This homework develops alternative theoretical formalisms to treat open quantum systems.

In class, we have look at a lot of physics of open quantum systems. We have mainly relied on the formalism of a master equation. In this homework, we will look at two alternative formalisms: the quantum trajectories method and the Heisenberg-Langevin method, which each give new analytic, numerical, and conceptual tools to tackle the physics of open quantum systems. With the addition of these techniques to your arsenal, you will have at your disposal the methods that are by far most commonly used to treat open quantum systems in quantum optics.

Problem 1. Quantum trajectories

This problem will walk you through the derivation of the *quantum trajectories* approach to open quantum systems. Then you will numerically implement of the method and use to explore the dynamics of a two-level system – astoundingly, there is still a bit of physics that we haven't milked from this! This technique will enable you to answer questions and treat situations that were difficult to approach with the master equation: What are the properties of the bath (the emitted photons), rather than the spin? What happens to the dynamics if one post-selects the measurement results based on what happened on some detector that is monitoring the dissipation?

Quantum trajectories is a method developed (remarkably, not until the 1990's) as a way to understand and solve the master equation. It often goes by other (rather misleading) names, such as: "wavefunction Monte Carlo," "quantum Monte Carlo," and "stochastic Schrödinger equation. (I strongly advise against these other names: they are more often used for other, much different – often more sophisticated – approaches).

Conceptually, the idea is to transform a master equation – that governs the evolution of the density matrix – into an average of equations governing pure quantum states $|\psi\rangle$. Note that thematically, this is in line with many things we've been doing in the course, starting with the first homework and lectures: going back and forth between three descriptions of open quantum systems as: (closed) system + environment $\longleftrightarrow$ (open) system with environment traced out $\longleftrightarrow$ classical average over closed quantum systems.

It turns out that this transformation from the density matrix to a classical average of pure state evolutions is possible, but comes at the cost that we have to include "quantum jumps": in addition to the usual Schrödinger evolution, there will be random, discrete quantum jumps from one pure state $|\psi\rangle$ to another pure state $|\psi'\rangle$. Averaging over all of these quantum jumps gives rise to the original master equation. Amusingly, this technique then gives a precise interpretation to the quantum jumps that pre-occupied early quantum theorists' debates! Interestingly, these jumps most naturally correspond to discrete changes in the observer's *knowledge*, not an inherent property of the state itself. (And the continuing debates as to whether there is any quantum state beyond that encapsulated by the observer's knowledge are for another course. . . .)

(a) We begin by deriving the quantum trajectories approach for a general master equation, leaving the Hamiltonian and jump operator arbitrary:

$$\partial_t \rho \quad = \quad -i[H,\rho] - J^\dagger J \rho - \rho J^\dagger J + 2 J \rho J^\dagger. \tag{1}$$

The only non-general part of this master equation is that we are assuming a single jump operator. The derivation is completely analogous for the general case in which multiple jump operators are summed over, but this will keep notation simple.

In class we showed how to group the evolution into terms involving an effective Hamiltonian H_{eff} and a "recycling" or "jump" term $2J\rho J^\dagger$. To begin the derivation, we want to consider the evolution of the state after an infinitesimal time δt: $\rho(t+\delta t) = \rho(t) + \delta t\, \partial_t \rho(t) + O(\delta t^2)$. We can group the right hand side into two terms: the "coherent" evolution (under non-Hermitian Hamiltonian H_{eff}) and the recycling term: $\rho(t+\delta t) = M_{\text{coh}}(t) + M_{\text{jump}}(t)$. Find M_{coh} and M_{jump}.

(b) We would like to apply the nice interpretation of adding density matrices: a density matrix $\rho = p_1\rho_1 + p_2\rho_2$ is equivalent to picking the quantum state ρ_1 with probability p_1 and ρ_2 with probability p_2. Your solution to the previous part is the sum of two terms, but not directly in this form – e.g., what is p_1? In particular, for this interpretation to be valid, ρ_j's have to be valid density matrices and p_j's have to be valid probabilities. Neither of the two terms in the previous part are valid density matrices

because their trace is not unity. However, they satisfy all other properties of the density matrix except this. So we can apply this interpretation if we write

$$\rho(t+\delta t) \quad = \quad p_{\rm coh}\rho_{\rm coh} + p_{\rm jump}\rho_{\rm jump} \tag{2}$$

if we define $\rho_j = M_j/p_j$ and $p_j = {\rm Tr}[M_j]$. Find p_j in terms of traces of ρ times jump operators.

