Open Quantum System

Lectures:

- Daniel Manzano, A short introduction to the Lindblad master equation (*all*)
- Breuer and Petruccione, The Theory of Open Quantum Systems (*ch. 3 - 4.3*)
- Daniel A. Lidar, Notes on the Theory of Open Quantum Systems (*up to ch. 12*)

October 29, 2023

Recap

Last time: derivation of the **Lindblad** equation

- General form:

$$\frac{d}{dt}\rho(t) = -i[H,\rho(t)] + \sum_{i,j=1}^{d^2-1} g_{i,j}\left(F_i\rho(t)F_j^\dagger - \frac{1}{2}\left\{F_j^\dagger F_i, \rho(t)\right\}\right)$$

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- Since $g_{i,j}$ - hermitian, can be diagonalized with real eigenvalues: $g = U\Lambda U^\dagger$, with $\Lambda = \mathrm{Diag}(\gamma_i)$. and $L_k = \sum_i U_{i,k}F_i$. Giving the diagonal form

$$\frac{d}{dt}\rho(t) = -i[H,\rho(t)] + \sum_{k=1}^{N^2-1} \gamma_k\left(L_k\rho L_k^\dagger - \frac{1}{2}\left\{L_k^\dagger L_k, \rho(t)\right\}\right) \quad (1)$$

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- Also, in the Heisenberg picture, for an operator $A(t)$

$$\frac{d}{dt}A = \mathcal{L}^\dagger A = i[H,A] + \sum_k \gamma_k\left(L_k^\dagger A L_k - \frac{1}{2}\left\{L_k^\dagger L_k, A\right\}\right) \quad (2)$$

Approximations: weak coupling

- Hamiltonian for system and bath

$$H_{\text{tot}} \equiv H = H_S \otimes \mathbb{I} + \mathbb{I} \otimes H_B + \alpha H_{\text{int}} \tag{3}$$

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- Back from the von-Neumann equation (in the Dirac's picture):

$$\begin{aligned}\rho(t)_{\text{tot}} &= \rho(0)_{\text{tot}} - i\alpha \int_0^t ds[H_{\text{int}}(s), \rho_{\text{tot}}(t)] \rightarrow \\ \frac{d}{dt}\rho(t)_{\text{tot}} &= \rho(0)_{\text{tot}} - i\alpha \int_0^t ds[H_{\text{int}}(s), \rho_{\text{tot}}(t)] \\ &\quad - \alpha^2 \int_0^t [H_{\text{int}}(s), [H_{\text{int}}(s), \rho_{\text{tot}}(t)]] + \mathcal{O}(\alpha^3)\end{aligned} \tag{4}$$

Approximations: weak coupling

- Explicitly taking the trace Tr_B, for $\rho_S \equiv \rho$, on gets

$$\frac{d}{dt}\rho(t) = -\alpha^2 \int_0^t \mathrm{Tr}_B \Big[[H_{\text{int}}(s), [H_{\text{int}}(s), \rho(t) \otimes \rho_B(t)]] \Big] \qquad (5)$$

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- Weak coupling limit:
  - $\alpha \ll 1$
  - Relaxation time of bath vs relaxation time of system
    $\tau_{B,\text{corr.}}, \tau_{B,\text{relax.}} \ll \tau_{\text{sys.}}$ with $\tau_{\text{sys.}} \sim |\omega - \omega'|^{-1}$ with ω - proper energy.

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- Corollary: $\rho_{\mathrm{tot}}(t) = \rho(t) \otimes \rho_B(t) \simeq \rho(t) \otimes \rho_B(0)$ giving

$$\frac{d}{dt}\rho(t) = -\alpha^2 \int_0^t \mathrm{Tr}_B\Big[[H_{\mathrm{int}}(s), [H_{\mathrm{int}}(s), \rho(t) \otimes \rho_B(0)]]\Big] \qquad (6)$$

but non-Markovian, since dependence in time τ - $0 < \tau < t$.

