Lindblad主方程（Lindblad master equation）

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Lindblad主方程（Lindblad master equation）是一种用于描述开放量子系统动力学的基本方程。所谓开放量子系统，指的是与外部环境有交互作用的量子系统，这种交互会导致系统的量子态随时间发生不可逆的变化，例如量子态的凝聚和去相干。

Lindblad主方程提供了一个数学框架，用于描述这种随时间演化过程，特别是当系统与外部环境的相互作用不能忽略时。它是一种非幺正（non-unitary）演化方程，区别于孤立量子系统中遵循的薛定谔方程（描述的是幺正演化）。

Lindblad方程的一般形式可以写为：

$$\frac{d\rho}{dt} = -\frac{i}{\hbar}[H,\rho] + \sum_k \left(L_k \rho L_k^\dagger - \frac{1}{2}\{L_k^\dagger L_k, \rho\} \right)$$

这里，ρ 是系统的密度算符（描述系统量子态的矩阵），H 是系统的哈密顿算符（描述系统的能量），$[H,\rho]$ 表示H和ρ的对易子，L_k 是与环境相互作用相关的算符，也被称为Lindblad算符或跃迁算符，$\{A,B\}$ 表示A和B的反对易子。

方程的第一项代表了系统内部的幺正演化，与薛定谔方程中的演化相同。第二项则代表了由于与环境相互作用导致的非幺正效应，如能量耗散和相干性丧失。

Lindblad方程在量子光学、量子信息科学以及其他涉及开放量子系统研究的领域中有着广泛的应用。通过这个方程，研究者能够模拟并分析开放系统的量子行为，以及它们如何受到周围环境的影响。

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对于一个三能级系统（通常指的是量子系统有三个可能的状态），描述退极化（depolarization）通道的Lindblad主方程可以特别设计来反映系统状态随时间因环境相互作用而发生的混合和退极化过程。退极化通道是一种量子通道，它使得量子态向最大混合态方向演化，这种过程会导致量子信息的丢失。

对于三能级系统，密度矩阵ρ可以用来描述系统的状态，它是一个3×3的矩阵。描述退极化的Lindblad方程需要引入一组适当的Lindblad算符L_k，这些算符描述了系统与其环境的相互作用，导致退极化效应。

具体地，对于退极化通道，我们可以定义一组Lindblad算符，它们作用于系统的各个基态之间，以此来模拟环境对系统状态的随机干扰。对于三能级系统，我们可能会选择一组描述状态之间跃迁的Lindblad算符，如下所示：

- $L_{jk} = \sqrt{\gamma_{jk}}|j\rangle\langle k|$，其中$\gamma_{jk}$是从态$k$到态$j$的退极化率，$j,k = 1,2,3$，并且$j \neq k$。

在这种情况下，Lindblad主方程可以写为：
$\frac{d\rho}{dt} = -\frac{i}{\hbar}[H,\rho] + \sum_{j\neq k}\left(L_{jk}\rho L_{jk}^{\dagger} - \frac{1}{2}\{L_{jk}^{\dagger}L_{jk},\rho\}\right)$

其中，H是系统的哈密顿算符，描述了系统内部的能量动力学。方程的第一项代表了系统的幺正演化，第二项则是非幺正演化项，其中包含了所有可能的态间跃迁引起的退极化效应。

这个方程通过组合幺正和非幺正的动力学，能够描述三能级系统在退极化通道作用下的时间演化。通过这种方式，可以分析系统如何因环境的作用而逐渐失去纯度和相干性，这对于量子信息处理和量子计算中的误差校正等领域非常重要。

Lindblad Master Equation Solver — QuTiP 4.7 Documentation

Unitary evolution

The dynamics of a closed (pure) quantum system is governed by the Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}\Psi = \hat{H}\Psi, \tag{1}$$

where Ψ is the wave function, $\hat{H}$ the Hamiltonian, and $\hbar$ is Planck's constant. In general, the Schrödinger equation is a partial differential equation (PDE) where both Ψ and $\hat{H}$ are functions of space and time. For computational purposes it is useful to expand the PDE in a set of basis functions that span the Hilbert space of the Hamiltonian, and to write the equation in matrix and vector form

$$i\hbar\frac{d}{dt}\left|\psi\right\rangle = H\left|\psi\right\rangle$$

where $\left|\psi\right\rangle$ is the state vector and H is the matrix representation of the Hamiltonian. This matrix equation can, in principle, be solved by diagonalizing the Hamiltonian matrix H. In practice, however, it is difficult to perform this diagonalization unless the size of the Hilbert space (dimensior of the matrix H) is small. Analytically, it is a formidable task to calculate the dynamics for systems with more than two states. If, in addition, we consider dissipation due to the inevitable interaction with a surrounding environment, the computational complexity grows even larger, and we have to resort to numerical calculations in all realistic situations. This illustrates the importance of numerica calculations in describing the dynamics of open quantum systems, and the need for efficient and accessible tools for this task.