(c) You have now almost completed the derivation of quantum trajectories. Let me state the algorithm as it presently appears; you will get the final algorithm by adding a simple observation to this. Presently, given a quantum state $\rho(t)$ and to get the new quantum state $\rho(t+\delta t)$, you randomly update it to be $\rho_{\rm coh}$ or $\rho_{\rm jump}$ with probability $p_{\rm coh}$ and $p_{\rm jump}$, respectively. [In your implementation, you can generate a random number r uniformly in $[0,1]$ and if $r < p_{\rm coh}$, you set the set the state to $\rho_{\rm coh}$; otherwise you set the state to $\rho_{\rm jump}$.] To get the full time dynamics, this is then repeated for many small times steps δt. One carries out this entire procedure N times (each time will have different dynamics due to the random numbers generated), and averages over these realizations. By the derivation, this will exactly reproduce the master equation evolution.

As stated, this algorithm is correct, but doesn't help too much since you still have to work with the full density matrix at each time step. However, if we assume the initial state is pure, a simplification becomes obvious. (A general mixed initial state can be treated with little additional complexity by diagonalizing $\rho_{\rm init} = \sum_{a=1}^{d} p_a \left|a\right\rangle\left\langle a\right|$ and doing d calculations with pure initial states, one for each term in the sum, but we restrict with pure initial states here.) In this case, argue that for an initial state $\left|\psi(t)\right\rangle$, the state at time $t+\delta t$ can be taken with probability $p_{\rm coh}$ to be the pure state $\left|\phi\right\rangle$ given by the time evolution under the effective Hamiltonian $H_{\rm eff}$ and with probability $p_{\rm jump}$ to be the state $\sqrt{2\delta t}J\left|\psi(t)\right\rangle / \sqrt{p_{\rm jump}}$.

The advantage of this algorithm over directly solving the master equation should now be apparent: at each time step, we only have to deal with a D-component state vector ($\left|\psi\right\rangle$), instead of a D^2-component density matrix (ρ). Since computationally solving the time-evolution equation scales as the square of the number of components, we now have an algorithm requiring $O(D^2)$ operations instead of $O(D^4)$; for large systems, this is an enormous computational advantage. It comes at the cost of having to average over N trajectories, but if $N \ll D^2$, this can still be a huge computational advantage.

In addition to the computational advantage, there is a conceptual advantage. We can interpret the dynamics as that of a closed system, except when it undergoes discrete jumps. This can be especially useful, for example, if the number of discrete jumps is small.

(d) For the master equation with Hamiltonian $H = \Omega S^x + \Delta S^z$ and jump operator $J = \Gamma\left|e\right\rangle\left\langle g\right|$, implement the algorithm you derived in the previous part to evolve the system in time, starting from an initial state $\left|g\right\rangle$. The algorithm is as follows:

- To obtain $\left|\psi(t+\delta t)\right\rangle$ from a state at time t, calculate $p_{\rm jump}$ and randomly, with probability $p_{\rm jump}$, set the new state to $\sqrt{2\delta t}J\left|\psi(t)\right\rangle / \sqrt{p_{\rm jump}}$, otherwise set it to the state coherently evolved with $H_{\rm eff}$.
- Iterate for as long times as you want to calculate.
- Repeat the two steps above over many random realizations, and construct averages of the desired quantities. Typically, one will need to use $\sim$ 10-100 realizations to begin obtaining good averages. Use as many as you need to get decent convergence (say within 5-10% over the important regimes of the dynamics).

One refers to this quantum trajectories algorithm as an "unraveling" of the master equation. In fact, there are different "unravelings" of the master equation, depending on what "detectors" one considers (obviously the results shouldn't depend on what set of detectors one sets up for the dissipation) – for example at each time one may detect photon numbers, but one could also detect various E-field quadratures, or measure in frequency space instead of time. Different unravelings may be beneficial to different circumstances.

(e) For the problem we are studying (sometimes called resonance fluorescence), let's set $\Delta = 0$ and work in units with $\Gamma = 1$; then numerically calculate and plot $\langle\sigma^x(t)\rangle$, $\langle\sigma^y(t)\rangle$, and $\langle\sigma^z(t)\rangle$ as a function of time for $\Omega = 0.1$, $\Omega = 1$, and $\Omega = 10$. These results should agree with what you would obtain from a master equation, which gives you a way to check them.

