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Lecture 8: Stochastic wave functions

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In the last lectures related to open quantum systems we talked a lot about "quantum jumps" associated to transitions between the states in the reservoir, concomitant with jumps between the states of the system, described by the $\hat{L}_m$ operators.

As a matter of fact the idea of jumps appeared very early in the history of quantum physics: Bohr introduced it to describe the sudden decay of an atom from one trajectory of the electron around the nucleus to a lower one. He postulated that an atom only emits light during the jump, contrarily to the prediction of classical electromagnetism where the electron should continuously radiate. This jump associated to the emission of light is also the way spontaneous emission in an atom was presented to you in highschool. However in the mind of many physicists in the early days of quantum mechanics, this was essentially a convenient image to understand what is going on but of little interest in practice as, according to what Schrödinger wrote in 1952, "...we are not experimenting with single particles...". Indeed all experiments until around 1980 were performed on large collections of atoms and one only had access to average behaviors. The density operator was initially introduced to describe this average for a system coupled to a reservoir, without having to think about the behavior of each individual component of the system.

In the late 1970's, the situation changed after Hans Dehmelt was able to trap a single electron in 1973, and, together with P. Toscheck, a single ion in 1980. The question of the evolution of a single quantum object coupled to a reservoir (for example the electromagnetic field surrounding it) came back on the scene. Today, in the context of the "second quantum revolution" that we described in the first lecture and which relies largely on the possibility to manipulate *individual* quantum objects, calculating their evolution is central.

Before getting to the formalism, let us show that this idea of quantum jumps is fruitful. Consider a two-level atom with states $|g\rangle, |e\rangle$, with a decay rate of the excited state Γ. We assume that the probability for the atom initially in $|e\rangle$ to decay during a time dt is $dp = \Gamma dt$. Importantly, we also assume that this probability is independent of the time t, i.e. the system has no memory of its past (this is the Markov approximation again...!). To calculate the probability $P_e(t)$ that the atom is still in $|e\rangle$ after a time t, we divide the interval $[0, t]$ into n steps of duration $dt = t/n$. For the atom to still be in $|e\rangle$ at t, it must not have decayed between $[0, dt]$, $[dt, 2dt]$.... The probability to not decay during an interval dt is $1 - dp$, and is independent of time (Markov), hence: $P_e(t) = (1 - dp)^n = (1 - \Gamma t/n)^n \to \exp(-\Gamma t)$ for $n \to \infty$. The picture is thus the following: take an ensemble of N atoms, all prepared in $|e\rangle$. A particular atom stays in $|e\rangle$ until a given time when it jumps to $|g\rangle$. Each atom will do the transition at a different time. If we record the number of atoms still in $|e\rangle$ for each interval $[kdt, (k + 1)dt]$, the

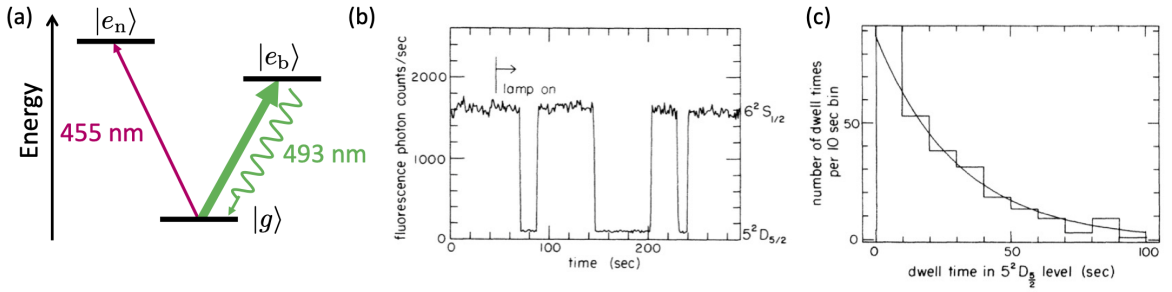

Figure 1: *(a) Simplified three-level structure of the Ba^+ ion used in the experiment of Hans Dehmelt [Phys. Rev. Lett.* **56**, *2797 (1986)]. (b) Fluorescence emitted at 493 nm as a function of time: when the lamp is turned on the atoms can be shelved in the state $|e_n\rangle$ where it does not emitted light. (c) Histogram of the dwell time in $|e_n\rangle$, together with an exponential fit to the data.*

corresponding histogram approximates an exponential decay.

