Open quantum systems – lecture 1

lecture
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suitable literature:

- H.-P. Breuer and F. Petruccione, *The Theory of Open Quantum Systems*, Oxford University Press, Oxford (2002).
- M. O. Scully and M. S. Zubairy, *Quantum Optics*, Cambridge University Press (1997).
- L. Mandel and E. Wolf, *Optical coherence and quantum optics*, Cambridge University Press (1995).
- N. G. van Kampen, *Stochastic processes in physics and chemistry*, Elsevier (1981).
- M. Schlosshauer, *Decoherence and the quantum-to-classical transition*, Springer (2007).
- H. M. Wiseman and G. J. Milburn, *Quantum Measurement and Control*, Cambridge University Press, Cambridge (2010).
- G. Schaller, *Open Quantum Systems Far from Equilibrium* Springer Lecture Notes in Physics **881**, Springer (2014).
- G. T. Landi, D. Poletti, and G. Schaller, *Non-equilibrium boundary driven quantum systems: models, methods and properties*, Reviews of Modern physics **in press**, arXiv:2104.14350.

Prerequisites

We summarize a few important concepts that should be familiar to everyone and fix the notation:

- We work in units where $\hbar = 1$ and $k_{\mathrm{B}} = 1$.
- We do not put hats on operators – it is clear from the context whether the quantity is an operator or not.
- General quantum systems can be conveniently described by a **density matrix**

$$\rho = \sum_n P_n \left|\Psi_n\right\rangle \left\langle\Psi_n\right| \,,$$

  where $\left|\Psi_n\right\rangle$ denote normalized $\left\langle\Psi_n|\Psi_n\right\rangle = 1$ states and $0 \leq P_n \leq 1$ with $\sum_n P_n = 1$ the corresponding probabilities. In this representation, the states need not necessarily be orthogonal, i.e., in general $\left\langle\Psi_n|\Psi_m\right\rangle \neq \delta_{nm}$. Density matrices fulfil the mathematical properties

$$\mathrm{Tr}\left\{\rho\right\} = 1 \,, \qquad \rho = \rho^\dagger \,, \qquad \left\langle\Psi\right| \rho \left|\Psi\right\rangle \geq 0 \qquad \forall \qquad \left|\Psi\right\rangle \,.$$

  Denoting the eigenvalues of a density matrix with λ_n, we see that $0 \leq \lambda_n \leq 1$ with $\sum_n \lambda_n = 1$, and the **spectral representation** of a density matrix

$$\rho = \sum_n \lambda_n \left|\Phi_n\right\rangle \left\langle\Phi_n\right| \qquad : \qquad \left\langle\Phi_n|\Phi_m\right\rangle = \delta_{nm}$$

  provides in general a different decomposition of a density matrix.

- A density matrix is called **pure**, if and only if

$$\rho_{\mathrm{p}} = \rho_{\mathrm{p}}^2 \,,$$

  i.e., $\rho_{\mathrm{p}} = \left|\Psi\right\rangle \left\langle\Psi\right|$ for some state $\left|\Psi\right\rangle$. Other density matrices are called **mixed**.

- While a solution of the Schrödinger equation obeys $\left|\dot{\Psi}\right\rangle = -\mathrm{i}H(t)\left|\Psi\right\rangle$, the density matrix obeys the **von-Neumann** evolution equation

$$\dot{\rho} = -\mathrm{i}\left[H(t), \rho\right] \,,$$

  where the indicated time-dependence in the Hamiltonian may arise either from externally driving a parameter or the use of a different picture such as the interaction picture.

  As such, the solution of the von-Neumann equation can be formally written as

$$\rho(t) = U(t)\rho_0 U^\dagger(t) \,,$$

where $U(t)$ is the **time evolution operator**, in general governed by the differential equation

$$\dot{U} = -\mathrm{i}H(t)U(t)\,.$$

Only if $H(t) \to H$ is constant, we can solve this differential equation by a **matrix exponential**

$$U(t) \to e^{-\mathrm{i}Ht} = \sum_{n=0}^{\infty} \frac{(-\mathrm{i})^n t^n}{n!} H^n\,.$$

