Introduction to Open Quantum Systems

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The study of open quantum systems allows physicists to model quantum mechanics and quantum field theories that contain interaction with an environment. This paper aims to showcase the fundamentals of the theory of open quantum systems, including the discussion of basic mathematical properties, derivation and intuition of the Lindblad master equation, and how the formal equations can be applied to a toy model of radiative damping.

I. INTRODUCTION

In undergraduate quantum mechanics the evolution of closed quantum systems, in which states evolve unitarily under a governing Hamiltonian, is often covered extensively. In such systems, the unitary evolution given by the Hamiltonian is crucial, and often the defining property of the system. However, in real world applications of quantum mechanics, as well as in systems interacting with thermal media, it is difficult to isolate a system from the environment, thus it is required that we develop an effective framework to model the interaction between an environment and the system of interest.

The study of open quantum systems aims to provide descriptions of systems that evolve while interacting with an environment by using first principle assumptions of quantum mechanics and statistical mechanics. One of the early attempts is the characterization of the quantum dynamical semigroup [4]. By constraining the dynamical equations and exploiting time hierarchies of the dynamics, physicists arrived at the Lindblad master equation.

With the formalism in hand, nuclear physicists started combining the Lindblad master equation with non-relativistic effective field theories to calculate evolution of nuclei and quarkonia in the quark gluon plasma [1], which enhances our understanding of thermal QCD. The Lindblad master equations are also widely utilized to study to quantum optical systems, with one notable example being quantum computing hardware development.

This paper aims to provide an overview of the basic mathematical formalisms of open quantum theory and showcase how the techniques involved can be applied to calculate radiative damping of a simple harmonic oscillator. The same description can then be extended to the so-called Caldeira-Leggett model of damped SHO, and even further to field theoretic approaches of heavy quarkonia disassociation.

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II. DENSITY MATRIX

First, we briefly review density matrices and the canonical ensemble, following [11]. Consider an isolated quantum system with an ensemble of states $\{|\psi_n\rangle\}$, each state $|\psi_n\rangle$ corresponds to a probability p_n, the density matrix of this system is given by

$$\rho = \sum_n p_n |\psi_n\rangle\langle\psi_n|. \tag{1}$$

The density matrix ρ is Hermitian, positive semi-definite, and satisfies $\mathrm{Tr}(\rho) = 1$. The expectation value of an observable $\mathcal{O}$ is given by

$$\langle\mathcal{O}\rangle = \mathrm{Tr}(\rho\mathcal{O}). \tag{2}$$

If a density matrix ρ_{AB} represents an ensemble of states that lie in the product space $\mathcal{H}_A \otimes \mathcal{H}_B$, one can trace over a subsystem

$$\rho_A = \mathrm{Tr}_B(\rho_{AB}). \tag{3}$$

After tracing over the degree of freedom in $\mathcal{H}_B$, ρ_A can be interpreted as an ensemble of states in $\mathcal{H}_A$.

If the system evolves under a known Hamiltonian H, ρ obeys the Liouville-von Neumann equation [12]

$$\frac{\partial\rho}{\partial t} = -i[H,\rho] = \mathcal{L}(\rho), \tag{4}$$

$$\rho(t) = U(t;0)\rho(0)U^\dagger(t;0) = \exp\left(\int_0^t \mathrm{d}t\,\mathcal{L}\right)\rho(0), \tag{5}$$

where U is the usual unitary time evolution operator $U(t_f, t_i) = e^{\mathcal{T}(i\int_{t_i}^{t_f} \mathrm{d}t\,H(t))}$, and $\mathcal{L}$ is often referred to as the Liouville super-operator.

