Advanced quantum mechanics
TD 3 : The Lindblad master equation as a stochastic evolution : the Monte Carlo wave function method

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1 Monte Carlo wave function or quantum jump method

We wish to describe the dynamics of a system S that is coupled to a (large) bath/environment E. While the Schrödinger equation deals with state vectors, which can only describe pure quantum states, our system S will be described by a density matrix $\hat{\rho}_S$ [1]. The dynamics of the system can be approximately described via the Lindblad master equation :

$$\frac{d}{dt}\hat{\rho}_S = \frac{1}{i\hbar}\left[\hat{H}_{eff}\hat{\rho}_S - \hat{\rho}_S\hat{H}_{eff}^\dagger\right] + \sum_i \hat{L}_i\hat{\rho}_S\hat{L}_i^\dagger \tag{1}$$

where the effective Hamiltonian

$$\hat{H}_{eff} = \hat{H}_0 - \frac{i\hbar}{2}\sum_i \hat{L}_i^\dagger\hat{L}_i \ , \tag{2}$$

contains a Hermitian part $\hat{H}_0$ and an anti-Hermitian part. The $\{\hat{L}_i\}$ are a set of so-called jump operators, describing the dissipative part of the dynamics.

We wish to reformulate Lindblad's master equation for $\hat{\rho}_S(t)$ in terms of a stochastic evolution of "wave functions", i.e. state vectors $|\phi(t)\rangle$ of S, such that averaging over all possible stochastic evolutions exactly gives the solution to the Lindblad equation :

$$\hat{\rho}_S(t) = \Big\langle\, |\phi(t)\rangle\langle\phi(t)| \,\Big\rangle \ , \tag{3}$$

with $\langle\ldots\rangle$ the average over all possible evolutions.

1. Assume that at time t the system is in the pure state $\hat{\sigma}_S(t) = |\phi(t)\rangle\langle\phi(t)|$. Show that at time $t+\delta t$, with δt arbitrarily small, the system is in a statistical mixture :

$$\hat{\sigma}_S(t+\delta t) = \left(1 - {\sum_k}' \delta\pi_k\right)|\phi_0\rangle\langle\phi_0| + {\sum_k}'\delta\pi_k\,|\phi_k\rangle\langle\phi_k| + \mathcal{O}[(\delta t)^2] \ , \tag{4}$$

with

$$\delta\pi_k = \delta t\,\langle\phi(t)|\,\hat{L}_k^\dagger\hat{L}_k\,|\phi(t)\rangle \ , \tag{5}$$

and

$$|\phi_k\rangle = \frac{\hat{L}_k\,|\phi(t)\rangle}{||\hat{L}_k\,|\phi(t)\rangle\,||} \ , \tag{6}$$

$$|\phi_0\rangle = \frac{e^{-i\hat{H}_{eff}\delta t/\hbar}\,|\phi(t)\rangle}{||e^{-i\hat{H}_{eff}\delta t/\hbar}\,|\phi(t)\rangle\,||} \ . \tag{7}$$

The prime in the sum over k indicates that the sum is limited to those k for which $\hat{L}_k\,|\phi(t)\rangle \neq 0$.

1. Note that if the subsystems S and E are entangled, then the state of the subsystem S (or E) is not pure.

2. Based on this result, formulate a numerical procedure to generate a particular stochastic evolution given the initial state $|\phi(t=0)\rangle$. In other words, describe an algorithm to generate $|\phi(t+\delta t)\rangle$ given $|\phi(t)\rangle$.

2 Spontaneous emission of a two-level atom

We consider a two-level atomic system S with ground and excited states $|g\rangle$ and $|e\rangle$ coupled to the vacuum radiation field. The bare (=no coupling) atomic Hamiltonian is

$$\hat{H}_0 = \hbar\omega_0 |e\rangle\langle e|$$

where ω_0 is the transition frequency. We use an effective *open-system* description : the environment's effect is modelled by Lindblad jump operators for describing dissipation/decoherence [2]. The master equation for the atomic density operator $\hat{\rho}(t)$ takes the Lindblad form with a single jump operator :

$$\hat{L} = \sqrt{\Gamma}\,|g\rangle\,\langle e|\ , \tag{8}$$

and with Γ the decay rate.
Going to the reference frame rotating with the atomic transition frequency, one can show that the hermitian part of the effective Hamiltonian $\hat{H}_{eff}$ is zero (you may verify this as an extra exercise).

1. (a) Write the equations of motions for the matrix elements $\rho_{ee}(t) \equiv \langle e|\hat{\rho}(t)|e\rangle$, $\rho_{gg}(t) \equiv \langle g|\hat{\rho}(t)|g\rangle$, $\rho_{eg}(t) \equiv \langle e|\hat{\rho}(t)|g\rangle$.
   (b) Express the solution of these equations at $t > 0$ as function of the initial values of the variables at $t = 0$.
2. We wish to recover this result with the wave function Monte Carlo method.
   (a) We consider the Monte Carlo wave function with the initial normalized state

   $$|\phi(0)\rangle = \alpha\,|g\rangle + \beta\,|e\rangle\ . \tag{9}$$

   Assuming that the system does not undergo any quantum jump between 0 and t, give the correctly normalized $|\phi_0(t)\rangle$.
   (b) Show that the wave function can undergo at most one jump between 0 and t. For this case, write its correctly normalized $|\phi_1(t)\rangle$ at time t.
   (c) The probability for not having any jump between 0 and t is given by the general formula

