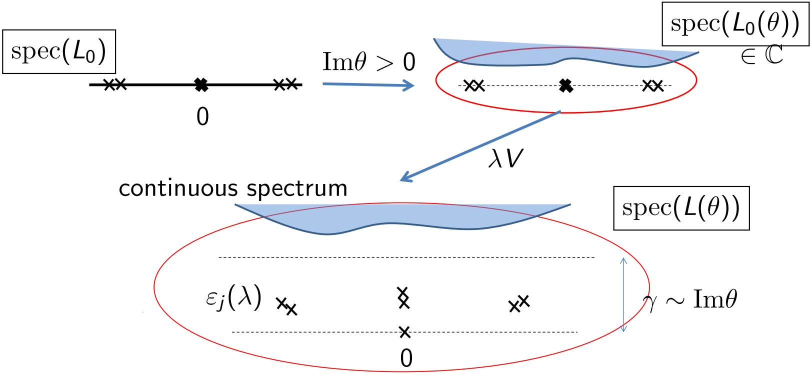


- Stationary states $\longleftrightarrow$ Null space (of L_0, L)
  - Non-interacting dynamics: multiple stationary states $|\varphi_j\rangle\langle\varphi_j| \otimes \rho_{\mathrm{R}}$
  - Interacting dynamics: single stationary state
    Equilibrum of system + reservoir under coupled dynamics

Resonances

Unstable eigenvalues become *complex* 'energies' = resonances = eigenvalues of a *spectrally deformed Liouville operator*.

Spectral deformation:
Transformation $U(\theta)$, $\theta \in \mathbb{C} \to L(\theta) = U(\theta) L U(\theta)^{-1}$



- $\varepsilon_0 = 0$ is simple eigenvalue, $\mathrm{Im}\,\varepsilon_j(\lambda) \propto \lambda^2 > 0$

Resonance representation of dynamics

- Spectral decomposition of $L(\theta)$

$$e^{itL(\theta)} \text{ ``}=\text{''} \sum_j e^{it\varepsilon_j} P_j + O(e^{-\gamma t})$$

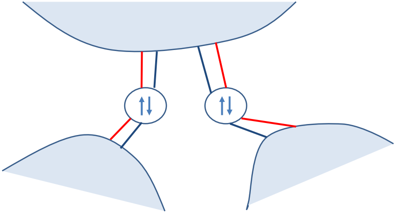
- Dynamics of system-reservoir observables A

$$\langle A \rangle_t = \sum_j e^{it\varepsilon_j} C_j(A) + O(e^{-\gamma t})$$

- Remainder decays more quickly than main term ($\gamma > \mathrm{Im}\varepsilon_j$)
- ε_j and C_j calculable by perturbation theory in λ
- For observables A of system alone, remainder is $O(\lambda^2 e^{-\gamma t})$
- *Return to equilibrium*. The coupled system approaches its joint equilibrium state: $\lim_{t\to\infty}\langle A \rangle_t = C_0(A)$.

Example: reduced dynamics of system

Two spins coupled to common and local reservoirs



Spin Hamiltonians $B_{1,2}\sigma^z_{1,2}$

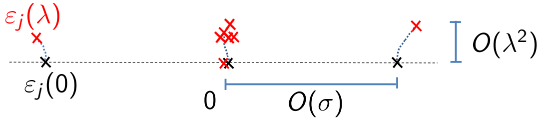
Interact.: energy exchange/dephasing: $\sigma^x_{1,2}/\sigma^z_{1,2} \otimes \sum g_k(a^\dagger_k + a_k)$

- Dynamics of two-spin reduced state ρ_t
  - *Thermalization* (convergence of diagonal of ρ_t): rate depends on exchange interaction only
  - *Decoherence* (decay of off-diagonals): rates depend on local & collective, exchange & dephasing interact. in a *correlated* way
  - *Entanglement*: estimates on entanglement preservation and entanglement death times for class of initial ρ_0

Isolated v.s. overlapping resonances

- $\begin{cases} \text{Energy level spacing of system } \sigma \\ \text{System-reservoir coupling constant } \lambda \end{cases}$
- $\begin{cases} \text{Isolated resonances regime: } \sigma >> \lambda^2 \\ \text{Overlapping resonances regime: } \sigma << \lambda^2 \end{cases}$

Isolated



Starting point: σ fixed, $\lambda = 0$

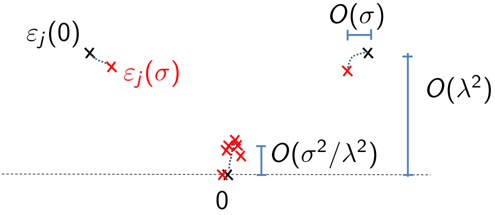
– Stationary system states: ρ_{S} diagonal in energy basis (H_{S})