When in thermal equilibrium under temperature T, the density matrix takes the form [10]

$$\rho = \frac{e^{-\beta H}}{\mathrm{Tr}(e^{-\beta H})} = \frac{1}{Z}\sum_n e^{-\beta E_n}|n\rangle\langle n|, \tag{6}$$

where E_n is the energy of the nth eigenstate $|n\rangle$, $\beta = \frac{1}{T}$ is the Boltzmann factor, and $Z = \mathrm{Tr}\left(e^{-\beta H}\right) = \sum_n e^{-\beta E_n}$ is the partition function. The average energy $\langle E\rangle$ of the system is given by

$$\langle E\rangle = -\frac{\mathrm{d}\ln Z}{\mathrm{d}\beta}. \tag{7}$$

The entropy S of this system is given by

$$S = -\operatorname{Tr}(\rho \ln \rho), \tag{8}$$

and its time evolution satisfies

$$\frac{\mathrm{d}S}{\mathrm{d}t} = -\operatorname{Tr}\left(\frac{\mathrm{d}\rho}{\mathrm{d}t}\ln\rho + \frac{\mathrm{d}\rho}{\mathrm{d}t}\right) = -\operatorname{Tr}(\mathcal{L}(\rho)\ln\rho). \tag{9}$$

III. DYNAMICS OF OPEN QUANTUM SYSTEMS

In this section, the two main approaches of open quantum system dynamics are introduced. Afterwards the Lindblad master equation which governs the evolution of open quantum systems is derived from both points of view. The first approach focuses on mathematical conditions of maps between density matrices, and the second approach uses perturbation theory.

After having obtained the Lindblad master equation, the physical meaning of its components are explained. For a complete pedagogical introduction and further details, the reader can refer to [2], which the main source of this section.

A. Mathematical Formulation

Let $\rho \mapsto M(\rho)$ be map from a density matrix to a density matrix, M is required to satisfy the following conditions.

- Linearity: linearity is required such that quantum operations are consistent with the ensemble interpretation of density matrices.

- Trace and Hermiticity preserving.

- Positivity and complete positivity: all density matrices of composite systems are mapped to density matrices.

We will refer to maps that satisfy these properties as completely positive trace-preserving (CPT) maps, or quantum operations. The restrictions on quantum operations result in the following statement.

Theorem 1 (Kraus representation theorem) *Let $\mathcal{H}$ be a Hilbert space with $N = \dim(\mathcal{H})$ and let ρ be a density matrix for states in $\mathcal{H}$. Any quantum operation $\rho \mapsto M(\rho)$ can be written as*

$$M(\rho) = \sum_{i=0}^{N^2-1} K_i \rho K_i^\dagger, \tag{10}$$

with K_i satisfying

$$\sum_{i=0}^{N^2-1} K_i^\dagger K_i = 1. \tag{11}$$

Such K_is are called Kraus operators. A complete proof of theorem 1 can be found in [7].

The Kraus operators are not unique for a given quantum operation. In fact, if

$$L_i = \sum_j u_{ij} K_j, \tag{12}$$

where u is a unitary map from $N \times N$ matrices to $N \times N$ matrices, then

$$\begin{aligned}
\sum_i L_i \rho L_i^\dagger &= \sum_{i,j,k} u_{ij} K_j \rho K_k^\dagger u_{ki}^* \\
&= \sum_{j,k} \delta_{jk} K_j \rho K_k^\dagger = \sum_i K_i \rho K_i^\dagger.
\end{aligned} \tag{13}$$

That is, L_i and K_i are equivalent representations of the same quantum operation.

An additional common assumption that is often imposed is that quantum operations are Markov processes, which promises that the evolution of the density matrix is local in time. The quantum operations thus form a one parameter semigroup parametrized by time t, that is, the time evolution can be given by

$$\rho(t) = M(t)\rho(0), \text{ with } M(t_1 + t_2) = M(t_1)M(t_2), \tag{14}$$

where the product should be understood as a sequential action of the operation. Thus at any moment

$$\rho(t + \mathrm{d}t) = M(\mathrm{d}t)\rho(t), \tag{15}$$

the evolution can be specified by finding $M(\mathrm{d}t)$.

Assume the the quantum system is evolved by a quantum operation after every small time step τ,

$$\rho(t+\tau) = \sum_{i=0}^{N^2-1} K_i \rho(t) K_i^\dagger = \rho(t) + \frac{\mathrm{d}\rho(t)}{\mathrm{d}t}\tau + O(\tau^2) \tag{16}$$

to match the orders of τ, K_i can be chosen as in [3], such that

$$\begin{aligned}
K_0 &= 1 + (G - iH)\tau, \\
K_i &= \sqrt{\gamma_i \tau} L_i, \text{ for } 1 \le i \le N^2 - 1,
\end{aligned} \tag{17}$$

where without loss of generality G and H are chosen to be Hermitian, and $\gamma_i > 0$ are chosen to have units $1/\tau$ in order to characterize decay rates.