- The expectation value of an operator can be obtained by performing the trace

$$\langle A \rangle = \mathrm{Tr}\left\{A\rho\right\} = \mathrm{Tr}\left\{\rho A\right\} = \sum_n \sum_m P_m \langle n| A |\Psi_m\rangle \langle \Psi_m|n\rangle = \sum_m P_m \langle \Psi_m| A |\Psi_m\rangle\ .$$

- Under a **projective measurement** of an observable O with spectral decomposition $O = O^\dagger = \sum_m O_m |m\rangle \langle m|$ with outcome m, the density matrix transforms as

$$\rho \to \rho^{(m)} = \frac{|m\rangle \langle m| \rho |m\rangle \langle m|}{P_m} \qquad : \qquad P_m = \mathrm{Tr}\left\{|m\rangle \langle m| \rho\right\}\ ,$$

where P_m is the probability for this measurement outcome.

- Of particular importance are the **canonical equilibrium state**

$$\rho_c = \frac{e^{-\beta H}}{\mathrm{Tr}\left\{e^{-\beta H}\right\}}$$

with given inverse temperature $\beta = 1/(k_B T)$ and Hamiltonian H, and the **grand-canonical equilibrium state**

$$\rho_{gc} = \frac{e^{-\beta(H-\mu N)}}{\mathrm{Tr}\left\{e^{-\beta(H-\mu N)}\right\}}\,,$$

with particle number operator N and chemical potential μ.

- At given average energy and particle number, the grand-canonical equilibrium state maximizes the **von-Neumann entropy**

$$S(\rho) \equiv -\mathrm{Tr}\left\{\rho \ln \rho\right\} = -\sum_n \lambda_n \ln \lambda_n\,,$$
$$S_{gc} = \beta\left[\langle H\rangle - \mu \langle N\rangle\right] + \ln \mathrm{Tr}\left\{e^{-\beta(H-\mu N)}\right\}\ .$$

- Matrix exponentials can be easily made explicit at the example of **Pauli matrices**

$$\sigma^x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\,, \qquad \sigma^y = \begin{pmatrix} 0 & -\mathrm{i} \\ +\mathrm{i} & 0 \end{pmatrix}\,, \qquad \sigma^z = \begin{pmatrix} +1 & 0 \\ 0 & -1 \end{pmatrix}\,.$$

Any two-level system (qubit) for example can be conveniently described by Pauli matrices. From the properties of the Pauli matrices $\sigma^\alpha \sigma^\beta + \sigma^\beta \sigma^\alpha = 2\delta_{\alpha\beta}\mathbf{1}$ one can for example conclude that for $n_x^2 + n_y^2 + n_z^2 = 1$ one has

$$e^{-\mathrm{i}\alpha[n_x\sigma^x + n_y\sigma^y + n_z\sigma^z]} = \cos(\alpha)\mathbf{1} - \mathrm{i}\sin(\alpha)\left[n_x\sigma^x + n_y\sigma^y + n_z\sigma^z\right]\,,$$

which can be useful to compute the time evolution operator of an undriven qubit.

- When two quantum systems with Hilbert spaces V and W interact, one can construct a basis of the joint Hilbert space C by **tensor products** of the basis vectors of the individual Hilbert spaces

$$|c_{ij}\rangle = |v_i\rangle \otimes |w_j\rangle \ ,$$

and the dimension of the composite system is the product of the individual dimensions $N_c = N_v N_w$.

- The problems we are aiming at are most conveniently treated within the language of second quantization. Thus, we represent operators mostly in terms of creation and annihilation (ladder) operators.

The **bosonic ladder operators** obey commutation relations

$$\left[b_k, b_q^\dagger\right] = \delta_{kq} \, , \qquad [b_k, b_q] = 0 \, ,$$

where k and q denote modes. The total particle number operator is then given by

$$N = \sum_k b_k^\dagger b_k \, .$$

A convenient basis choice are then the **Fock states** defined as the eigenstates of the particle number operator. For a system with N modes we can label them by N integer numbers with

$$|n_1, n_2, \ldots, n_N\rangle = |n_1\rangle \otimes |n_2\rangle \otimes \ldots \otimes |n_N\rangle \qquad n_i \in \{0, 1, 2, 3, \ldots\} \, .$$