(f) The previous parts of this problem give a new method that reproduces the results of a quantum master equation. However, this method also allows us to calculate new things that are not be easily treated with the master equation. The rest of this problem explores such aspects of quantum trajectories.

As one example, we can calculate the state conditioned on the measurement record (i.e. how many photons were emitted and when). Here you will consider a simple example. Calculate $\langle S^y(t)\rangle$ and $\langle S^z(t)\rangle$ for cases (i.e. trajectories) where no photons were emitted in the interval $[0, t]$. In other words, choose the trajectories in your simulation where this is true and calculate the averages over this subset of trajectories. Perform this calculation for $\Omega = 0.1$, $\Omega = 1$, and $\Omega = 10$. (Recall that we did the $\Omega = 0$ calculation analytically in class.)

(g) As another example of a quantity easily obtained from trajectories but less obviously attainable from the master equation, consider the waiting time distribution of emission events. That is, given that an emission happens at time t_1, calculate the probability distribution $P(\tau)$ of waiting times for the next event – i.e. the probability that the next event occurs at $t_1 + \tau$. Calculate $P(\tau)$ for $\Omega = 0.1$, $\Omega = 1$, and $\Omega = 10$.

Problem 2. Heisenberg-Langevin

Here you will consider the Heisenberg-Langevin approach is an approach to open quantum dynamics equivalent to the master equation. The master equation is formulated in the Schrödinger picture, where the state $\rho(t)$ evolves and observables are stationary. The Heisenberg-Langevin approach is then the equivalent calculation in the Heisenberg picture, where observables evolve in time and the state is time-independent. Much like the Heisenberg picture for closed systems, this approach is especially useful for systems that are nearly classical, since the Heisenberg equations of motion are simply the classical equations of motion with the classical variables replaced with operators.

(a) Go through Sec. 8.4.2 of Lukin's notes. The key point is that in addition to non-Hermitian Hamiltonian terms, giving a damping of field operators $b(t)$ through the Heisenberg equations of motion, there is an additional fluctuation term: $\partial_t b = i[H_{\text{eff}}, b] + f$ where f is a fluctuation operator. The commutation relations of f are tied to the rate of damping in H_{eff} (an example of a fluctuation-dissipation relation). This is all explained in Lukin's 8.4.2 and Chap 9. (Nothing is due here; this is just the background and derivation.)

(b) Consider a cavity with photon loss coupled to the electromagnetic vacuum. The Heisenberg-Langevin equation gives $\partial_t a = -\frac{\kappa}{2}a + \hat{f}$ where f is an operator with the expectation values

$$\langle f(t)\rangle = 0 \tag{3}$$
$$\langle f(t)f^\dagger(t')\rangle = \kappa\delta(t-t') \tag{4}$$
$$\langle f^\dagger(t)f(t')\rangle = 0. \tag{5}$$

Take f to commute with a and $a^\dagger$. Note that the fluctuation operator strengths ($\langle f(t)f^\dagger(t')\rangle$) and the damping κ are related. This is an example of the fluctuation-dissipation relation. You can solve this equation to give the x-quadrature

$$x(t) = x(0)e^{-\kappa t/2} + \int_0^t dt' \, \frac{e^{-\kappa(t-t')/2}}{\sqrt{2}} \left(f(t') + f^\dagger(t')\right). \tag{6}$$

Use this to calculate $\langle x(t)\rangle$ for an initial coherent state $|\alpha\rangle$ and an initial two-photon Fock state $|n = 2\rangle$. These coherences are just exponential decays regardless of the initial state.

(c) Calculate the variance in the quadrature, $\langle x^2(t)\rangle - \langle x(t)\rangle^2$, for these two initial states.

In closing, I would like to mention some methods that we will *not* cover, but are important in physics to treat nonequilibrium quantum dynamics of both closed and open systems. Perhaps most prominent in physics are the Keldysh or equivalent Kadanoff-Baym approaches for nonequilibrium dynamics. These naturally generalize to open quantum systems – in fact, they are most often applied to many-body quantum systems, where when one looks at simple observables, they effectively look like open systems any ways where all of the non-monitored degrees of freedom serve as the "bath". A main advantage of these formalisms is that they allow one to treat non-Markovian situations on equal footing as Markovian ones. However, they are relatively formidable formalisms and additionally are basically intractable in general, requiring dramatic approximations to make progress. One also finds "influence functionals" (tracing back to Feynman) and approaches based around "Caldeira-Leggett" models on a fairly regular basis. Some googling will quickly turn up references for all of these approaches, and I'm happy to discuss them with interested parties.