

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 is often mentioned, in which states evolve unitarily under a governing Hamiltonian that is given and considered a defining property of the system. However, in the real world it is difficult to isolate a system from the environment it interacts with, and often times we need to effectively model the interaction between the environment and the system of interest.

The study of open quantum systems aims to develop descriptions of systems that evolve while interacting with an environment using first principle assumptions of quantum mechanics and statistical mechanics. One of the early attempts is the characterization of the quantum dynamical semigroup [4]. Using several techniques, some physical and some mathematical, 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 theory to calculate evolution of nuclei and quarkonia in a high temperature and low energy limit [1], which enhances our understanding of the structure of QCD and in particular the behavior of quark gluon plasmas.

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 in the case of calculating radiative damping of a simple harmonic oscillator.

II. DENSITY MATRIX

The introduction to density matrices presented in [11] is briefly summarized below. Consider an isolated quantum system with an ensemble of states $\{|\psi_n\rangle\}$, each with probabilities p_n , the density matrix of this system is given by

$$\rho = \sum_n p_n |\psi_n\rangle\langle\psi_n|. \quad (1)$$

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

$$\langle\mathcal{O}\rangle = \text{Tr}(\rho\mathcal{O}). \quad (2)$$

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

$$\rho_A = \text{Tr}_B(\rho_{AB}). \quad (3)$$

After which 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]

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

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

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

A thermal state in equilibrium under temperature T has a density matrix of the form [10]

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

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

$$\langle E \rangle = -\frac{d \ln Z}{d\beta}. \quad (7)$$

The entropy S of this system and the time evolution of S are given by

$$S = -\text{Tr}(\rho \ln \rho), \quad (8)$$

$$\frac{dS}{dt} = -\text{Tr}\left(\frac{d\rho}{dt} \ln \rho + \frac{d\rho}{dt}\right) = -\text{Tr}(\mathcal{L}(\rho) \ln \rho). \quad (9)$$

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III. DYNAMICS OF OPEN QUANTUM SYSTEMS

In the section, the two main approaches of open quantum system dynamics are introduced, and the Lindblad master equation, the equation that 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 makes use of perturbation theory and tracing over an environment bath.

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], 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 demanded 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*

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

with K_i satisfying

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

Such K_i s 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

$$L_i = \sum_j u_{ij} K_j, \quad (12)$$

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

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

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

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

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

$$\rho(t + dt) = M(dt)\rho(t), \quad (15)$$

the evolution can be specified by finding $M(dt)$.

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

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

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

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

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

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

(16) can then be simplified

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

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

(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

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

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 interaction picture,

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

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

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

As shown above, operators in interaction picture are indicated by a tilde.

We can 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.

We can then solve for the evolution of $\tilde{\rho}$,

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

By substituting (32) into (30) the Redfield equation can be obtained

$$\begin{aligned} \frac{d\tilde{\rho}_S}{dt} &= -i \text{Tr}_B([\tilde{V}(t), \tilde{\rho}(0)]) \\ &\quad - \int_0^t dt_1 \text{Tr}_B([\tilde{V}(t), [\tilde{V}(t_1), \tilde{\rho}(t_1)]]) \end{aligned} \quad (33)$$

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

In the above, to go from (33) to (34), scale separation is implemented. 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

$$\begin{aligned} \tilde{V}(t) &= \sum_{\alpha, \omega} e^{i(H_S + H_B)t} S_{\alpha, \omega} \otimes B_{\alpha} e^{-i(H_S + H_B)t} \\ &= \sum_{\alpha, \omega} e^{-i\omega t} S_{\alpha, \omega} \otimes \tilde{B}_{\alpha}(t) = \sum_{\alpha, \omega} e^{i\omega t} S_{\alpha, \omega}^{\dagger} \otimes \tilde{B}_{\alpha}^{\dagger}(t). \end{aligned} \quad (37)$$