By the trace preserving condition (11) the form of G can be fixed

$$(1 + 2G\tau) + \sum_{i=1}^{N^2-1} \gamma_i L_i^\dagger L_i \tau = 1 \Rightarrow G = -\frac{1}{2}\sum_{i=1}^{N^2-1} \gamma_i L_i^\dagger L_i. \tag{18}$$

(16) can then be simplified

$$\rho(\tau) = \rho + \{G, \rho\}\tau - i[H, \rho]\tau + \sum_{i \geq 1} \gamma_i L_i \rho L_i^\dagger \tau$$

$$= \rho - i[H, \rho]\tau + \sum_{i \geq 1} \gamma_i \left(L_i \rho L_i^\dagger - \frac{1}{2}\{L_i^\dagger L_i, \rho\} \right)\tau,$$
(19)

$$\frac{\partial \rho}{\partial t} = -i[H, \rho] + \sum_i \gamma_i \left(L_i \rho L_i^\dagger - \frac{1}{2}\{L_i^\dagger L_i, \rho\} \right). \quad (20)$$

(20) is the so called Lindblad master equation, it describes the most general form of Markovian evolution of quantum systems.

B. Physical Derivation

Alternatively, consider a system S that interacts with an environment bath B. Only knowledge of S can be probed, therefore specific forms of B should not be assumed. The total Hilbert space of quantum states can be written as

$$\mathcal{H} = \mathcal{H}_S \otimes \mathcal{H}_B. \quad (21)$$

In general, the Hamiltonian by which the system evolves can be written as

$$H = H_S + H_B + V, \quad (22)$$

where H_S only acts on $\mathcal{H}_S$, H_B only acts on $\mathcal{H}_B$, and V contains all the cross terms. V can further be written as a sum

$$V = \sum_\alpha S_\alpha \otimes B_\alpha = V^\dagger. \quad (23)$$

Denote the time evolution operator due to H as U, and that due to $H_S + H_B$ as U_0.

The total density matrix evolves by

$$\rho(t) = U(t;0)\rho(0)U^\dagger(t;0). \quad (24)$$

The observable system density matrix is then given by tracing over the bath

$$\rho_S(t) = \text{Tr}_B(U(t;0)\rho(0)U^\dagger(t;0)). \quad (25)$$

We assume that the initial state is separable $\rho(0) = \rho_S(0) \otimes \rho_B(0)$. $\rho_B(0)$ is Hermitian, positive-semidefinite, so it admits an orthonormal spectral decomposition

$$\rho_B(0) = \sum_\mu p_\mu |\mu\rangle\langle\mu|, \text{ with } p_\mu \geq 0. \quad (26)$$

$\rho_S(t)$ can be written as

$$\rho_S(t) = \sum_\mu \langle\mu| U(t;0)\rho_S(0) \otimes \sum_\nu p_\nu |\nu\rangle\langle\nu| U^\dagger(t;0) |\mu\rangle$$

$$= \sum_{\mu,\nu} \langle\mu| U(t;0)\sqrt{p_\nu}|\nu\rangle \rho_S(0) \langle\nu| \sqrt{p_\nu}U^\dagger(t;0) |\mu\rangle. \quad (27)$$

By identifying $K_{\mu\nu} = \langle\mu| U(t;0)\sqrt{p_\nu} |\nu\rangle$, the quantum operation on ρ_S, obtained from tracing over unitary evolution of ρ, obeys theorem 1.

We now attempt to write down a concrete evolution map mainly following the treatment in [2]. To simplify the derivation, we go to the interaction picture,

$$\widetilde{V}(t) = U_0^\dagger(t;0)VU_0(t;0), \quad (28)$$

$$\tilde{\rho}(t) = U_0^\dagger(t;0)\rho(t)U_0(t;0), \quad (29)$$

$$\frac{d\tilde{\rho}_S(t)}{dt} = -i\,\text{Tr}_B([\widetilde{V}(t), \tilde{\rho}(t)]). \quad (30)$$

As shown above, operators in interaction picture are indicated by a tilde. We then assume there is a time scale separation in the system

$$\tau_{\text{damp}} \gg \tau_{\text{coarse}} \gg \tau_B, \quad (31)$$

where τ_{damp} is the characteristic time scale of the system's decay rate, τ_{coarse} is τ from last section, the time scale between each quantum operation, and τ_B is the time scale for bath fluctuation, which is also the time for memory of the system to be lost. Intuitively, the bath always restores thermal equilibrium much faster than than any other interaction between the bath and the system.