One can show that

$$\begin{aligned} b_k^\dagger \, |n_1, \ldots, n_k, \ldots, n_N\rangle &= \sqrt{n_k + 1} \, |n_1, \ldots, n_k + 1, \ldots, n_N\rangle \ , \\ b_k \, |n_1, \ldots, n_k, \ldots, n_N\rangle &= \sqrt{n_k} \, |n_1, \ldots, n_k - 1, \ldots, n_N\rangle \ . \end{aligned}$$

Consequently, we can represent all Fock states by acting with creation operators on the **vacuum state**

$$|n_1, \ldots, n_N\rangle = \prod_k \frac{(b_k^\dagger)^{n_k}}{\sqrt{n_k!}} \, |0, \ldots, 0\rangle \ .$$

In contrast, **fermionic ladder operators** obey anticommutation relations

$$\left\{f_k, f_q^\dagger\right\} = \delta_{kq} \, , \qquad \{f_k, f_q\} = 0 \, ,$$

where $\{A, B\} = AB + BA$. The total particle number operator is again given by

$$N = \sum_k f_k^\dagger f_k \, ,$$

and the Fock states are labeled by

$$|n_1, n_2, \ldots, n_N\rangle \qquad n_i \in \{0, 1\} \, .$$

The creation and annihilation operators act similarly as in the bosonic case, and likewise one can construct the Fock states by acting with creation (raising) operators on the vacuum state. However, note that there is an ambiguity in the sign of the Fock states, since the different creation operators anti-commute.

- For a bosonic Hamiltonian

$$H = \sum_k \omega_k b_k^\dagger b_k$$

with single-particle energies ω_k one can for the grand-canonical equilibrium state show for $\mu < \omega_k \ : \ \forall k$ that

$$\langle a_k \rangle = \mathrm{Tr}\left\{ a_k \frac{e^{-\beta(H-\mu N)}}{\mathrm{Tr}\left\{e^{-\beta(H-\mu N)}\right\}} \right\} = 0\,,$$
$$\left\langle a_k^\dagger a_q \right\rangle = \mathrm{Tr}\left\{ a_k^\dagger a_q \frac{e^{-\beta(H-\mu N)}}{\mathrm{Tr}\left\{e^{-\beta(H-\mu N)}\right\}} \right\} = \delta_{kq} \frac{1}{e^{\beta(\omega_k-\mu)}-1} \equiv \delta_{kq} n_B(\omega_k)\,,$$

where $n_B(\omega)$ is the **Bose-Einstein distribution** (often used with $\mu = 0$).

- For a fermionic Hamiltonian

$$H = \sum_k \epsilon_k f_k^\dagger f_k$$

with single-particle energies ϵ_k one can for the grand-canonical equilibrium state generally ($\mu \in \mathbb{R}$) show that

$$\langle f_k \rangle = \mathrm{Tr}\left\{ f_k \frac{e^{-\beta(H-\mu N)}}{\mathrm{Tr}\left\{e^{-\beta(H-\mu N)}\right\}} \right\} = 0\,,$$
$$\left\langle f_k^\dagger f_q \right\rangle = \mathrm{Tr}\left\{ f_k^\dagger f_q \frac{e^{-\beta(H-\mu N)}}{\mathrm{Tr}\left\{e^{-\beta(H-\mu N)}\right\}} \right\} = \delta_{kq} \frac{1}{e^{\beta(\epsilon_k-\mu)}+1} \equiv \delta_{kq} n_F(\epsilon_k)\,,$$

where $n_F(\omega)$ is the **Fermi-Dirac distribution** (also Fermi function).

- The term **universe** denotes the model universe as a whole, it can be split into a part of interest of the universe, which we call **system** and the rest, which we call **reservoir**. We will mostly be concerned with model universes where the reservoir actually behaves as a standard reservoir (i.e., it is approximately inert).

- A linear map that takes a valid density matrix ρ into another valid density matrix ρ' while preserving the density matrix properties is given by

$$\rho' = \sum_\alpha K_\alpha \rho K_\alpha^\dagger \qquad : \qquad \sum_\alpha K_\alpha^\dagger K_\alpha = \mathbf{1}\,.$$

Here, the operators K_α can be called Kraus operators.