In 1986, three experiments observed quantum jumps using individual ions [1, 2, 3]. The principle of the experiments was the same for all, even if the exact atomic structure was a bit different. The simplified level structure involves two transitions from the ground state $|g\rangle$ (see Fig. 1): one couples to a state $|e_n\rangle$ with a narrow transition (decay rate Γ_n), the other coupled to $|e_b\rangle$ (decay rate $\Gamma_b \gg \Gamma_n$). An incoherent light continuously excites the $|g\rangle - |e_b\rangle$ transition and one monitors the fluorescence emitted by the ion. At a given time, the experimentalists turn on a second incoherent light tuned on the $|g\rangle - |e_n\rangle$ transition. They observed that the ion stops emitting light for some time before it emits again. The interpretation consists in saying that when the light on the narrow transition is on, the ion jumps from $|g\rangle$ to $|e_n\rangle$ where it stays for a duration $\sim 1/\Gamma_n$. The histogram of the durations during which the fluorescence if off gives an exponential decay, with a rate Γ_n. This experiment demonstrating the existence of quantum jumps (that are now more than a simple image...) was a shock for many physicists. Since then the formalism of stochastic wave function, which we will describe in this lecture, has been developed to put all these on firm ground.

1 Stochastic wave function

The idea was developed theoretically in the late 1980's by several physicists. The article by J. Dalibard, Y. Castin and K. Moelmer in [4] is a masterpiece of pedagogy and elegance and you are strongly encouraged to read it. In this work, the stochastic wave function was introduced using the Wigner-Weisskopf method applied to an atom and the surrounding vacuum field considered as a reservoir. Here we will start from the Kraus formalism that we have developed in the previous lectures to explain the idea.

Consider a system $\mathcal{S}$ (e.g. a two-level atom) coupled to a reservoir $\mathcal{R}$, described at a time t by a *separable* state:

$$|\psi_{SR}(t)\rangle = |\psi_S(t)\rangle \otimes |\chi_0\rangle \ , \tag{1}$$

with $|\chi_0\rangle$ the state of the reservoir. We have learned in lecture 6 that the state at a

later time $t + dt$ is

$$|\psi_{SR}(t+dt)\rangle = \sum_m [\hat{M}_m(t,dt)\,|\psi_S(t)\rangle] \otimes |\chi_m\rangle \ , \tag{2}$$

where the $|\chi_m\rangle$'s are various states of $\mathcal{R}$, orthogonal to $|\chi_0\rangle$, and the $\hat{M}_m(t,dt)$ are the Kraus operators. We can single out the case where the state of the reservoir is unchanged ("no click") and the cases where a transition occurs ("detection of a click"):

$$|\psi_{SR}(t+dt)\rangle = \hat{M}_0\,|\psi_S(t)\rangle] \otimes |\chi_0\rangle + \sum_{m\neq 0} [\hat{M}_m\,|\psi_S(t)\rangle] \otimes |\chi_m\rangle \ . \tag{3}$$

Hence, the state of the system $\mathcal{S}$ *conditioned* on the absence of click (i.e. the reservoir is unchanged) is:

$$|\psi_S(t+dt)\rangle = \frac{\hat{M}_0\,|\psi_S(t)\rangle}{\|\hat{M}_0\,|\psi_S(t)\rangle\,\|} \ , \tag{4}$$

while the state of $\mathcal{S}$ following a click that brings the reservoir into the state $|\chi_{m\neq 0}\rangle$ is

$$|\psi_S(t+dt)\rangle = \frac{\hat{M}_m\,|\psi_S(t)\rangle}{\|\hat{M}_m\,|\psi_S(t)\rangle\,\|} \ . \tag{5}$$