We then use perturbation theory to solve for the evolution of $\tilde{\rho}$,

$$\tilde{\rho}(t) = \tilde{\rho}(0) - i\int_0^t dt_1[\widetilde{V}(t_1), \tilde{\rho}(t_1)]. \quad (32)$$

By substituting (32) into (30), we obtain the Redfield equation

$$\frac{d\tilde{\rho}_S}{dt} = -i\,\text{Tr}_B([\tilde{V}(t), \tilde{\rho}(0)])$$

$$- \int_0^t dt_1 \text{Tr}_B([\tilde{V}(t), [\tilde{V}(t_1), \tilde{\rho}(t_1)]]) \quad (33)$$

$$= -\int_0^\infty ds\,\text{Tr}_B\left([\tilde{V}(t), [\tilde{V}(t-s), \tilde{\rho}_S(t) \otimes \rho_B(0)]]\right). \quad (34)$$

In the above, to go from (33) to (34), scale separation condition is imposed. First, since $\tau_{\text{coarse}} \gg \tau_B$, $\text{Tr}_B([\tilde{V}(t), \tilde{\rho}(0)])$ can be set to 0 by shifting parameters of the initial state. Then, since $\tau_{\text{damp}} \gg \tau_{\text{coarse}}$, $\tilde{\rho}(t_1) \approx \tilde{\rho}(t)$. Lastly, in the weak coupling limit and τ_B being the smallest time scale,

$$\tilde{\rho}(t) = \tilde{\rho}_S(t) \otimes \rho_B(0). \quad (35)$$

Now we turn to the treatment in [5]. The interaction Hamiltonian V admits a spectral decomposition

$$V = \sum_{\alpha,\omega} S_{\alpha,\omega} \otimes B_\alpha. \quad (36)$$

such that in the interaction picture

$$\tilde{V}(t) = \sum_{\alpha,\omega} e^{i(H_S+H_B)t} S_{\alpha,\omega} \otimes B_\alpha e^{-i(H_S+H_B)t}$$

$$= \sum_{\alpha,\omega} e^{-i\omega t} S_{\alpha,\omega} \otimes \tilde{B}_\alpha(t) = \sum_{\alpha,\omega} e^{i\omega t} S_{\alpha,\omega}^\dagger \otimes \tilde{B}_\alpha^\dagger(t). \tag{37}$$

Substituting (37) back in to (34) one obtains

$$\frac{d\tilde{\rho}_S}{dt} = \int_0^\infty ds\, \mathrm{Tr}_B \left(\tilde{V}(t)\rho(t)\tilde{V}(t-s) + \tilde{V}(t-s)\rho(t)\tilde{V}(t) - \tilde{V}(t)\tilde{V}(t-s)\rho(t) - \rho(t)\tilde{V}(t)\tilde{V}(t-s) \right) \tag{38}$$

$$= \sum_{\omega,\alpha,\beta} \Gamma_{\alpha\beta}(\omega) \left(S_{\beta,\omega}\tilde{\rho}_S S_{\alpha,\omega}^\dagger - S_{\alpha,\omega}^\dagger S_{\beta,\omega}\tilde{\rho}_S \right) + \mathrm{h.c.}, \text{ where} \tag{39}$$

$$\Gamma_{\alpha\beta}(\omega) = \int_0^\infty ds\, e^{i\omega s} \mathrm{Tr}_B(\tilde{B}_\alpha^\dagger(t)\tilde{B}_\beta(t-s)\rho_B) = \int_0^\infty ds\, e^{i\omega s} \mathrm{Tr}_B(\tilde{B}_\alpha^\dagger(s)\tilde{B}_\beta(0)\rho_B). \tag{40}$$

