Week 10

PHY 435 / 635 Decoherence and Open Quantum Systems
Instructor: Sebastian Wüster, IISER Bhopal, 2018

These notes are provided for the students of the class above only. There is no warranty for correctness, please contact me if you spot a mistake.

In the previous section we had seen that revival features of coherences (or Purity) can correctly be captured by non-Markovian methods, but not with Markovian ones. The Redfield method used there is conceptually simple to derive, but not very efficient for larger systems (the Refield tensor $R_{ab;cd}$ has N^4 components for N system basis states).

In the next section we thus list several advanced methods that can be used to tackle challenging non-Markovian open quantum problems. The purpose is merely to provide you with keywords for further reading when needed.

5.2 Methods for Non-Markovian Open Quantum System Dynamics

Further reading: "Dynamics of non-Markovian open quantum systems", I. de Vega and D. Alonso, Rev. Mod. Phys. **89** 015001 (2017).

5.2.1 Stochastic Schrödinger equations

A fairly basic problem that already arises for Markovian open quantum systems, is that even if we restrict ourselves to a small number M of basis states in the Hilbert-space, the density matrix $\hat{\rho}$ has $M \times M$ elements, compared to M elements in a quantum state $|\,\Psi\,\rangle$, which complicated numerical solutions. For intermediate system sizes, this problem can efficiently be overcome using the

Quantum Jump Monte Carlo Method
Consider the Lindblad Master equation (4.24). Instead of it, we evolve a Schrödinger equation with a *non-Hermitian* effective Hamiltonian $\hat{H}_{\rm eff}$:

$$i\hbar\frac{d}{dt}|\,\Psi_{\mathcal{S}}\,\rangle = \hat{H}_{\rm eff}|\,\Psi_{\mathcal{S}}\,\rangle \equiv \left(\hat{H}_{\mathcal{S}} - i\hbar\sum_{\mu}\hat{L}_{\mu}^{\dagger}\hat{L}_{\mu}\right)|\,\Psi_{\mathcal{S}}\,\rangle. \tag{5.20}$$

After one numerical time-step δt, the wavefunction will have norm $\langle\,\Psi_{\mathcal{S}}\,|\,\Psi_{\mathcal{S}}\,\rangle = 1-\sum_{\mu}\delta p_{\mu} < 1$, for very small δp_{μ}. The latter are given by $\delta p_{\mu} = \delta t\langle\,\Psi_{\mathcal{S}}\,|\hat{L}_{\mu}^{\dagger}\hat{L}_{\mu}|\,\Psi_{\mathcal{S}}\,\rangle$.

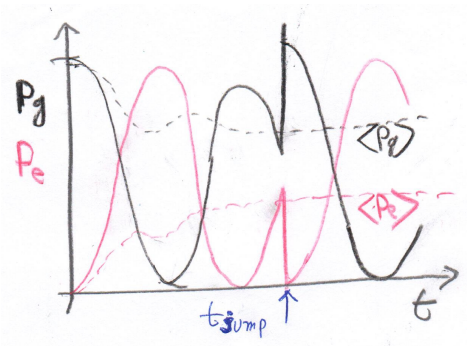
Using random numbers, we then perform a quantum jump with probability $p = \sum_\mu \delta p_\mu$, by projecting the wavefunction onto any of the states $\hat{L}_\mu |\, \Psi_\mathcal{S} \,\rangle$ with probability δp_μ, and then renormalizing the state to unity.
The density matrix in the end is obtained by averages over many realisations of this procedure, according to

$$\hat{\rho} = \overline{|\, \Psi_\mathcal{S} \,\rangle\langle\, \Psi_\mathcal{S} \,|}, \tag{5.21}$$

where $\overline{\cdots}$ is the stochastic average.
See: K. Molmer, Y. Castin, and J. Dalibard, J. Opt. Soc. Am. B **10**, 524 (1993).

- The decohering effects of the environment enter here through the randomness of the jumps.
- Solving the evolution of the probability distributions underlying the density matrix through actual stochastic processes is called unravelling of the Master equation. Note that there may be multiple differing unravellings of any given Master equation.
- While they are mainly mathematical tricks, unravelling still also can give additional intuitive ideas of the physical origin of some decoherence phenomena, see below.

Quantum Jump trajectories for driven two-level atom:



left: Consider again the first example in section 4.6 (at $T = 0$). The sketch on the left shows how the populations in the ground and excited state would look in a single trajectory (realisation) of quantum jump Monte Carlo. The atom tries to undergo the usual Rabi oscillations, which are interrupted and reset at random moments t_{jump}. Averaging over many of those looses all the oscillatory features and can give us a picture like the right one in the earlier example (also shown on the left as dotted lines).

Noise also allows efficient tackling of non-Markovian scenarios, such as in

Non-Markovian Quantum State Diffusion (NMQSD)
Here the system evolves according to the stochastic differential equation (SDE) ($\hbar = 1$, single μ)

$$\frac{d}{dt}|\,\Psi_{\mathcal{S}}\,\rangle = -i\hat{H}_{\mathcal{S}}|\,\Psi_{\mathcal{S}}\,\rangle + \hat{S}|\,\Psi_{\mathcal{S}}\,\rangle z(t) - \hat{S}^{\dagger}\int_0^t ds\;\; C(t,s)\hat{O}(t,s,z)ds|\,\Psi_{\mathcal{S}}\,\rangle. \tag{5.22}$$

Here $z(t)$ is a complex random process that has correlations $\overline{z^*(t)z(s)} = C(t,s)$, $\overline{z(t)s(t)}$, where $C(t,s)$ is the bath correlation function (4.15). $\hat{O}$ is an additional operator to be determined from some complicated procedure. See: L. Diósi, N. Gisin, and W. T. Strunz, Phys. Rev. A **58, 1699 (1998).**

- Non-Markovian effects can enter through the bath correlation function $C(t)$.
- As before, the density matrix is obtained through stochastic averaging.

