Dynamics of Open Quantum Systems

Matt Krems

Department of Physics, University of California, San Diego, La Jolla, CA 92093-0319
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In this paper, I discuss open quantum systems in terms of the Lindblad quantum master equation, quantum operations, and the Schrödinger-Langevin equation. These allow one to study open quantum systems in a systematic way, as long as certain assumptions apply to the system being studied. A formal derivation of the Lindblad quantum master equation, which describes the time evolution of density matrices, is presented, and an example demonstrating its utility is included. This example is also discussed in terms of a quantum operation. Quantum operations are briefly introduced and their use in relation to the Lindblad master equation is discussed. Additionally, the inability of the Lindblad master equation to describe mixed state quantum systems in which the Hamiltonian is a function of the microstates warrants the Schrödinger-Langevin equation. A derivation of the Schrödinger-Langevin equation is presented using an ansatz and imposing that the average norm of the microstate is conserved.

Quantum mechanics is currently the core theory for understanding the laws of physics. Essentially every physicist is familiar with quantum mechanics relating to closed systems which obey so-called unitary evolution. Although many important conclusions about our universe can be derived when considering closed quantum systems, it is a simple fact that in the real world, there are no perfectly closed systems, except perhaps the universe as a whole. Open quantum systems, in contrast to closed quantum systems, cannot, in general, be represented in terms of a unitary time evolution. When dealing with open quantum systems, it is often useful to formulate an equation of motion which involves a system's **density matrix** or **statistical operator**. This type of equation of motion is called a **quantum master equation**.

The density matrix is useful for characterizing a mixed state, that is a system which contains a number of quantum states all weighted by a classical probability (this is in contrast to the intrinsic probabilistic nature of a quantum state), p_i. It contains all the physically relevant information one can possibly obtain about an ensemble. The density matrix is defined as

$$\hat{\rho}(t) = \sum_i p_i |\psi_i(t)\rangle\langle\psi_i(t)| \qquad (1)$$

where $\sum_i p_i = 1$ and the $|\psi_i(t)\rangle$ are a complete set of normalized state vectors called **microstates** which evolve in time according to the Schrödinger equation (note that I set $\hbar = 1$ here and for the rest of this paper)

$$i\frac{d}{dt}|\psi(t)\rangle = \hat{H}(t)|\psi(t)\rangle. \qquad (2)$$

The time evolution of a microstate is given by $|\psi(t)\rangle\rangle = \hat{U}(t, t_0)|\psi(t_0)\rangle$ where $\hat{U}(t, t_0)$ is the **time translation operator** defined as

$$\hat{U}(t, t_0) = \hat{T}\left\{exp\left[-i\int_{t_0}^{t} dt' \hat{H}(t')\right]\right\} \qquad (3)$$

and $\hat{T}$ denotes the chronological time-ordering operator. It is important to explicitily distinguish between a mixed state and pure state. A **pure state** or pure ensemble is one in which $p_i = 1$ for some $|\psi_i(t)\rangle$ with $i = n$ for example and $p_i = 0$ for all other conceivable state kets. The density operator is written as $\hat{\rho} = |\psi_n(t)\rangle\langle\psi_n(t)|$ for this pure state. A **mixed state** is one in which there is more than one non-zero p_i for an ensemble. Nonetheless, all density matrices must have the following properties,

$$\hat{\rho}^\dagger = \hat{\rho} \quad Tr\{\hat{\rho}\} = 1 \quad \langle\psi_i|\hat{\rho}|\psi_i\rangle \geq 0 \quad \forall \; |\psi_i\rangle \, \epsilon \, \mathcal{H}, \quad (4)$$

that is, the density operator must be Hermitian, have unit trace, and be positive semi-definite. By taking a time derivative of $\hat{\rho}(t)$, defined by Eq.(1) and using the Schrödinger equation, Eq.(2), I arrive at

$$\frac{d}{dt}\hat{\rho}(t) = -i\sum_i p_i \left[\hat{H}|\psi_i\rangle\langle\psi_i| + |\psi_i\rangle\langle\psi_i|\hat{H}\right]. \qquad (5)$$