We now apply the Markov approximation: the Kraus operators only depend on the time step dt: $\hat{M}_m(t,dt) = \hat{M}_m(dt)$. This also allows us to say that the system and reservoir are not entangled at t, as implied in Eq. (1). We then use the expressions of the operators seen in Lecture 6:

$$M_0(dt) \quad = \mathbb{1} - \frac{i}{\hbar} H_{\text{eff}}\,dt \quad \text{with} \quad H_{\text{eff}} = H_S - \frac{i}{2}\sum_{m\neq 0} L_m^\dagger L_m \ , \tag{6}$$

$$M_{m\neq 0}(dt) \ = L_m\sqrt{dt} \ . \tag{7}$$

The probability that a jump in the reservoir from $|\chi_0\rangle$ to $|\chi_m\rangle$ occurs during dt is, according to the rule on POVM given in Lecture 3:

$$dp_m = \langle\psi_S|\,\hat{M}_m^\dagger \hat{M}_m\,|\psi_S\rangle = \langle\psi_S|\,\hat{L}_m^\dagger \hat{L}_m\,|\psi_S\rangle\ dt \ . \tag{8}$$

Hence the probability that a click occurs, i.e. a transition in $\mathcal{R}$ irrespective of its final state, is $dp = \sum_{m\neq 0} dp_m$. Calling $\langle\psi_S|\sum_{m\neq 0}\hat{L}_m^\dagger\hat{L}_m\,|\psi_S\rangle = \gamma$, the probability to get a click during dt is $dp = \gamma dt$. After this jump occurs the reservoir relaxes to the state $|\chi_0\rangle$ in a very short time τ_c (see Lecture 7), and one can assume for the following time step dt again a separable $\mathcal{S}-\mathcal{R}$ state: $|\psi_{SR}(t+dt)\rangle = |\psi_S(t+dt)\rangle \otimes |\chi_0\rangle$.

Let us now come back to the evolution of the state of the system when no detection

occurs. Using Eq. (6), we obtain:

$$\begin{aligned}
\|\hat{M}_0 |\psi_S(t)\rangle\|^2 &= \langle\psi_S| \hat{M}_0^\dagger \hat{M}_0 |\psi_S\rangle && (9)\\
&= \langle\psi_S| (\mathbb{1} + \frac{i}{\hbar} H_{\text{eff}}^\dagger \, dt)(\mathbb{1} - \frac{i}{\hbar} H_{\text{eff}} \, dt) |\psi_S\rangle && (10)\\
&= \langle\psi_S| (\mathbb{1} + \frac{i}{\hbar} (H_{\text{eff}}^\dagger - H_{\text{eff}}) \, dt) |\psi_S\rangle + \mathcal{O}(dt^2) && (11)\\
&= \langle\psi_S| (\mathbb{1} - \sum_{m\neq 0} \hat{L}_m^\dagger \hat{L}_m \, dt) |\psi_S\rangle + \mathcal{O}(dt^2) && (12)\\
&= \langle\psi_S| (\mathbb{1} - \sum_{m\neq 0} \hat{M}_m^\dagger \hat{M}_m) |\psi_S\rangle + \mathcal{O}(dt^2) && (13)\\
&\approx 1 - dp \; . && (14)
\end{aligned}$$

Hence,

$$|\psi_S(t+dt)\rangle = \frac{\mathbb{1} - i H_{\text{eff}}/\hbar \, dt}{\sqrt{1-dp}} \; |\psi_S(t)\rangle \; . \tag{15}$$

Equation 15 calls for an important remark, which shows the subtlety of the approach. Naively, one would have thought that the evolution of the system in the absence of detection should be governed by a unitary evolution under H_S and not H_{eff}:

$$|\psi_S(t+dt)\rangle \propto (\mathbb{1} - i H_S/\hbar \, dt) \; |\psi_S(t)\rangle \; . \tag{16}$$