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  - $s \mapsto s - t$, since interaction is neglected for a large Δt.
  - Integral boundary $t \to \infty$.
- Yielding the Redfield equation:

$$\frac{d}{dt}\rho(t) = -\alpha^2 \int_0^\infty \mathrm{Tr}_B \Big[[H_{\text{int}}(s), [H_{\text{int}}(s-t), \rho(t) \otimes \rho_B(0)]] \Big] \quad (7)$$

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- Expansion of S_k in the form

$$S_k = \sum_{\omega} S_k(\omega) \quad \text{,with } S_k(\omega) = \sum_{\substack{\varepsilon - \varepsilon' = \\ = \omega \in \sigma(H_S)}} \Pi_{\varepsilon} S_k \Pi_{\varepsilon'} \tag{8}$$

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- Properties of the defined operators:
  - $[H_S, S_k(\omega)] = -\omega S_k(\omega) \quad \text{and} \quad [H_S, S_k^\dagger(\omega)] = +\omega S_k(\omega)$
  - $[H_S, S_k^\dagger(\omega) S_l(\omega)] = 0$
  - $S_k^\dagger(\omega) = S_k(-\omega)$
  - $$\sum_\omega S_k(\omega) = \sum_\omega S_k^\dagger(\omega) = S_k \tag{9}$$

Rotating wave approximation

- The decomposition of H_{int} and the interaction picture gives

$$\begin{aligned} H_{\text{int}} &= \sum_{k,\omega} S_k(\omega) \otimes E_k \to \\ H_{\text{int}}(t) &= \sum_{k,\omega} e^{-i\omega t} S_k(\omega) \otimes E_k(t) \end{aligned} \tag{10}$$

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- Expanding the commutators, one gets

$$\begin{aligned} \frac{d}{dt}\rho(t) = \sum_{\substack{\omega,\omega' \\ k,l}} \Big(& e^{i(\omega'-\omega)t}\Gamma_{kl}(\omega)[S_l(\omega)\rho(t), S_k^\dagger(\omega')] + \\ & + e^{i(\omega-\omega')t}\Gamma_{kl}^*(\omega')[S_l(\omega), \rho(t) S_k^\dagger(\omega')] \Big) \end{aligned} \tag{11}$$

- With defining

$$\Gamma_{kl}(\omega) \equiv \int_0^\infty ds\ e^{i\omega s}\mathrm{Tr}_B[B_k^\dagger(t) \otimes B_l(t-s)\rho_B(0)] \tag{12}$$

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- Rotating wave approximation: only resonant terms $\omega = \omega'$ are kept.

Rotating wave approximation

- One obtains

$$\frac{d}{dt}\rho(t) = \sum_{\omega}\sum_{k,l}\Big(\Gamma_{k,l}(\omega)[S_l(\omega)\rho(t), S_k^{\dagger}(\omega)] + \Gamma_{lk}^{*}(\omega)[S_l(\omega), \rho(t)S_k^{\dagger}(\omega)]\Big) \tag{13}$$

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- One can rewrite the term Γ_{kl} into the hermitian and non-hermitian parts:

$$\Gamma_{kl}(\omega) = \frac{1}{2}\gamma_{kl}(\omega) + i\pi_{kl}, \quad \pi_{kl}(\omega) \equiv \frac{1}{2i}(\Gamma_{kl}(\omega) - \Gamma_{kl}^{*}(\omega)) \\ \gamma_{kl}(\omega) \equiv \Gamma_{kl}(\omega) + \Gamma_{kl}^{*}(\omega) = \\ = \int_{-\infty}^{\infty} ds\; e^{i\omega s}\mathrm{Tr}_B[S_k^{\dagger}(s)S_l(0)\rho_B(0)] \tag{14}$$

Rotating wave approximation

- Now, back to the Schrodinger picture, one gets

$$\begin{aligned}\frac{d}{dt}\rho(t) =& - i[H + H_{\mathrm{LS}}, \rho(t)] + \sum_{\substack{\omega \\ k,l}} \gamma_{kl}(\omega) \cdot \\ & \cdot \left(S_l(\omega)\rho(t)S_k^\dagger(\omega) - \frac{1}{2}\left\{ S_k(\omega)^\dagger S_l(\omega)^\dagger, \rho(t) \right\} \right)\end{aligned} \tag{15}$$

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- The additional term H_{LS} - the Lamb Shift Hamiltonian, defined by

$$H_{\text{LS}} = \sum_{\substack{\omega, \\ k,l}} \pi_{kl}(\omega) S_k^\dagger(\omega) S_l(\omega) \tag{16}$$

- With recalling the terms S_k - the basis of the decomposition of the interaction Hamiltonian $H_{\text{int}} = \sum_k S_k \otimes B_k$ and $S_k(\omega) = \sum_{\varepsilon' - \varepsilon} \Pi_\varepsilon S_k \Pi_{\varepsilon'}$.

