4

Quantum trajectories

In the previous chapter we discussed various methods – operator sum representation and master equation – to study the dynamics of an open quantum system. In this chapter we discuss a numerical approach to solve the master equation namely, quantum trajectory approach. This technique was first introduced in [43, 163, 44, 45, 42].

In this chapter we will discuss the basics of quantum trajectory approach. We start with the perturbative expansion for the density operator ρ for the system S interacting with the bath B. This is followed by the section on unravelling the Lindblad master equation and the Monte Carlo simulations.

4.1 Perturbative expansion for the density operator

Consider the master equation

$$\dot{\rho} = \mathcal{L}\rho \tag{4.1}$$

for the density operator ρ. $\mathcal{L}$ is the Liouvillian. In general, the Liouvillian $\mathcal{L}$ can be written as the sum of an unperturbed part $\mathcal{L}_0$ and a small perturbation S, such that

$$\mathcal{L} = \mathcal{L}_0 + S. \tag{4.2}$$

The formal solution of Eq. (4.1) is

$$\rho_S(t) = e^{(\mathcal{L}_0+S)t}\rho_S(0). \tag{4.3}$$

For the perturbation expansion of $\rho(t)$, consider the operator:

$$\mathcal{A} = \exp\left((\mathcal{L}_0 + S)t\right) \tag{4.4}$$

and let

$$\mathcal{B} = e^{-\mathcal{L}_0 t}\mathcal{A}. \tag{4.5}$$

From here we get

$$\begin{aligned}\dot{\mathcal{B}} &= -\mathcal{L}_0 e^{-\mathcal{L}_0 t}\mathcal{A} + e^{-\mathcal{L}_0 t}(\mathcal{L}_0 + S)\mathcal{A} \\ &= e^{-\mathcal{L}_0 t}(S)\mathcal{A} \\ &= e^{-\mathcal{L}_0 t} S e^{\mathcal{L}_0 t}\mathcal{B}.\end{aligned} \tag{4.6}$$

This give rise to a formal solution

$$\mathcal{B}(t) = \mathcal{I} + \int_0^t \dot{\mathcal{B}}(s)ds \tag{4.7}$$

$$\Rightarrow \mathcal{A} = e^{\mathcal{L}_0 t}\left(\mathcal{I} + \int_0^t e^{-\mathcal{L}_0 s} S e^{\mathcal{L}_0 s}\mathcal{B}ds\right). \tag{4.8}$$

Repeating this process give rise to the identity

$$\begin{aligned}\mathcal{A} = \sum_{m=0}^{\infty}\int_0^t dt_m \int_0^{t_m} dt_{m-1}\cdots\int_0^{t_2} dt_1 \\ \times e^{\mathcal{L}_0(t-t_m)} S e^{\mathcal{L}_0(t_m - t_{m-1})} S \cdots S e^{\mathcal{L}_0 t_1}\end{aligned} \tag{4.9}$$

and hence we get

$$\begin{aligned}e^{(\mathcal{L}_0+S)t} = \sum_{m=0}^{\infty}\int_0^t dt_m \int_0^{t_m} dt_{m-1}\cdots\int_0^{t_2} dt_1 \\ \times e^{\mathcal{L}_0(t-t_m)} S e^{\mathcal{L}_0(t_m - t_{m-1})} S \cdots S e^{\mathcal{L}_0 t_1}\end{aligned} \tag{4.10}$$

with $\{t_m\}$ a monotonically increasing sequence.

The integrand in Eq. (4.10) describes a single quantum trajectory for the initial state $\rho(0)$, The terms $\exp[\mathcal{L}_0(t_m - t_{m-1})]$ represents continuous time-evolution in the intervals $[t_{m-1}, t_m)$, while S represents discontinuous quantum jumps at time $\{t_m\}$. Eq (4.10) can be interpreted as a generalized sum over all the possible "jump" pathways that the system might follow during its evolution from time $t = 0$ to time t.

One can choose different $\mathcal{L}_0$ and S depending on the experimental setup or the requirement of the problem. Different choices of $\mathcal{L}_0$ and S give rise to different trajectories or unravellings. In the next section we will discuss the quantum trajectory for a specific $\mathcal{L}_0$ and S for Lindblad master equation.