   $$P(t) = ||e^{-iH_{eff}t/\hbar}\,|\phi(0)\rangle\,||^2\ . \tag{10}$$

   Calculate $P(t)$ explicitly.
   (d) Show that the probability for having no jump up to time $t \to \infty$ is non-zero. Give its value as a function of β.
   (e) Calculate $\left\langle\, |\phi(t)\rangle\,\langle\phi(t)|\,\right\rangle_{\text{jump}}$ by averaging over all possible trajectories for the fixed initial state.
   (f) By averaging the previous expression for $\left\langle\, |\phi(t)\rangle\,\langle\phi(t)|\,\right\rangle_{\text{jump}}$ over a probability distribution of α and β, show that one retrieves the expression for $\rho(t)$ found in the first question.

2. Alternatively, if we would use a *closed-system* description of the coupled atom + field, then we would consider a Jaynes–Cummings Hamiltonian (in the rotating-wave approximation).

3 Coherent cavity field

Now consider a cavity with a single mode of frequency ω. The cavity Hamiltonian is

$$H = \hbar\omega\hat{a}^\dagger\hat{a} \ , \tag{11}$$

with $\hat{a}$ and $\hat{a}^\dagger$ the ladder operators of the cavity mode. Assume that the photons populating the cavity are initially in a coherent state [3]. A coherent state $|\alpha\rangle$ is defined as the eigenstate of the annihilation operator $\hat{a}$:

$$\hat{a}|\alpha\rangle = \alpha|\alpha\rangle. \tag{12}$$

In the Fock (photon number) basis, $|\alpha\rangle$ has the expansion

$$|\alpha\rangle = e^{-\frac{|\alpha|^2}{2}} \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}}|n\rangle \ , \tag{13}$$

with n the number of photons. So, the initial density operator reads

$$\hat{\rho}(0) = |\alpha\rangle \langle\alpha| \ . \tag{14}$$

Due to imperfections, photons might escape the cavity. We again use the effective *open-system* description and model the losses through the Lindblad master equation with jump operator $\hat{L} = \sqrt{\kappa}\hat{a}$, corresponding to the loss of a photon. Here, κ is the photon loss rate. Like in the previous exercise, we consider the reference frame turning at the frequency of the mode, such that the hermitian part of the effective Hamiltonian is zero. We thus have the master equation :

$$\frac{d\hat{\rho}}{dt} = \kappa \left[\hat{a}\hat{\rho}\hat{a}^\dagger - \frac{1}{2}\{\hat{a}^\dagger\hat{a}, \hat{\rho}\}\right] \ . \tag{15}$$

(a) Calculate the density operator $\hat{\rho}(t)$ with the Monte Carlo wave function method. Does the system stay in a pure state ?

(b) Calculate $\langle\hat{a}^\dagger\hat{a}\rangle\,(t)$.

(c) Assume that the system is initially in a Schrödinger cat state

$$|\psi(0)\rangle = \frac{1}{\sqrt{\mathcal{N}}}\big(\,|\alpha\rangle + |-\alpha\rangle\,\big), \tag{16}$$

with normalization factor $\mathcal{N} = 2 + 2e^{-2|\alpha|^2}$. Explain in a qualitative way how decoherence manifests itself in the Monte Carlo wave function method.

(d) [*Bonus*] Show that the density matrix at time t for the case of initial cat state is given by

$$\hat{\rho}(t) = \frac{1}{\mathcal{N}}\Big(|\alpha_t\rangle\langle\alpha_t| + |-\alpha_t\rangle\langle-\alpha_t| + e^{-2(1-e^{-\kappa t})|\alpha|^2}\ (|\alpha_t\rangle\langle-\alpha_t| + |-\alpha_t\rangle\langle\alpha_t|)\Big), \tag{17}$$

with $\alpha_t = \alpha e^{-\kappa t/2}$. Start from the *physically motivated ansatz* that the operator $|\alpha\rangle\langle\beta|$ evolves under photon loss as

$$|\alpha\rangle\langle\beta| \ \mapsto \ f_{\alpha\beta}(t)\,|\alpha_t\rangle\langle\beta_t|,$$

3. Coherent states are the quantum states that most closely resemble classical light (i.e. described by classical fields).

where $\alpha_t = \alpha e^{-\kappa t/2}$, $\beta_t = \beta e^{-\kappa t/2}$, and $f_{\alpha\beta}(t)$ is a scalar prefactor that accounts for decoherence of the off-diagonal term [4]. Hint : use

$$\hat{a}^\dagger |\alpha\rangle = \left(\frac{\partial}{\partial \alpha} + \frac{\alpha^*}{2} \right) |\alpha\rangle \ , \tag{18}$$

which can, e.g., be shown starting from the Fock representation.

(e) We define the *decoherence time* T as the time when the off-diagonal terms have decayed significantly, e.g. by a factor e^{-1}. Use Eq. (17) of the previous question to determine the decoherence time in case of a macroscopic cat state (i.e. $|\alpha|^2 \gg 1$). Compare this to the photon decay time. What can you conclude ?

4. There are a number of alternative ways of calculating $\hat{\rho}(t)$ without relying on such Ansatz (e.g. via Kraus operators or by projecting onto the Fock basis). These all give the same result.