Perturbation: $\lambda \neq 0$ small

– Unique stationary system state: equilibrium $\propto \mathrm{e}^{-\beta H_{\mathrm{S}}}$

– All decay times $\propto 1/\lambda^2$

Overlapping



Starting point: λ fixed, $\sigma = 0$

– Stationary system states: ρ_{S} diagonal in the interaction operator eigenbasis (G)

Perturbation: $\sigma \neq 0$ small

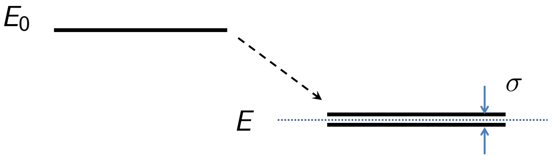
– Unique stationary system state: equilibrium $\propto \mathrm{e}^{-\beta H_{\mathrm{S}}}$

– Emergence of *two* time-scales

  ◦ $t_1 \propto 1/\lambda^2$: approach of quasi-stationary states

  ◦ $t_2 \propto \lambda^2/\sigma^2 \gg t_1$: quasi-stat. states decay into equilibrium

A donor-acceptor model



$$H = \begin{pmatrix} E_0 & 0 & 0 \\ 0 & E+\sigma/2 & 0 \\ 0 & 0 & E-\sigma/2 \end{pmatrix} + H_{\mathrm{R}} + \lambda \begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix} \otimes \varphi(g)$$

- $H_{\mathrm{R}} = \sum_k \omega(k) a_k^\dagger a_k$ and $\varphi(g) = \frac{1}{\sqrt{2}} \sum_k (g_k a_k^\dagger + h.c.)$, reservoir spatially infinitely extended and at thermal equilibrium.
- Donor-acceptor transition induced by environment.

Degenerate acceptor, $\sigma = 0$

- Stationary system states are convex span of equilibrium state $\rho_1 \propto \mathrm{e}^{-\beta H_\mathrm{S}} + O(\lambda^2)$ and of $\rho_2 \propto |0\ 1\ \ -1\rangle\langle 0\ 1\ \ -1|$.
- Asymptotic system state ($t \to \infty$) depends on initial state $\rho(0)$

$$\rho(\infty) = \begin{pmatrix} p & 0 & 0 \\ 0 & \frac{1}{2}(1-p) & \alpha(p) \\ 0 & \alpha(p) & \frac{1}{2}(1-p) \end{pmatrix} + O(\lambda^2),$$

where p depends on $\rho(0)$

- Final state is approached on time-scale $t_1 \propto 1/\lambda^2$,

$$\rho(t) - \rho(\infty) = O(\mathrm{e}^{-t/t_1}),$$

Lifted acceptor degeneracy, $0 < \sigma \ll \lambda^2$

• The total system (donor-acceptor + environment) has *single* stationary state: the *coupled* equilibrium state. Reduced to donor-acceptor system, it is (modulo $O(\lambda^2)$)

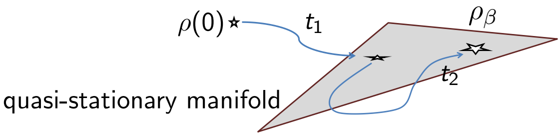
$$\rho_\beta \propto \mathrm{e}^{-\beta H_{\mathrm{S}}}$$

• Final state is approached on time-scale $t_2 \propto \lambda^2/\sigma^2$ $(\gg t_1)$

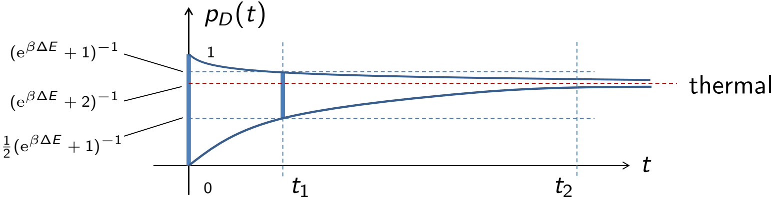
$$\rho(t) - \rho_\beta = O(\mathrm{e}^{-t/t_2}),$$

• Manifold of stationary states for $\sigma = 0$ becomes quasi-stationary (decays on time-scale t_2)

- Arbitrary initial state $\rho(0)$ approaches quasi-stationary manifold, then decays to the unique equilibrium ρ_β.



- Evolution of donor-probability, $p_D(t) = [\rho(t)]_{11}$



- $p_D(0) \in [0,1]$, $p_D(t_1) = \frac{1}{2}\frac{1+p_D(0)}{e^{\beta\Delta E}+1}$, $p_D(t_2) = \frac{1}{e^{\beta\Delta E}+2}$ (equil.)

Based on collaborations with

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