5.2.2 Path Integral Methods

There are a couple of advanced methods based on Feynman's Path Integral (see advanced QM lectures), which we list here only in order for you to be able to place the abbreviations when you encounter them. See the review for references.

- Quasiadiabatic propagator path integral (QUAPI)
- Path integral Monte Carlo schemes (PIMC)
- Hierarchical Equation of Motion (HEOM)

5.3 Non-Markovian Dynamics and Information Flow

Further reading: "Colloquium: Non-Markovian dynamics in open quantum systems", H.-P. Breuer *et. al*, Rev. Mod. Phys. **88** 021002 (2016).

It turns out that information theoretic concepts can offer some interesting insight into Non-Markovian Dynamics. We have to first generalize the concepts of distinguishable states and overlap to density matrices.

Orthogonal density matrices Open quantum system "states" (density matrices) are called orthogonal, if their support is orthogonal. Diagonalizing the density matrix $\hat{\rho} = \sum_n p_n|\,n\,\rangle\langle\,n\,|$, the support is spanned by the vectors $\{|\,n\,\rangle, p_n \neq 0\}$, that is all eigenvectors with non-zero eigenvalue.

We introduce the

Trace distance of two density matrices $\hat{\rho}_1$, $\hat{\rho}_2$ as

$$D(\hat{\rho}_1, \hat{\rho}_2) \equiv \frac{1}{2}||\hat{\rho}_1 - \hat{\rho}_2||, \tag{5.23}$$

where we define the norm of an operator as $||\hat{O}|| = \sqrt{\hat{O}^\dagger \hat{O}} (= \sum_j |o_j|^2)$. The expression as sum over mod-squares of eigenvalues o_j requires a Hermitian $\hat{O}$.

- One can show that $D(\hat{\rho}_1, \hat{\rho}_2) = 0$ iff $\hat{\rho}_1 = \hat{\rho}_2$ and $D(\hat{\rho}_1, \hat{\rho}_2) = 1$ iff $\hat{\rho}_1$ and $\hat{\rho}_2$ are orthogonal. In this sense the trace distance is a measure of the distinguishability of two density matrices.

Returning to the concept of reduced system evolution as a dynamical map (4.2), where $\hat{\rho}_\mathcal{S}(t) = \hat{V}(t,0)[\hat{\rho}_\mathcal{S}(0)]$ (we introduced the extra label 0, indicating time propagation from $t = 0$ to t), one can see that in the Markovian case we have

Divisible maps: For times $t > s > 0$, we have

$$\hat{\rho}_\mathcal{S}(t) = \hat{V}(t,0)[\hat{\rho}_\mathcal{S}(0)] = \hat{V}(t,s)[\hat{V}(s,0)[\hat{\rho}_\mathcal{S}(0)]]. \tag{5.24}$$

The dynamical map $\hat{V}(t,0)$ is then called divisible.

One (=mathematicians) can further show that under trace preserving positive map[7], the trace distance between any two density matrices can only be reduced. This implies

$$D(\hat{\rho}_1(t), \hat{\rho}_2(t)) \leq D(\hat{\rho}_1(0), \hat{\rho}_2(0)) \tag{5.25}$$

for Markovian evolution (where $\hat{\rho}_1(t) = \hat{V}(t,0)[(\hat{\rho}_1(0)]$ etc.).

We now interpret the distinguishability (and hence the trace distance) of two density matrices as the level of information content of the system. Since D must decrease for Markovian evolution, , information always flows one way from the system to the environment in that case. In contrast, in the non-Markovian case it can also flow back into the system.

These concepts than allow the definition of a "measure" of non-Markovianity, that can *quantify* to what degree a system is non-Markovian. One defines the

[7] This means any physically reasonable map.

Measure for the "Non-Markovianity" of the time evolution of some open quantum systems:

$$\mathcal{NM} = \max_{\rho_{S^{(1,2)}}} \left[\int_{\sigma>0} dt\, \sigma(t) \right], \tag{5.26}$$

where $\sigma(t) = \frac{d}{dt} D(\hat{\rho}_1(t), \hat{\rho}_2(t))$.

- In words the above definition implies this algorithm: (i) Start with all possible pairs of density matrices $\hat{\rho}_1(0)$, $\hat{\rho}_2(0)$ in the system. Evolve these in time (or measure their time evolution), and determine the time evolution of the trace distance. (iii) Only for those time intervals where it is increasing we integrate this up. (iv) The measure $\mathcal{NM}$ is finally the maximal result for all initial states.
- Since we typically cannot really maximise over all possible pairs of initial states, just maximising over many pairs should already give us a solid lower bound.
- Different measures for this also exist in the literature.

6 Applications of Decoherence

For those interested I recommend reading chapters 6,7 of SD, "decoherence in action" and "decoherence and quantum computing" as a "reward" for the effort put into following this lecture. These contain interesting descriptions of real world experiments and technologies where the concepts learnt are absolutely crucial.