However, this is not the case. To understand this, consider a two-level atom in a state $|\psi_S(t)\rangle = \alpha |g\rangle + \beta |e\rangle$ with a decay rate Γ for $|e\rangle$. We assume the free hamiltonian $H_S = \hbar\omega_0 |e\rangle\langle e|$. Then $|\psi_S(t+dt)\rangle = \alpha |g\rangle + \beta \, e^{-i\omega_0 dt} |e\rangle$. Hence the probability to find the atom in $|e\rangle$ does not change as the time evolves, which is not compatible with the idea that it may decay during dt. In fact, the absence of detection of a photon coming from the atom as the time increases makes it *more likely* that the atom is found in its ground state: no detection therefore implies a non hermitian evolution of the state!

2 Quantum trajectories

We are now equipped with the necessary ingredients to calculate the evolution of the stochastic wave function as a function of time. We first split the interval between 0 and t into time-steps $dt = t/n$. For each time step we calculate the probability $dp = \gamma dt$ to undergo a jump. We compare this probability to a random number r drawn from a uniform distribution in $[0, 1]$. The procedure is then:

1. If $r \geq dp$, the wavefunction evolves according to

$$|\psi_S(t+dt)\rangle = \frac{\mathbb{1} - i H_{\text{eff}}/\hbar \, dt}{\sqrt{1-dp}} \; |\psi_S(t)\rangle \; . \tag{17}$$

2. If $r < dp$, the wavefunction undergoes a jump and the final state is $|\psi_S(t+dt)\rangle = \hat{L}_m |\psi(t)\rangle / \sqrt{dp_m/dt}$ with a probability dp_m/dp.

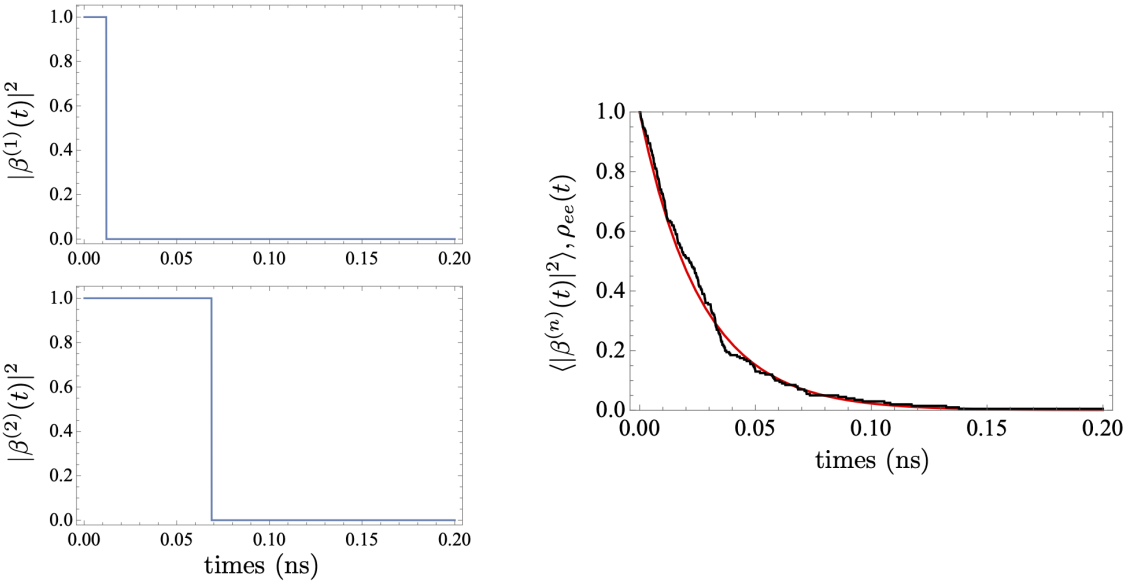

Figure 2: *(Left) Examples of quantum trajectories for an atom initially excited. (Right) Average over 200 trajectories, together with the solution of the Bloch equation.*

A particular sequence of choices for each step dt is called a *quantum trajectory*: it consists in a succession of periods of continuous, coherent-like evolution of the wave function, followed by jumps at random times.

