Lecture 25: Quantum Trajectories Continued

Quantum Monte-Carlo Wavefunction

The statistical evolution of ~~of~~ the pure state in each dt

$$|\psi(t)\rangle \xrightarrow{1-dp} |\phi_0(t)\rangle \quad \text{(No jump)}$$

$$|\psi(t)\rangle \xrightarrow{dp} |\phi_1(t)\rangle \quad \text{(Jump)}$$

gives a method of simulating the master equation.

(i) Suppose $\hat{\rho}(0) = |\psi(0)\rangle\langle\psi(0)|$ a pure state

(ii) Choose a very small grid $\Delta t \ll \frac{1}{\omega}$ ← eigenvalue of $\hat{H}$

(iii) Calculate $dp(t) \equiv \Gamma dt \langle\psi(t)|\hat{\sigma}_+\hat{\sigma}_-|\psi(t)\rangle$ at time t

(iv) At any time t pick a random number ϵ, $0 \le \epsilon \le 1$

(a) If $\epsilon < dp(t)$, jump $|\tilde{\psi}(t)\rangle = \hat{\sigma}_-|\psi(t)\rangle$

(b) Else $|\tilde{\psi}(t+\Delta t)\rangle = e^{-i\hat{H}_{eff}\Delta t/\hbar}|\psi(t)\rangle$

(v) Renormalize $|\psi\rangle = \dfrac{|\tilde{\psi}\rangle}{\|\tilde{\psi}\|}$

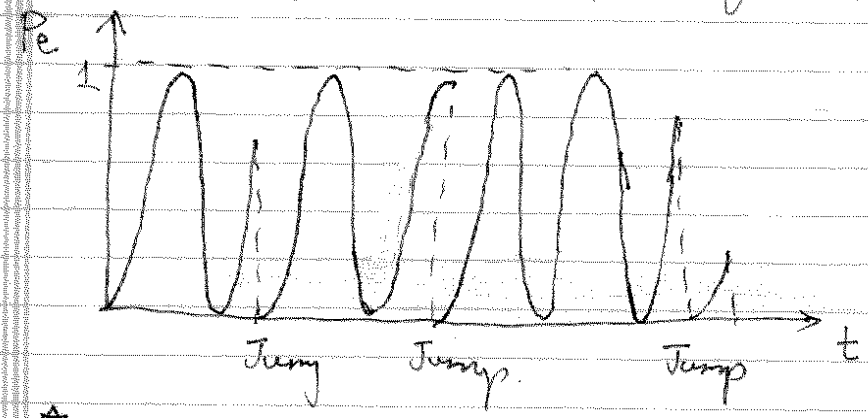
Each $|\psi(t)\rangle$ is known as a quantum trajectory.

If we average over different runs, with quasi-random #s ϵ, we recover the probabilities expected for the density operator

$$\Rightarrow \boxed{\hat{\rho}(t) = \langle\langle |\psi(t)\rangle\langle\psi(t)| \rangle\rangle_{\text{average over many runs}}}$$

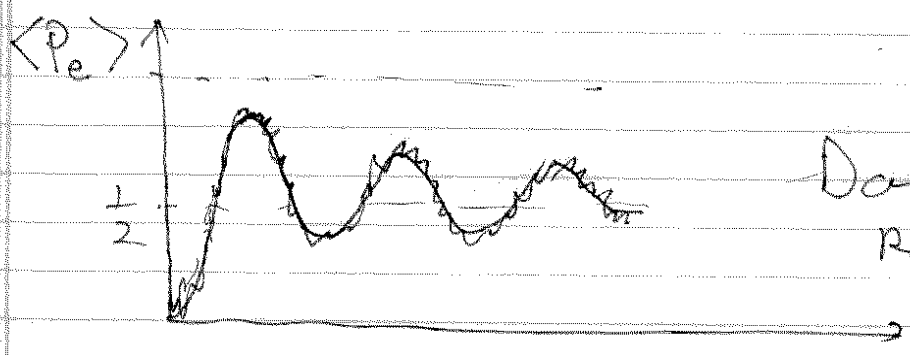
In certain circumstances this is preferred method for simulation rather than direct integration of the master eqn. Whereas $\hat{\rho}$ has $O(D^2)$ elements $|\psi\rangle$ has $O(D)$ for D = dim (Hilbert space). Thus, if memory is an issue, for ~~very~~ very large Hilbert spaces, this is very efficient.