As long as $\hat{H}$ is not a function of the microstates, $|\psi_i\rangle$, i.e. $\hat{H} \neq \hat{H}(|\psi_i\rangle)$, one can take $\hat{H}$ out of the sum and write this as

$$\frac{d}{dt}\hat{\rho}(t) = -i\left[\hat{H}(t), \hat{\rho}(t)\right], \qquad (6)$$

which is the **Liouville-von Neumann equation**. This must be supplied with an initial condition, $\hat{\rho}(t_0)$. The solution is

$$\hat{\rho}(t) = \hat{U}(t, t_0)\hat{\rho}(t_0)\hat{U}^\dagger(t, t_0) \qquad (7)$$

The Liouville-von Neuman equation gives the dynamics of a closed quantum system. We would like to extend this equation to include open quantum systems.

First, we need to decide on what we mean by an open quantum system. We would like to consider the interaction of our system, denoted by S, with an external environment or reservoir, denoted by R. The Hilbert space of

the total system is given by the tensor product, denoted by $\otimes$, of the Hilbert space of the total system and the reservoir. Thus, I can write the Hamiltonian in the form

$$\hat{H} = \hat{H}_S \otimes \hat{I}_R + \hat{I}_S \otimes \hat{H}_R + \hat{H}_{SR} \qquad (8)$$

where $\hat{I}_R$ and $\hat{I}_S$ are the identity operators in their respective Hilbert spaces, and $\hat{H}_S$ is the Hamiltonian of the open system S, $\hat{H}_R$ is the Hamiltonian of the environment R, and $\hat{H}_{SR}$ is the Hamiltonian describing the interaction between the system and the environment. Also, we assume that $\left[\hat{H}_S \otimes \hat{I}_R, \hat{I}_S \otimes \hat{H}_R\right] = 0$. We could, in principle, use Eq.(6), to determine the dynamics of the closed quantum system containing the system and reservior. However, this requires worrying about a bunch of extra degress of freedom associated with the reservoir. We would be determining the detailed dynamics of the reservoir, which we are not interested in and which, in principle, are incredibly difficult to follow. We would like to find a new equation of motion for only the system, but we would like to include the effects of the reservoir. If the system is composed of noninteracting identical particles, we can write

$$\hat{H}_S \otimes \hat{I}_R = \sum_n \varepsilon_n c_n^\dagger c_n \qquad (9)$$

with $\left\{c_n, c_{n'}^\dagger\right\} = \delta_{nn'}$ and $\{c_n, c_{n'}\} = 0$ for fermions and $\left[c_n, c_{n'}^\dagger\right] = \delta_{nn'}$ and $[c_n, c_{n'}] = 0$ for bosons. Assume $\hat{H}_{SR} = \sum_{n \neq n'} f_{nn'} c_n^\dagger c_n$ where the $f_{nn'}$ contains the operators for R and satisfy $f_{nn'} = f_{n'n}^\dagger$. Note that $\hat{H}_S \otimes \hat{I}_R$ is in the Hiblert space of $S \otimes R$ and the interaction is expanded in terms of the eigenstates of $\hat{H}_S \otimes \hat{I}_R$ including off-diagonal terms introduced by the operator $f_{nn'}$. The density matrix $\hat{\rho}_R$ of the reservoir can be expanded in terms of the eigenlevels $|r\rangle$ of $\hat{I}_S \otimes \hat{H}_R$

$$\hat{\rho}_R = \sum_r F(E_r)|r\rangle\langle r| \qquad (10)$$

where E_r is the eigenvalue corresponding to $|r\rangle$ and $F(E_r)$ is the thermal equilibrium distribution. Let $\hat{\rho}_S(t)$ be the density matrix of the system and $\hat{\rho}_C(t)$ be the total density matrix, then