Let us apply this procedure to the case of a single two-level atom driven by a laser at frequency ω with a Rabi frequency Ω. There, in the rotating frame approximation, $H_S = -\hbar\Delta|e\rangle\langle e| + (\hbar\Omega/2)(\sigma_+ + \sigma_-)$, with $\Delta = \omega - \omega_0$. As seen in Lecture 7, a single jump operator $L_- = \sqrt{\Gamma}\,\sigma_-$ contributes, so that $H_{\rm eff} = H_S - i(\hbar\Gamma/2)\sigma_+\sigma_-$ ($\sigma_+\sigma_- = |e\rangle\langle e|$). If we write the state of the atom as $|\psi_S(t)\rangle = \alpha(t)\,|g\rangle + \beta(t)\,|e\rangle$, the case 1 corresponds to the evolution:

$$\begin{pmatrix}\alpha(t+dt)\\ \beta(t+dt)\end{pmatrix} = \frac{1}{\sqrt{1-dp}}\begin{pmatrix}1 & -i\frac{\Omega}{2}dt\\ -i\frac{\Omega}{2}dt & 1+(i\Delta-\frac{\Gamma}{2})dt\end{pmatrix}\begin{pmatrix}\alpha(t)\\ \beta(t)\end{pmatrix}\ . \tag{18}$$

Here, the probability $dp = \langle\psi_S|\,\hat{L}_-^\dagger L_-\,|\psi_S\rangle\ dt = \Gamma|\langle e|\psi_S\rangle|^2\,dt = \Gamma|\beta(t)|^2\,dt$. Hence, when no jump occurs, using $\sqrt{1-dp} \approx 1 - dp/2$ and keeping only the first order terms in dt:

$$\alpha(t+dt) = \left(1+\frac{\Gamma dt}{2}|\beta(t)|^2\right)\alpha(t) - i\frac{\Omega dt}{2}\beta(t) \tag{19}$$

$$\beta(t+dt) = \left(1-\frac{\Gamma dt}{2}|\alpha(t)|^2 + i\Delta dt\right)\beta(t) - i\frac{\Omega dt}{2}\alpha(t)\ . \tag{20}$$

In the opposite case where a jump occurs, $|\psi_S(t+dt)\rangle = |g\rangle$. The result of such a simulation is shown in Fig. 2 for the case where $\Omega = 0$, and the atom is initially in the excited state ($\beta(0) = 1$). We also show the average over many trajectories, where we recover the exponential decay.

Figure 3 presents the case of an atom driven by a laser, on resonance with the transition ($\Delta = 0$), switched on at $t = 0$. The trajectory consists of Rabi oscillations