Thus, for the case at hand — a two-level atom driven by laser and coupled to the vacuum a given quantum trajectory might be



e.g.
Highly saturated
$\Delta = 0$
$\Omega = 10\Gamma$

Averaged over <u>many</u> trajectories $\Rightarrow$ dephasing



Damped Rabi flopping

Here, the "smooth" curve is the exact solution to the master equation and the "noisy" curve is average over many trajectories. The "noise" is due to the fact that we took a finite # of runs. It is a numerical "experiment" averaged over a finite number of equivalent to measuring the fluorescence for a finite number of atoms in a true experiment (counting statistics).

To determine the efficacy of our ~~[illegible]~~ simulation we must do a proper error analysis.

Statistics of the QMC method

Suppose we take N trajectories.

$$\Rightarrow \langle \hat{A} \rangle_N \equiv \frac{1}{N} \sum_{i=1}^{N} \langle \phi^{(i)}_{(t)} | \hat{A} | \phi^{(i)}_{(t)} \rangle \equiv \langle\langle \hat{A}_L \rangle\rangle$$

approximates the true value $\langle \hat{A} \rangle \equiv \mathrm{Tr}(\hat{\rho} \hat{A})$

The statistical error $\delta A_N \equiv \frac{\Delta A_N}{\sqrt{N}} = \sqrt{\langle (\langle \hat{A} \rangle_N - \langle \hat{A} \rangle)^2 \rangle}$

where $\Delta A_N^2 \equiv \langle\langle \hat{A}_L^2 \rangle\rangle - \langle \hat{A} \rangle_N^2$

$$= \frac{1}{N} \left(\sum_{i=1}^{N} \langle \phi^{(i)} | \hat{A} | \phi^{(i)} \rangle^2 \right) - \langle \hat{A} \rangle_N^2$$

is the sample variance

Signal to noise: $\frac{\langle \hat{A} \rangle}{\delta A_N} = \sqrt{N} \frac{\langle \hat{A} \rangle}{\Delta A_N} \gg 1$

$$\Rightarrow \text{Require } \boxed{\sqrt{N} \gg \frac{\Delta A_N}{\langle \hat{A} \rangle}}$$

"Local" vs. "Global" operators:

- If $\hat{A} = |j\rangle\langle j|$ $\quad \hat{A}^2 = \hat{A}$ $\Rightarrow \begin{cases} \langle \hat{A} \rangle \sim \frac{1}{D} & D = \dim \mathcal{H} \\ \Delta A^2 \sim \frac{1}{D} & D \gg 1 \end{cases}$

$\Rightarrow$ Require $N \gg D$

$\Rightarrow$ Better to solve master equation directly

- If Eigenspace of $\hat{A}$ is of order D

$$\Delta A \sim \langle \hat{A} \rangle \Rightarrow \sqrt{N} \gg 1$$

$\Rightarrow$ Good state for N large compared to unity

General case: Linblad form

We can generalize our procedure for "unraveling" the master equation in stochastically evolving quantum trajectories for a general class of the "Linblad" form

$$\frac{\partial \hat{\rho}}{\partial t} = -\frac{i}{\hbar}[\hat{H}, \hat{\rho}] + \sum_{m=1}^{M}\left(-\frac{1}{2}\left(\hat{C}_m^{\dagger}\hat{C}_m\hat{\rho} + \hat{\rho}\hat{C}_m^{\dagger}\hat{C}_m\right) + \hat{C}_m\rho\hat{C}_m^{\dagger}\right)$$

where $\{\hat{C}_m\}$ of M operators are known as the jump operators (sometime Linblad operators)

e.g. Two-level atom plus thermal reservoir

$$\hat{C}_1 = \sqrt{\Gamma(\bar{n}+1)}\,\hat{\sigma}_- \qquad \hat{C}_2 = \sqrt{\Gamma\bar{n}}\,\hat{\sigma}_+$$