$$\hat{\rho}_S(t) = \sum_r \langle r|\hat{\rho}_C(t)|r\rangle = Tr_R\left\{\hat{\rho}_C(t)\right\}. \qquad (11)$$

where Tr_R denotes the partial trace over the reservoir degrees of freedom. Thus, we can recover the density matrix of the system we are interested in by integrating over the reservoir degress of freedom. Additionally, at $t = 0$, we assume

$$\hat{\rho}_C(t) = \hat{\rho}_S(0) \otimes \hat{\rho}_R, \qquad (12)$$

thus saying there is no interation at exactly time zero. We choose $\hat{H}_0 = \hat{H}_S \otimes \hat{I}_R + \hat{I}_S \otimes \hat{H}_R$ to be the unperturbed Hamiltonian, and using the time translation operator defined perviously, we can write, in the interaction picture

$$i\frac{\partial}{\partial t}\hat{U}^{(I)}(t, t_0) = \hat{H}_{SR}^{(I)}(t)\hat{U}^{(I)}(t, t_0) \qquad (13)$$

where $\hat{H}_{SR}^{(I)}(t) = \sum_{n \neq n'} f_{nn'}^{(I)}(t)e^{i(\varepsilon_n - \varepsilon_{n'})t}c_n^\dagger c_{n'}$ with $f_{nn'}^{(I)}(t) = e^{i(\hat{I}_S \otimes \hat{H}_R)t}f_{nn'}e^{i(\hat{I}_S \otimes \hat{H}_R)t}$. At $t > 0$ we have

$$\hat{\rho}_C^{(I)}(t) = \hat{U}^{(I)}(t, 0)\hat{\rho}_C(0)\hat{U}^{(I)\dagger}(t, 0). \qquad (14)$$

After expanding $\rho_S^{(I)}(t)$ to second order with respect to $\hat{H}_{SR}$ and assuming that $Tr\rho_R f_{nn'} = 0$ we have

$$\hat{\rho}_S^{(I)}(t) - \hat{\rho}_S(0) = it\left[\hat{\rho}_S(0), \Sigma_R\right] - t\left\{\hat{\rho}_S(0), \Sigma_I\right\} + \sum_{r,r'} F(E_R) \times$$

$$\int_0^t \int_0^t \sum_{m \neq m'} \sum_{n \neq n'} dt_1 dt_2 e^{i[(\varepsilon_n - \varepsilon_{n'})t_1 + (\varepsilon_m - \varepsilon_{m'})t_2]}\langle r|f_{nn'}^{(I)}(t_1)|r'\rangle$$

$$\langle r'|f_{mm'}^{(I)}(t_2)|r\rangle c_n^\dagger c_{n'}\hat{\rho}_S(0)c_m^\dagger c_{m'} \qquad (15)$$

where Σ_R and Σ_I are the real and imaginary parts of

$$\Sigma = \frac{i}{t}\sum_{r,r'} F(E_R)\int_0^t dt_1 \int_0^{t_1} dt_2\langle r|\hat{H}_{SR}^{(I)}(t_1)|r'\rangle\langle r'|\hat{H}_{SR}^{(I)}(t_2)|r\rangle \qquad (16)$$

If one assumes that the reservoir is Markovian or "memoryless" that is, in more precise language that there is no correlation between different transitions, one can say that only those terms with $(n, n') = (m, m')$ do not vanish in the expansion. We can then set

$$w_{n'n} = \sum_{r,r'} F(E_R)|\langle r|f_{nn'}|r'\rangle|^2 \delta_{E_n + E_r, E_{n'} + E_{r'}} \qquad (17)$$

as the transition rate for particles to jump from n to n', such that

$$\Sigma_I = \frac{1}{2}\sum_{n \neq n'} w_{n'n} c_n^\dagger c_{n'} c_{n'}^\dagger c_n. \qquad (18)$$