4.2 Unravelling the Lindblad master equation

Consider the Lindblad form of master equation (see Eq. (3.48)):

$$\begin{aligned}\dot{\rho}(t) &= -i[H,\rho] + \mathcal{D}\rho \\ &= -i[H,\rho] + \sum_j 2\gamma_j F_j \rho F_j^\dagger - \gamma_j [F_j^\dagger F_j \rho + \rho F_j^\dagger F_j].\end{aligned} \tag{4.11}$$

In this equation we choose F_i to be jump operators. The terms $F_i^\dagger F_i \rho/2$ and $\rho F_i^\dagger F_i/2$ describes the loss of population from the current states. The term $F_i \rho F_i^\dagger$ can be understood as the density matrix after the transition described by F_i; such transition can be interpreted as "quantum trajectory".

Now we can write:

$$\mathcal{L}_0 = -i[H,\rho] + \sum_j 2\gamma_j - \gamma_j [F_j^\dagger F_j \rho + \rho F_j^\dagger F_j] \tag{4.12}$$

and

$$S = \sum_i S_i, \tag{4.13}$$

where

$$S_i\rho = F_i\rho F_i^\dagger. \tag{4.14}$$

The unperturbed Liouvillian $\mathcal{L}_0$ can be written as

$$\mathcal{L}_0 = -i[H_{eff}\rho - \rho H_{eff}], \tag{4.15}$$

where

$$H_{eff} = H - i\sum_j \gamma_j [F_j^\dagger F_j]. \tag{4.16}$$

This non-hermitian Hamiltonian generates non-unitary time-evolution and we can write the non-unitary Schrödinger equation

$$i\frac{d}{dt}|\psi(t)\rangle = H_{eff}|\psi(t)\rangle. \tag{4.17}$$

This confirms that the unperturbed part of the Liouvillian $\mathcal{L}_0$ give rise to non-unitary coherent time-evolution for the initial state $\rho(0)$. This coherent evolution is interrupted by non-deterministic jumps S_i. The probability of the jump in a particular time interval Δt can be calculated as:

$$\begin{aligned} p_{c,i}(t) &= \mathrm{tr}(S_i\rho_c(t))\Delta t, \\ &= 2\gamma_i \mathrm{tr}(F_i\rho_c(t)F_i^\dagger)\Delta t, \\ &= 2\gamma_i \langle F_i^\dagger F_i\rangle \Delta t, \end{aligned} \tag{4.18}$$

where ρ_c is the density matrix in a particular trajectory. It is often called conditioned density operator. The probability to find at least one jump in the time interval $[t, t+\Delta t)$ due to any of the S_i is given by:

$$p_c(t) = \sum_i p_{c,i}(t). \tag{4.19}$$

4.3 Monte Carlo simulation

Monte Carlo simulation provides the most useful implementation of the quantum trajectory. This section outlines a Monte Carlo algorithm for the generation of stochastic quantum trajectories based on the unravelling of the Lindblad master equation developed thus far.

In the simulation, time is discrete with a time-step Δt. We start with an arbitrary state $|\Psi(0)\rangle$. Let $|\Psi(t)\rangle$ be the state at time t. Then we

1. evolve the state $|\Psi(t_{n+1})\rangle$ as:

$$|\Psi(t_{n+1})\rangle = \exp(-iH_{eff}\Delta t)|\Psi(t_n)\rangle. \tag{4.20}$$

2. Normalise the state:

$$|\Psi(t_{n+1})\rangle = \frac{|\Psi(t_{n+1})\rangle}{\sqrt{\langle\Psi(t_{n+1})|\Psi(t_{n+1})\rangle}}. \tag{4.21}$$

3. Calculate the probability for the jump:

$$\begin{aligned} p_{c,i}(t_n) &= \langle\Psi(t_n)|F_i^\dagger F_i|\Psi(t_n)\rangle\Delta t, \\ P_c(t_n) &= \sum_i p_{c,i}(t_n). \end{aligned} \tag{4.22}$$

4. Draw a random number r_n from a uniform distribution in the interval $[0, 1)$ and compare it with P_c.

   (a) If $P_c(t_n) \geq r_n$, a jump occurs. The new instantaneous state of the system is $|\Psi(t_{n+1})\rangle = F_i|\Psi(t_n)\rangle$.

   (b) If $P_c(t_n) < r_n$, go to step 1