Damped oscillator $\quad \Downarrow \hat{a} \qquad \Downarrow \hat{a}^{\dagger}$

The Linblad form was studied in 1976, ~~pre~~ arising in any system-reservoir Markovian dynamics,

As before we can "unravel" to Master equation by integrating, starting with a pure state

~~Given $|\psi(t)\rangle = |\psi(t)\rangle$~~

First note $\left.\frac{\partial\hat{\rho}}{\partial t}\right|_{\text{Hom, Hamm}} + \left.\frac{\partial\hat{\rho}}{\partial t}\right|_{\text{Decay}} = -\frac{i}{\hbar}[\hat{H}_{eff}, \hat{\rho}]$

where $\hat{H}_{eff} = \hat{H} - \frac{1}{2}\sum_m \hat{C}_m^{\dagger}\hat{C}_m$

Given $\hat{\rho}(t) = |\psi(t)\rangle\langle\psi(t)|$

$$\Rightarrow \hat{\rho}(t+dt) = |\tilde{\phi}_0(t,dt)\rangle\langle\tilde{\phi}_0(t,dt)| + \sum_{m=1}^{M}|\tilde{\phi}_m(t,dt)\rangle\langle\tilde{\phi}_m(t+dt)|$$

$$= \delta p_0|\phi_0(t,dt)\rangle\langle\phi_0(t,dt)| + \sum_{m=1}^{M}(\delta p_m)\,|\phi_m(t,dt)\rangle\langle\phi_m(t,dt)|$$

$\hat{\rho}(t+dt)$ is a statistical mixture of $M+1$ states

with $|\tilde{\phi}_m(t,dt)\rangle = \sqrt{dt}\,\hat{C}_m|\psi(t)\rangle$

$$|\phi_m(t,dt)\rangle = \frac{|\tilde{\phi}_m(t,dt)\rangle}{\|\tilde{\phi}_m\|} = \frac{\hat{C}_m|\psi(t)\rangle}{\|\hat{C}_m|\psi(t)\rangle\|}$$

$$\delta p_m = \|\tilde{\phi}_m\|^2 = dt\,\langle\psi(t)|\hat{C}_m^\dagger\hat{C}_m|\psi(t)\rangle$$

$$|\tilde{\phi}_0(t,dt)\rangle = \left(1-\frac{i}{\hbar}\hat{H}_{eff}dt\right)|\psi(t)\rangle \approx e^{-\frac{i}{\hbar}\hat{H}_{eff}dt}|\psi(t)\rangle$$

$$|\phi_0(t,dt)\rangle = \frac{|\tilde{\phi}_0\rangle}{\|\tilde{\phi}_0\|}$$

$$\delta p_0 = \|\tilde{\phi}_0\|^2 = 1 - \frac{i}{\hbar}dt\,\langle\psi(t)|\left(\hat{H}_{eff}^\dagger - \hat{H}_{eff}\right)|\psi(t)\rangle$$

$$= 1 - \sum_m \langle\psi(t)|\hat{C}_m^\dagger\hat{C}_m|\psi(t)\rangle dt$$

$$= 1 - \sum_m \delta p_m \equiv 1 - \delta p$$

Thus, for the general Linblad form, we can define a generalized Monte-Carlo simulation

$$\boxed{|\psi(t)\rangle} \xrightarrow[\text{jump}]{\delta p} \begin{cases} \xrightarrow{\delta p_1} \\ \vdots \\ \xrightarrow{\delta p_m} \end{cases} |\psi(t+dt)\rangle = \frac{\hat{C}_m|\psi(t)\rangle}{\|\hat{C}_m|\psi(t)\rangle\|}$$

$$\xrightarrow[1-\delta p]{\text{no jump}} |\psi(t+dt)\rangle = e^{-\frac{i}{\hbar}\hat{H}_{eff}dt}|\psi(t)\rangle$$

First we pick a random # $0<\epsilon<1$. If $\delta p \equiv \sum_m \langle\psi(t)|\hat{C}_m^\dagger\hat{C}_m|\psi(t)\rangle < \epsilon \Rightarrow$ Jump.