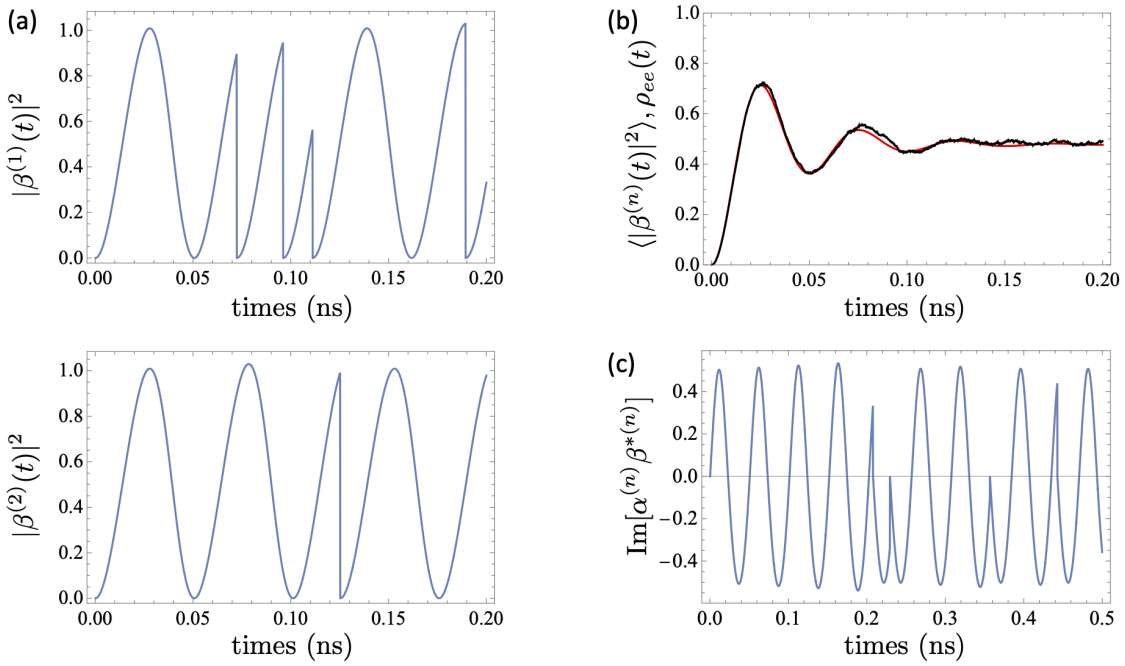

Figure 3: *(a) Examples of quantum trajectories for an atom in* $|g\rangle$ *at* $t = 0$*, driven by a resonant laser with Rabi frequency* Ω*. (b) Average over 1000 trajectories, together with the solution of the Bloch equations. (c) Evolution of the atomic dipole* $\langle D^{(n)}(t)\rangle \propto \mathrm{Im}[\alpha^{(n)}\beta^{*(n)}]$ *associated to a quantum trajectory.*

that are interrupted by jumps from $|e\rangle$ to $|g\rangle$ at random times. When averaging over many trajectories, one recovers the solution of the Bloch equations for a two-level atom.

The stochastic wavefunction approach is not a new concept that we need to add to quantum physics. It is simply a new, fruitful way of looking at the evolution of open quantum systems. As an example of physical insight that it provides, consider again a two-level atom driven by a laser (detuning Δ, Rabi frequency Ω). The solution of the steady-state solution for the coherences is:

$$\rho_{eg}^{\mathrm{st}} = -i\frac{\Omega}{2}\frac{\Gamma/2 + i\Delta}{\Delta^2 + \Omega^2/2 + \Gamma^2/4} \ . \tag{21}$$

This expression predicts that at high intensity of the laser ($\Omega \gg \Gamma$), $\rho_{eg}^{\mathrm{st}} \approx 0$ i.e. the average atomic dipole $\langle D\rangle \propto \rho_{eg} \approx 0$. This fact is not so obvious but the stochastic wave function provides a nice interpretation: consider the evolution of the coherence of the two-level atom $\alpha^{(n)}(t)\beta^{*(n)}(t)$ during a particular trajectory, as represented in Fig. 3(c). It undergoes oscillations interrupted by jumps at random times, exactly as in the classical description of an oscillating dipole undergoing random collisions which dephase the dipole. Due to the random phase shift associated to each jump, the average of the dipole is 0 and one recovers the result of the Bloch equations.

3 The Lindblad form recovered

We have seen in the last section that the average over many quantum trajectories reproduces the solution of the Bloch equations in the case of the two-level system (Fig. 2,3). As a sanity check let us show that in the general case, the average over many different quantum trajectories corresponding to different stochastic wave functions $|\psi^{(n)}(t)\rangle$ leads to the Lindblad equation for the average density operator of the system $\mathcal{S}$:

$$\rho(t) = \frac{1}{N}\sum_n \rho^{(n)}(t) \quad \text{with} \quad \rho^{(n)}(t) = |\psi_S^{(n)}(t)\rangle \langle\psi_S^{(n)}(t)| \ . \tag{22}$$