We ignore Σ_R [1], and arrive at an equation in the Schrödinger picture

$$\frac{d}{dt}\hat{\rho}_S(t) = -i\left[\hat{H}_S, \hat{\rho}_S(t)\right] - \frac{1}{2}\sum_{n \neq n'}\left\{\hat{A}_{n'n}^\dagger \hat{A}_{n'n}, \hat{\rho}_S(t)\right\} + \sum_{n \neq n'} \hat{A}_{n'n}\hat{\rho}_S(t)\hat{A}_{n'n}^\dagger. \qquad (19)$$

where we have set $\hat{A}_{n'n} = \sqrt{w_{n'n}}c_{n'}^\dagger c_n$. This is the **Lindblad master equation**. It is more commonly written in

a form where all of the operators are expanded in terms of the eigenstates of the system itself. The common form is

$$\frac{d}{dt}\hat{\rho}_S(t) = -i\left[\hat{H}_S, \hat{\rho}_S\right] - \frac{1}{2}\hat{V}^\dagger\hat{V}\hat{\rho}_S - \frac{1}{2}\hat{\rho}_S\hat{V}^\dagger\hat{V} + \hat{V}\hat{\rho}_S\hat{V}^\dagger,$$ (20)

where the $\hat{V}$ are now operators representing the effect of the reservoir on the system. We have essentially eliminated the detailed dynamics of the reservoir in this form. To arrive at the Lindblad master equation, we have made three important assumptions. Eq.(12) says that the system and reservoir are initially uncorrelated and there interaction is turned on at $t > 0$. In expanding $\hat{\rho}_S^{(I)}(t)$ to second order, we have made the assumption that the interaction of the system with the reservoir is weak. Finally, we have assumed the reservoir itself has no correlations between different transitions, thus being "memoryless".

We can use the Lindblad equation for a very simple example involving a two level atom coupled to the vacuum, undergoing spontaneous emission [2]. The coherent part of the atom's evolution is described by the Hamiltonian

$$\hat{H} = \omega\hat{\sigma}_z/2$$

where ω is the energy difference of the atomic levels and $\hat{\sigma}_z$ is one of the Pauli matrices defined by

$$\hat{\sigma}_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad \hat{\sigma}_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \qquad \hat{\sigma}_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$ (21)

The $\hat{V}$ operator is defined as $\sqrt{\gamma}\hat{\sigma}_-$ where γ is the rate of spontaneous emission and $\hat{\sigma}_-$ is the atomic lowering operator defined as

$$\hat{\sigma}_- = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}.$$

From the definition one can simply see that this operator connects the excited state to the ground state of this two-level system. The Lindblad equation for this example becomes

$$\frac{d}{dt}\hat{\rho} = -i\left[\hat{H}, \hat{\rho}\right] + \gamma\left[2\hat{\sigma}_-\hat{\rho}\hat{\sigma}_+ - \hat{\sigma}_+\hat{\sigma}_-\hat{\rho} - \hat{\rho}\hat{\sigma}_+\hat{\sigma}_-\right]$$

where $\hat{\sigma}_+ \equiv \hat{\sigma}_-^\dagger$ is the atomic raising operator. One can switch to the interaction picture by writing

$$\hat{\rho}^{(I)}(t) = e^{i\hat{H}t}\hat{\rho}(t)e^{-i\hat{H}t},$$

$$\hat{\sigma}_-^{(I)} = e^{i\hat{H}t}\hat{\sigma}_- e^{-i\hat{H}t} = e^{-i\omega t}\hat{\sigma}_-,$$

and

$$\hat{\sigma}_+^{(I)} = e^{i\hat{H}t}\hat{\sigma}_+ e^{-i\hat{H}t} = e^{i\omega t}\hat{\sigma}_+.$$

The equation of motion for $\hat{\rho}^{(I)}$ is now

$$\frac{d}{dt}\hat{\rho}^{(I)} = \gamma\left[2\hat{\sigma}_-\hat{\rho}^{(I)}\hat{\sigma}_+ - \hat{\sigma}_+\hat{\sigma}_-\hat{\rho}^{(I)} - \hat{\rho}^{(I)}\hat{\sigma}_+\hat{\sigma}_-\right].$$