To pick which jump occurs, $\Pi_m \equiv \frac{\delta p_m}{\delta p}$ is its probability. Choose another random number.

If no jump evolve by $\hat{H}_{eff}$. Repeat

Further considerations

The procedure outlined, while formally correct is not necessarily very efficient, only accurate to order δt in the true time step. For very small δt, the probability of a jump $\delta p = \sum_m c_m^\dagger c_m \, \delta t \ll 1$.

$\Rightarrow$ Most of the time a jump does not occur and we "waste" "random" numbers in our algorithm.

A more efficient procedure is to use a "waiting time" or "delay function". For the simple case studies in Lect #24, decaying atom in the absence of a driving field we found the probability that no jump occurs for a duration τ

$$P(\tau) = |c_g|^2 + e^{-\Gamma\tau}|c_e|^2 = \| e^{-iH_{eff}\tau/\hbar}|\psi(0)\rangle\|^2$$

$$|\psi(0)\rangle = c_g|g\rangle + c_e|e\rangle$$

More generally, we have $P(\tau)$ satisfying

$$P(\tau+d\tau) = \delta p_0(\tau, d\tau)\, P(\tau)$$

$$= \langle\psi(\tau)| e^{\frac{i}{\hbar}(H_{eff}-H_{eff}^\dagger)d\tau} |\psi(\tau)\rangle \; P(\tau)$$

where $$|\psi(\tau)\rangle = \frac{e^{-\frac{i}{\hbar}H_{eff}\tau}|\psi(0)\rangle}{\sqrt{\langle\psi(0)| e^{\frac{i}{\hbar}(H_{eff}^\dagger - H_{eff})\tau}|\psi(0)\rangle}}$$

Solution: $P(\tau) = \| e^{-iH_{eff}\tau}|\psi(0)\rangle\|^2$

Thus, an efficient MCWF simulation can be generated picking a random number and evolving $|\psi\rangle$ deterministically by $e^{-iH_{eff}t/\hbar}$ until $\|\tilde{\psi}(\tau)\|^2 \equiv \langle\psi(0)| e^{+\frac{i}{\hbar}(H_{eff}^\dagger - H_{eff})\tau}|\psi(0)\rangle < \epsilon$.

Then jump, renormalize, and repeat.

Waiting time distribution for resonance fluorescence

Let us return to our simple problem problem of resonance fluorescence of a two-level atom.

For $\Delta = 0$ $\quad \hat{H}_{eff} = -i\hbar\frac{\Gamma}{2}|e\rangle\langle e| - \frac{\hbar\Omega}{2}\left(|e\rangle\langle g| + |g\rangle\langle e|\right)$

This is equivalent to the Rabi flopping Hamiltonian we studied in Lecture #3 with $\Delta \to -i\frac{\Gamma}{2}$ (taking also the zero of energy at the ground state)

There we found for $|\psi(0)\rangle = |g\rangle$

$$|\psi(t)\rangle = e^{-\frac{i}{\hbar}\hat{H}t}|\psi(0)\rangle$$

$$= e^{-i\Delta t/2}\left\{\left(\cos\left(\frac{\tilde{\Omega}t}{2}\right) + i\frac{\Delta}{\tilde{\Omega}}\sin\left(\frac{\tilde{\Omega}t}{2}\right)\right)|g\rangle + \left(i\frac{\Omega}{\tilde{\Omega}}\sin\left(\frac{\tilde{\Omega}t}{2}\right)\right)|e\rangle\right\}$$

where $\tilde{\Omega} = (\Omega^2 + \Delta^2)^{1/2}$

Now for the case with decay, and on resonance

$\Delta \Rightarrow -i\frac{\Gamma}{2}$, $\quad \tilde{\Omega} \Rightarrow \sqrt{\Omega^2 - \frac{\Gamma^2}{4}}$ $\quad$ (real for $\Omega > \frac{\Gamma}{2}$ saturated)