For simplicity, we will do it on the case of a two level system with the excited state having a decay rate Γ. Then $H_{\rm eff} = H_S - i(\hbar\Gamma/2)\sigma_+\sigma_-$. Consider first the evolution of $\rho^{(n)}(t)$ from t to $t+dt$: during this time step, the system can either undergo a jump (probability $1-dp$) or not (probability dp). If it does not undergo a jump the wave function changes from $|\psi_S^{(n)}(t)\rangle$ to $|\psi_S^{(n)}(t+dt)\rangle \approx (1 - iH_{\rm eff}dt/\hbar)\,|\psi_S^{(n)}(t)\rangle\,/\sqrt{1-dp}$. Otherwise $|\psi_S^{(n)}(t+dt)\rangle = |g\rangle$. Hence:

$$\begin{aligned}
\rho^{(n)}(t+dt) &= (1-dp)\,\rho^{(n)}_{\rm nojump}(t+dt) + dp\,\rho^{(n)}_{\rm jump}(t+dt) && (23)\\
&= (1-dp)\,\frac{1-iH_{\rm eff}t/\hbar}{\sqrt{1-dp}}\,|\psi_S^{(n)}(t)\rangle\langle\psi_S^{(n)}(t)|\,\frac{1+iH_{\rm eff}^\dagger t/\hbar}{\sqrt{1-dp}} + dp\,|g\rangle\langle g| && (24)\\
&= \rho^{(n)}(t) - \frac{i}{\hbar}[H_S\rho^{(n)}(t) - \rho^{(n)}(t)H_S]dt && (25)\\
&\quad -\frac{\Gamma}{2}[\sigma_+\sigma_-\rho^{(n)}(t) + \rho^{(n)}(t)\sigma_+\sigma_-]\,dt + \Gamma\,dt\,|g\rangle\,\rho^{(n)}_{ee}(t)\,\langle g| \ . && (26)
\end{aligned}$$

Remember that $\rho^{(n)}_{ee}(t) = \langle e|\,\rho^{(n)}(t)\,|e\rangle$, $\sigma_+ = |e\rangle\langle g|$, and $\sigma_- = |g\rangle\langle e|$. We then obtain:

$$\frac{d\rho^{(n)}}{dt} = \frac{1}{i\hbar}[H_S,\rho^{(n)}] + \frac{\Gamma}{2}(\sigma_+\rho^{(n)}\sigma_- - \sigma_+\sigma_-\rho^{(n)} - \rho^{(n)}\sigma_+\sigma_-) \ . \tag{27}$$

Hence, when averaging over many trajectories:

$$\frac{d\rho}{dt} = \frac{d}{dt}\left(\frac{1}{N}\sum_n \rho^{(n)}(t)\right) = \frac{1}{i\hbar}[H_S,\rho] + \frac{\Gamma}{2}(\sigma_+\rho\sigma_- - \sigma_+\sigma_-\rho - \rho\sigma_+\sigma_-) \ . \tag{28}$$

We (of course...) recover the Lindblad form and can interpret the operator ρ as the density operator of the system $\mathcal{S}$.

One can also calculate the average value of any observable $\hat{A}$: consider a trajectory (n) corresponding to a wave function $|\psi^{(n)}(t)\rangle$. Calculate $\langle\hat{A}\rangle^{(n)}(t) = \langle\psi^{(n)}(t)|\hat{A}|\psi^{(n)}(t)\rangle$, and $\langle\hat{A}\rangle(t) = \sum_n\langle\hat{A}\rangle^{(n)}(t)/N$, with N the number of trajectories.

4 Discussion of the method

Besides yielding a nice intuition about the time evolution of open many-body quantum systems, the stochastic wave function is an important tool to calculate their dynamics.

Think of an ensemble of N qubits interacting with each other. The density matrix has 2^{2N} coefficients. For $N \gtrsim 25$, solving the master equation consisting of $2^{2N}/2$ coupled equations is not feasible on any computer today and in the foreseeable future. However the stochastic wave function approach requires solving "only" 2^N coupled equations, of course at the price of averaging over many trajectories. In most cases, a number $N_r \approx 1000-10000$ of realizations is enough, and in any case does not grow exponentially with the number of particles, hence providing a huge gain in the number of equations to solve.

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