And decomposing $\Gamma_{\alpha\beta}$ into the real and imaginary component $\Gamma_{\alpha\beta} = \frac{1}{2}\gamma_{\alpha\beta} + i\delta_{\alpha\beta}$ yields

$$\frac{d\tilde{\rho}_S}{dt} = -i[H_{LS}, \tilde{\rho}_S] + D(\tilde{\rho}_S), \tag{41}$$

$$H_{LS} = \sum_{\omega,\alpha,\beta} \delta_{\alpha\beta}(\omega) S_{\alpha,\omega}^\dagger S_{\beta,\omega}, \ D(\tilde{\rho}_S) = \sum_{\omega,\alpha,\beta} \gamma_{\alpha\beta}(\omega) \left(S_{\beta,\omega}\tilde{\rho}_S S_{\alpha,\omega}^\dagger - \frac{1}{2}\{S_{\alpha,\omega}^\dagger S_{\beta,\omega}, \tilde{\rho}_S\} \right). \tag{42}$$

Going back to Schrödinger picture and diagonalizing $\gamma_{\alpha\beta}$ reproduces (20) [2, 5].

To use the master equation, one would construct a model of the interaction Hamiltonian V, and a model of the bath ρ_B. A common ansatz for the bath is an ensemble of states in thermal equilibrium,

$$\rho_B = \frac{e^{-\beta H_B}}{\mathrm{Tr}_B(e^{-\beta H_B})} \tag{43}$$

as previously mentioned.

C. The Lindblad Master Equations

We now focus on interpreting the Lindblad master equation in standard form (20), the main reference of this subsection is [9]. First, (20) can be rewritten

$$\frac{\partial\rho}{\partial t} = -i\left(H_{\mathrm{eff}}\rho - \rho H_{\mathrm{eff}}^\dagger \right) + \sum_i \gamma_i L_i \rho L_i^\dagger, \tag{44}$$

where

$$H_{\mathrm{eff}} = H - \frac{i}{2}\sum_i \gamma_i L_i^\dagger L_i. \tag{45}$$

Consider one component of the density matrix

$$\rho(t) \supset p_n |\psi_n(t)\rangle\langle\psi_n(t)| \tag{46}$$

evolving an infinitesimal time dt, this results in

$$\rho(t+dt) \supset p_n(1 - iH_{\mathrm{eff}}dt) |\psi_n(t)\rangle\langle\psi_n(t)| (1 + iH_{\mathrm{eff}}^\dagger dt)$$
$$+ p_n \sum_i \gamma_i dt L_i |\psi_n(t)\rangle\langle\psi_n(t)| L_i^\dagger + O(dt^2). \tag{47}$$

There are three implications of (47). To begin, H the Hermitian component of H_{eff} describes the usual unitary time evolution of states under the known Hamiltonian,

$$|\psi_n(t+dt)\rangle = (1 - iHdt) |\psi_n(t)\rangle.$$

The second implication is that the probability of staying in $|\psi_n(t+dt)\rangle$ is not constant. Rather,

$$p_n ||(1 - iH_{\mathrm{eff}}dt) |\psi_n(t)\rangle ||^2$$
$$= p_n \langle\psi_n(t)| \left(1 - \sum_i \gamma_i L_i^\dagger L_i dt\right) |\psi_n(t)\rangle \tag{48}$$

$$\Rightarrow \frac{dp_n}{dt} = -\sum_i \gamma_i \langle\psi_n(t)| L_i^\dagger L_i |\psi_n(t)\rangle p_n. \tag{49}$$

The non-Hermitian component $-\frac{i}{2}\sum_i \gamma_i L_i^\dagger L_i$ generates exponential decays. In particular, a pure state would evolve towards a mixed state. The third implication lies in the second component of (47), it is responsible for characterizing the probability of discrete transitions between states with probability

$$p\big(|\psi_n\rangle \to L_i |\psi_n\rangle\big) = p_n \gamma_i dt \langle\psi_n| L_i^\dagger L_i |\psi_n\rangle. \tag{50}$$