The unnormalized wavefunction under the no-jump condition

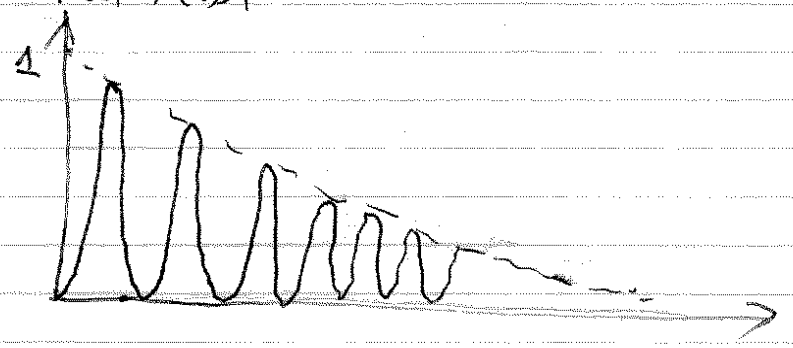
$$|\tilde{\psi}(t)\rangle = e^{-\frac{i}{\hbar}\hat{H}_{eff}t}|\psi(0)\rangle$$

$$= e^{-\frac{\Gamma}{4}t}\left\{\left(\cos\left(\frac{\tilde{\Omega}t}{2}\right) + \frac{\Gamma}{2\tilde{\Omega}}\sin\left(\frac{\tilde{\Omega}t}{2}\right)\right)|g\rangle + i\frac{\Omega}{\tilde{\Omega}}\sin\left(\frac{\tilde{\Omega}t}{2}\right)|e\rangle\right\}$$

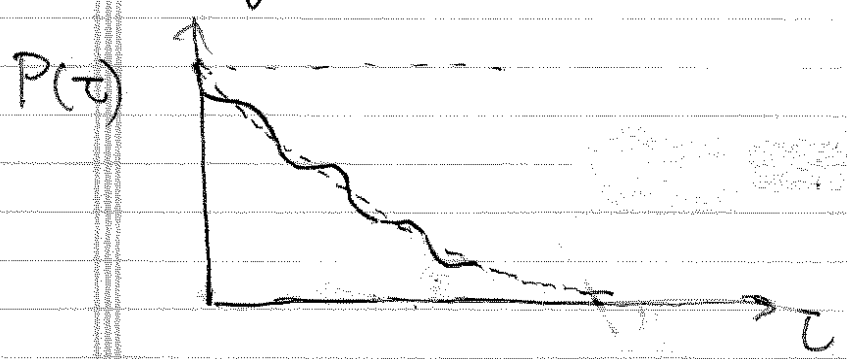
where $\tilde{\Omega} = \sqrt{\Omega^2 - \frac{\Gamma^2}{4}}$

~~The~~ In its unnormalize form, the probability to be in the excited state decays as it oscillates

$\tilde{P}_e(t) = |\langle e|\tilde{\Psi}(t)\rangle|^2$



Waiting function $\langle\tilde{\Psi}(t)|\tilde{\Psi}(t)\rangle = e^{-\frac{\Gamma}{2}t}\left[\left(\cos\left(\frac{\tilde{\Omega}}{2}t\right) + \frac{\Gamma}{2\tilde{\Omega}}\sin\left(\frac{\tilde{\Omega}t}{2}\right)\right)^2 + \frac{\Omega^2}{\tilde{\Omega}^2}\sin^2\left(\frac{\tilde{\Omega}t}{2}\right)\right]$



Normalized wavefunction

$P_e(t) = \tilde{P}_e(t) / \langle\tilde{\Psi}(t)|\tilde{\Psi}(t)\rangle$