This can be solved using a Bloch vector representation (popular in quantum information) for $\hat{\rho}^{(I)}$ which is defined by

$$\hat{\rho} = \frac{\hat{I} + \lambda \cdot \sigma}{2}.$$ (22)

The solution is

$$\lambda_x = \lambda_x(0)e^{-\gamma t}$$

$$\lambda_y = \lambda_y(0)e^{-\gamma t}$$

$$\lambda_z = \lambda_z(0)e^{-2\gamma t} + 1 - e^{-2\gamma t}.$$

This problem is an example of the application of the Lindblad equation to include energy dissipation. This example can be seen as an instance of the spin-boson model, in which a small, finite dimensional quantum system interacts with a bath of simple harmonic oscillators. The original motivation for studying the spin-boson model was to examine the effect of dissipation on macroscopic tunneling of the flux trapped in a SQUID (Superconducting QUantum Interference Device) [3].

This evolution describe by the Lindblad equation is equivalent to that of a **quantum operation**, $\mathcal{E}$, written as

$$\hat{\rho}' \equiv \mathcal{E}(\hat{\rho}).$$ (23)

We can use the so called **operator-sum representation** to write the quantum operation as

$$\mathcal{E}(\hat{\rho}) = \sum_k \hat{E}_k\hat{\rho}\hat{E}_k^\dagger$$ (24)

where the $\hat{E}_k$ are called the **Kraus operators** and are defined as $\hat{E}_k = \langle e_k|\hat{U}|e_0\rangle$ where $|e_0\rangle$ is the initial state of the environment (there is no loss of generality by assuming a pure state) and $|e_k\rangle$ is the kth element of the orthonormal basis for the state space of the environment. For our two-level system, we have

$$\hat{\rho}^{(I)}(t) = \hat{E}_0\hat{\rho}^{(I)}(0)\hat{E}_0^\dagger + \hat{E}_1\hat{\rho}^{(I)}(0)\hat{E}_1^\dagger.$$

with the Kraus operators, $\hat{E}_i$, defined as

$$\hat{E}_0 = \begin{pmatrix} 1 & 0 \\ 0 & \sqrt{1-\gamma'} \end{pmatrix} \qquad \hat{E}_1 = \begin{pmatrix} 0 & \sqrt{\gamma'} \\ 0 & 0 \end{pmatrix}$$

with $\gamma' = 1 - e^{-2t\gamma}$. A quantum operation is a general tool for describing the evolution of quantum systems in a wide variety of circumstances, including stochastic

changes to quantum states. Like the Lindblad case, this quantum operation is a description of energy dissipation. The particular operators presented here are those of a quantum operation called **amplitude damping**. This type of problem is useful for describing the general features of energy dissipation in a quantum system whether it be an atom spontaneously emitting a photon, a spin system at high temperature reaching equilibrium with its environment, or the state of a photon in an interferometer or cavity when it is subject to scattering and attenuation. This type of characterization a quantum operation is a general tool for describing the evolution of open quantum systems. Apparently, it is actually more general than the Lindblad equation approach. Since solving the Lindblad equation allows one to determine the time dependence of a density matrix, the result can also be express as a quantum operation defined by

$$\hat{\rho}(t) = \sum_k \hat{E}_k(t)\hat{\rho}(0)\hat{E}_k^\dagger(t), \tag{25}$$

where $\hat{E}_k(t)$ are time-dependent operation elements, determined from the solution of the master equation. A quantum process, however, cannot always be written down as a master equation since quantum operations may describe non-Markovian dynamics. A quantum operation formalism only describes quantum state changes and not continuous time evolution. The quantum operation formalism directly resembles the mathematical form for a quantum measurement. See [2] for more dicussion on this.