IV. EXAMPLE: RADIATIVE DAMPING

Now we apply the Lindblad equation to a simple example. Consider a simple harmonic oscillator with frequency ω coupled to an external oscillating scalar field, analogous to light, via the following Hamiltonian [6]

$$V = \int d\Omega\, \lambda(\Omega)(ab_\Omega^\dagger + a^\dagger b_\Omega) \tag{51}$$

$$= \int d\Omega\, \frac{\lambda(\Omega)}{2}\Big((a + a^\dagger)(b_\Omega + b_\Omega^\dagger) - (a - a^\dagger)(b_\Omega - b_\Omega^\dagger)\Big), \tag{52}$$

where a and $a^\dagger$ are the creation and annihilation operators for the SHO and b and $b^\dagger$ are the creation and annihilation operators for the external scalar field. V is designed to resemble the classical electromagnetic interaction of a particle in an electromagnetic field

$$V \supset -q\vec{v} \cdot \vec{A} + q\Phi. \tag{53}$$

In the interaction picture, by using

$$e^{i\omega(a^\dagger a + \frac{1}{2})t} a\, e^{-i\omega(a^\dagger a + \frac{1}{2})t} = a e^{-i\omega t}, \tag{54}$$

the interacting potential becomes

$$\widetilde{V} = \int d\Omega\, \lambda(\Omega) e^{i(N_a\omega + N_b\Omega)t}(ab_\Omega^\dagger + a^\dagger b_\Omega)e^{-i(N_a\omega + N_b\Omega)t}$$

$$= \int d\Omega\, \lambda(\Omega)(ab_\Omega^\dagger e^{-i(\omega-\Omega)t} + a^\dagger b_\Omega e^{i(\omega-\Omega)t}). \tag{55}$$

which is in the form of (37). In parallel with quantum field theory, calculating $\Gamma_{\alpha\beta}(\omega)$ is equivalent to calculating correlation functions of the external scalar field. Roughly speaking, the correlators take the form

$$\Gamma_{\alpha\beta}(\omega) \sim \int_0^\infty ds\, e^{i\omega s} \sum_\mu p_\mu \langle \mu|\, b_\Omega^{(\dagger)} e^{-i(\omega-\Omega)s} b_\Omega^{(\dagger)}\, |\mu\rangle \tag{56}$$

which are obtained using (26) and (40). These terms thus produce non-zero jump operators

$$S_1 = a\ ,\ \Gamma_{11}(\omega) \sim \lambda(\omega)^2(\langle N_B\rangle + 1);$$
$$S_2 = a^\dagger\ ,\ \Gamma_{22}(\omega) \sim \lambda(\omega)^2\, \langle N_B\rangle \tag{57}$$

that effect the SHO's dynamics.

A special case is a 0 temperature bath, in which $\langle N_B\rangle = 0$. As any absorption would not happen in such a bath, the only allowed jump operator is $L \sim a$ [7]. The Lindblad equation in the interaction picture thus read

$$\frac{\partial\rho}{\partial t} = \gamma\left(a\rho a^\dagger - \frac{1}{2}\{a^\dagger a, \rho\}\right). \tag{58}$$

The expectation value of the SHO number operator decays exponentially, as shown below

$$\frac{d\langle N\rangle}{dt} = \frac{d}{dt}\operatorname{Tr}(N\rho) = \operatorname{Tr}\left(\gamma N\left(a\rho a^\dagger - \frac{1}{2}a^\dagger a\rho - \frac{1}{2}\rho a^\dagger a\right)\right)$$

$$= -\gamma \operatorname{Tr}\big(a^\dagger(aa^\dagger - a^\dagger a)a\rho\big) = -\gamma \operatorname{Tr}(N\rho)$$

$$= -\gamma\langle N\rangle \tag{59}$$

$$\Rightarrow \langle N(t)\rangle = e^{-\gamma t}\langle N(0)\rangle. \tag{60}$$

On the contrary, one expects a non-zero $\langle N(t\to\infty)\rangle$ in a finite temperature bath due to non-zero stimulation.

V. CONCLUSION

The Lindblad master equation serves as a powerful tool for analyzing open quantum system dynamics. As demonstrated in the examples, it involves relatively simple calculations in order to operate in this framework. However, we must remind ourselves that in the strongly interacting regime or in systems without clear time scale separation, the aforementioned formulae have to be applied with caution. Further studies with such considerations in mind is still an active area of research [8], and applications of different forms of master equations in other fields of physics are still being proposed and discussed.

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