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

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

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

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

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

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

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

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,

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

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

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

where

$$H_{\text{eff}} = H - \frac{i}{2} \sum_i \gamma_i L_i^\dagger L_i. \quad (45)$$

Consider one component of the density matrix

$$\rho(t) \supset p_n |\psi_n(t)\rangle \langle \psi_n(t)| \quad (46)$$

evolving an infinitesimal time dt , this results in

$$\begin{aligned} \rho(t+dt) \supset & p_n (1 - iH_{\text{eff}}dt) |\psi_n(t)\rangle \langle \psi_n(t)| (1 + iH_{\text{eff}}^\dagger dt) \\ & + p_n \sum_i \gamma_i dt L_i |\psi_n(t)\rangle \langle \psi_n(t)| L_i^\dagger + O(dt^2). \end{aligned} \quad (47)$$

There are three implications of (47). To start with, 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,

$$\begin{aligned} p_n & \|(1 - iH_{\text{eff}}dt) |\psi_n(t)\rangle\|^2 \\ & = p_n \langle \psi_n(t) | (1 - \sum_i \gamma_i L_i^\dagger L_i dt) | \psi_n(t) \rangle \end{aligned} \quad (48)$$

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

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

$$p(|\psi_n\rangle \rightarrow L_i |\psi_n\rangle) = p_n \gamma_i dt \langle \psi_n | L_i^\dagger L_i | \psi_n \rangle. \quad (50)$$

IV. EXAMPLE: RADIATIVE DAMPING

Consider a simple harmonic oscillator with frequency ω coupled to an external oscillating scalar field, analogous to light, via the following Hamiltonian [6]

$$\begin{aligned} V &= \int d\Omega \lambda(\Omega) (ab_\Omega^\dagger + a^\dagger b_\Omega) \\ &= \int d\Omega \frac{\lambda(\Omega)}{2} \left((a + a^\dagger)(b_\Omega + b_\Omega^\dagger) - (a - a^\dagger)(b_\Omega - b_\Omega^\dagger) \right), \end{aligned} \quad (51)$$

$$(52)$$

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

$$H_{\text{int}} \supset -q\vec{v} \cdot \vec{A} + q\Phi. \quad (53)$$

In the interaction picture, by using

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

the interacting potential becomes

$$\begin{aligned} \tilde{V} &= \int d\Omega \lambda(\Omega) e^{i(N_a \omega + N_b \Omega)t} (ab_\Omega^\dagger + a^\dagger b_\Omega) e^{-i(N_a \omega + N_b \Omega)t} \\ &= \int d\Omega \lambda(\Omega) (ab_\Omega^\dagger e^{-i(\omega - \Omega)t} + a^\dagger b_\Omega e^{i(\omega - \Omega)t}). \end{aligned} \quad (55)$$

which is in the form of (37).

In parallel with quantum field theory, calculating the corresponding $\Gamma_{\alpha\beta}(\omega)$ is equivalent to calculating the correlation function of the external scalar field.

One can then continue analyzing the behavior of this system by considering integrals of the form

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

obtained using (26) and (40), which produce the non-zero terms

$$\begin{aligned} S_1 &= a, \quad \Gamma_{11}(\omega) \sim \lambda(\omega)^2 (\langle N_B \rangle + 1); \\ S_2 &= a^\dagger, \quad \Gamma_{22}(\omega) \sim \lambda(\omega)^2 \langle N_B \rangle. \end{aligned} \quad (57)$$

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

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

It can be shown that the expectation value of the number operator decays exponentially .

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

$$\begin{aligned} &= -\gamma \text{Tr} \left(a^\dagger (a a^\dagger - a^\dagger a) \rho \right) = -\gamma \text{Tr}(N\rho) \\ &= -\gamma \langle N \rangle \end{aligned} \quad (59)$$

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

On the contrary, for a finite temperature bath, one can expect a non-zero $\langle N(t \rightarrow \infty) \rangle$ due to stimulation from the bath.

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 more applications of different forms of master equations in other fields of physics are still being probed.

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