The Lindblad equation has other limitations as well. Consider a mixed state with a Hamiltonian which is a function of the microstates themselves, i.e. $\hat{H} = \hat{H}(|\psi_i\rangle)$. As an example, when using Density Functional Theory (DFT), the Hamiltonian is a function of the density, n, where $n = \sum_i |\psi_i\rangle\langle\psi_i|$. Thus, the Hamiltonian is different for each element of the ensemble, $|\psi_i\rangle$. One can see from Eq.(5) that there is, in general, no closed equation of motion such as the Lindblad equation, for a system like this where $\hat{\rho}$ is a mixed state. Therefore, we must try to find a stochastic differential equation to include the effects of an environment. If a damping term is included in the Schrödinger equation, probability is no longer conserved [4]. However, we can try to compensate for this loss by adding a fluctuating term. This results in a form for the Schrödinger-Langevin equation. To find this equation, we start with

$$\frac{d}{dt}|\psi(t)\rangle = -i\hat{H}|\psi(t)\rangle - \hat{U}|\psi(t)\rangle + \ell(t)\hat{V}|\psi(t)\rangle \tag{26}$$

where $\hat{U}$ and $\hat{V}$ are operators to be specified and $\ell(t)$ is a random fluctuating term usually taken to be white noise:

$$\langle \ell(t)\rangle = 0 \qquad \langle \ell(t)\ell^*(t')\rangle = \delta(t-t') \tag{27}$$

The Hamiltonian here is the one for the system we are interested in, analogous to $\hat{H}_S$ in the derivation of the Lindblad master equation, and $\hat{V}$ will again be the operator representing the interaction of the system with the reservoir. For small Δt, one obtains

$$|\psi(t+\Delta t)\rangle = \left[1 - i\hat{H}\Delta t - \hat{U}\Delta t + \int_t^{t+\Delta t'} \ell(t')dt'\hat{V}\right]|\psi(t)\rangle.$$

For the Hermitian conjugate, we have

$$\langle\psi(t+\Delta t)| = \langle\psi(t)|\left[1 - i\hat{H}\Delta t - \hat{U}\Delta t + \hat{V}^\dagger \int_t^{t+\Delta t'} \ell^*(t')dt'\right].$$

If we take the scalar product and average over ℓ, we get

$$\langle\psi(t+\Delta t)|\psi(t+\Delta t)\rangle = \langle\psi(t)|\psi(t)\rangle - 2\langle\psi(t)|\hat{U}|\psi(t)\rangle + \langle\psi(t)|\hat{V}^\dagger\hat{V}|\psi(t)\rangle.$$

From this, we can see that the average norm is conserved when $2\hat{U} = \hat{V}^\dagger\hat{V}$. Thus, we have found the form of the **Schrödinger-Langevin equation**:

$$\frac{d}{dt}|\psi(t)\rangle = -i\hat{H}|\psi(t)\rangle - \frac{1}{2}\hat{V}^\dagger\hat{V}|\psi(t)\rangle + \ell(t)\hat{V}|\psi(t) \tag{28}$$

In it's most general form, it can be written as

$$\frac{d}{dt}|\psi(t)\rangle = -i\hat{H}|\psi(t)\rangle - \frac{1}{2}\sum_a \hat{V}_a^\dagger\hat{V}_a|\psi(t)\rangle + \sum_a \ell_a(t)\hat{V}_a|\psi(t). \tag{29}$$

The Schrödinger-Langevin equation is useful for applications such as Stochastic Time Dependent Current Density Functional Theory (Stochastic TD-CDFT) [5], which one can use to study many-particle systems in interaction with external baths. Stochastic TD-CDFT has been used to describe the interaction of an excited quantum system with an external environment and its subsequent decay into the ground state, which has been previously impossible using standard DFT methods [6]. In this paper, it is shown that for He$^+$, the dynamics calculated using the Lindblad master equation and those calculated using Stochastic TD-CDFT (employing the Schrödinger-Langevin equation) give comparable results. The results of this study can be discussed in terms of quantum measurement theory.

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