Rotating wave approximation

- Using the diagonalization of the equation, one gets the LGKS equation with the Lamb Shift Hamiltonian and the jump operators.

$$\begin{aligned}\frac{d}{dt}\rho(t) =& - i[H + H_{\mathrm{LS}}, \rho(t)]+ \\ &\sum_{i,\omega}\left(L_i(\omega)\rho(t)L_i^\dagger(\omega) - \frac{1}{2}\left\{ L_i^\dagger L_i(\omega), \rho(t)\right\}\right) = \mathcal{L}\rho(t)\end{aligned} \tag{17}$$

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- $\rightarrow$ Decomposition of the interaction Hamiltonian H_{int} into the basis $S_k \otimes B_k$
- $\rightarrow$ Decomposition of the basis elements via $S_k(\omega)$, defined using the spectra of the system H_S.
- $\rightarrow$ Substituting into the Redfield, identifying elements, separating into Hermitian/non-Hermitian and diagonalizing. Obtaining the Lindblad equation with the Lamb Shift contribution, which is dependent on the spectrum of the system H_S.

Other special cases: Optical, High temperature, Brownian motion, Nonlinear mean field, Nonlinear mean field laser master equations.

Exact example - spin-boson

- Spin coupled to a boson bath. Hamiltonian given by

$$\begin{aligned} H &= H_S + H_B + H_I = H_0 + H_{\text{int}} = \\ &= \frac{\omega_0}{2}\sigma_z + \sum_k \omega_k b_k^\dagger b_k + \sum_k \sigma_z \otimes \left(\lambda_k b_k^\dagger + \lambda_k^* b_k\right) \end{aligned} \tag{18}$$

  with ω_k - mode frequencies of the bosonic bath, g_k - the coupling constants to the bosonic bath, b - the bosonic creation and anihilation operators obeying $[b_i, b_j^\dagger] = \delta_{i,j}$. $\sigma_z = |0\rangle\langle 0| - |1\rangle\langle 1|$ - the Pauli z operator.

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- The interaction Hamiltonian evolution (in the Dirac's picture)

$$H_{\text{int}} = \sum_k \sigma_z \otimes \left(\lambda_k b_k^\dagger e^{i\omega_k t} + \lambda_k^* b_k e^{-i\omega_k t}\right) \tag{19}$$

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- The former obeys the commutations:

$$\begin{aligned} [H_{\text{int}}(t), H_{\text{int}}(s)] &= -2i \sum_k \sin(\omega(t-s)) = -2i\phi(t-s) \\ &= \quad [H_{\text{int}}(t), [H_{\text{int}}(s), H_{\text{int}}(r)]] = 0 \end{aligned} \tag{20}$$

Exact example - spin-boson

- **Goal - find the system's density matrix**

$$\rho_S(t) = \mathrm{Tr}_B[U(t)\rho_S(0) \otimes \rho_B(0)U^\dagger(t)] \tag{21}$$

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- After some algebra, one can write

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- The integrations yield

$$-i\int_0^t H(s)ds = \sigma_z \otimes \sum_k (\alpha_k^* a_k - \alpha_k a_k^\dagger) \qquad \text{with} \;\; \alpha_k(t) = \frac{\lambda_k^*(e^{i\omega_k t}) - 1}{\omega_k} \tag{23}$$

Exact example - spin-boson

- For the integral of the commutator -

$$\sigma_z^2 \otimes \sum_k \mathrm{Im}\left[\frac{1 - e^{i\omega_k t} + i\omega_k t}{\omega_k^2}\right] \tag{24}$$

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- After some tedious simplifications, and by defining

$$f(t) \equiv \sum_k \mathrm{Im}\left[|\lambda_k|^2 \frac{e^{i\omega_k t} - i\omega_k t - 1}{\omega_k^2}\right] \tag{25}$$

one can write the evolution operator

$$U(t) = e^{if(t)} \prod_k \exp\left(\sigma_z \otimes \left[\alpha_k(t) a_k - \alpha_k(t)^* a_k^\dagger\right]\right) \tag{26}$$