Non-unitary evolution

While the evolution of the state vector in a closed quantum system is deterministic, open quantum systems are stochastic in nature. The effect of an environment on the system of interest is to induce stochastic transitions between energy levels, and to introduce uncertainty in the phase difference between states of the system. The state of an open quantum system is therefore described in terms of ensemble averaged states using the density matrix formalism. A density matrix ρ describes a probability distribution of quantum states $|\psi_n\rangle$, in a matrix representation $\rho = \sum_n p_n |\psi_n\rangle \langle\psi_n|$, where p_n is the classical probability that the system is in the quantum state $|\psi_n\rangle$. The time evolution of a density matrix ρ is the topic of the remaining portions of this section.

The Lindblad Master equation

The standard approach for deriving the equations of motion for a system interacting with its environment is to expand the scope of the system to include the environment. The combined quantum system is then closed, and its evolution is governed by the von Neumann equation

$$\dot{\rho}_{\rm tot}(t) = -\frac{i}{\hbar}[H_{\rm tot}, \rho_{\rm tot}(t)], \tag{2}$$

the equivalent of the Schrödinger equation (1) in the density matrix formalism. Here, the total Hamiltonian

$$H_{\rm tot} = H_{\rm sys} + H_{\rm env} + H_{\rm int},$$

includes the original system Hamiltonian $H_{\rm sys}$, the Hamiltonian for the environment $H_{\rm env}$, and a term representing the interaction between the system and its environment $H_{\rm int}$. Since we are only term representing the interaction between the system and its environment $H_{\rm int}$. Since we are only interested in the dynamics of the system, we can at this point perform a partial trace over the environmental degrees of freedom in Eq. (2), and thereby obtain a master equation for the motion of the original system density matrix. The most general trace-preserving and completely positive form of this evolution is the Lindblad master equation for the reduced density matrix $\rho = {\rm Tr}_{\rm env}[\rho_{\rm tot}]$

$$\dot\rho(t) = -\frac{i}{\hbar}[H(t), \rho(t)] + \sum_n \frac{1}{2}\left[2C_n\rho(t)C_n^\dagger - \rho(t)C_n^\dagger C_n - C_n^\dagger C_n\rho(t)\right] \tag{3}$$

where the $C_n = \sqrt{\gamma_n}A_n$ are collapse operators, and A_n are the operators through which the environment couples to the system in $H_{\rm int}$, and γ_n are the corresponding rates. The derivation of Eq. (3) may be found in several sources, and will not be reproduced here. Instead, we emphasize the approximations that are required to arrive at the master equation in the form of Eq. (3) from physical arguments, and hence perform a calculation in QuTiP:

- **Separability:** At $t = 0$ there are no correlations between the system and its environment such that the total density matrix can be written as a tensor product $\rho^I_{\rm tot}(0) = \rho^I(0) \otimes \rho^I_{\rm env}(0)$.
- **Born approximation:** Requires: (1) that the state of the environment does not significantly change as a result of the interaction with the system; (2) The system and the environment remain separable throughout the evolution. These assumptions are justified if the interaction is weak, and if the environment is much larger than the system. In summary, $\rho_{\rm tot}(t) \approx \rho(t) \otimes \rho_{\rm env}$.
- **Markov approximation** The time-scale of decay for the environment $\tau_{\rm env}$ is much shorter than the smallest time-scale of the system dynamics $\tau_{\rm sys} \gg \tau_{\rm env}$. This approximation is often deemed a "short-memory environment" as it requires that environmental correlation functions decay on a time-scale fast compared to those of the system.
- **Secular approximation** Stipulates that elements in the master equation corresponding to transition frequencies satisfy $|\omega_{ab} - \omega_{cd}| \ll 1/\tau_{\rm sys}$, i.e., all fast rotating terms in the interaction picture can be neglected. It also ignores terms that lead to a small renormalization of the system energy levels. This approximation is not strictly necessary for all master-equation formalisms (e.g., the Block-Redfield master equation), but it is required for arriving at the Lindblad form (3) which is used in `qutip.mesolve`.

For systems with environments satisfying the conditions outlined above, the Lindblad master equation (3) governs the time-evolution of the system density matrix, giving an ensemble average of the system dynamics. In order to ensure that these approximations are not violated, it is important that the decay rates γ_n be smaller than the minimum energy splitting in the system Hamiltonian. Situations that demand special attention therefore include, for example, systems strongly coupled to their environment, and systems with degenerate or nearly degenerate energy levels.

For non-unitary evolution of a quantum systems, i.e., evolution that includes incoherent processes such as relaxation and dephasing, it is common to use master equations. In QuTiP, the function `qutip.mesolve` is used for both: the evolution according to the Schrödinger equation and to the master equation, even though these two equations of motion are very different. The `qutip.mesolve` function automatically determines if it is sufficient to use the Schrödinger equation (if no collapse operators were given) or if it has to use the master equation (if collapse operators were given). Note that to calculate the time evolution according to the Schrödinger equation is easier and much faster (for large systems) than using the master equation, so if possible the solver will fall back on using the Schrödinger equation.

What is new in the master equation compared to the Schrödinger equation are processes that describe dissipation in the quantum system due to its interaction with an environment. These environmental interactions are defined by the operators through which the system couples to the environment, and rates that describe the strength of the processes.

原 Lindblad 方程：

$$\dot{\rho}(t) = -\frac{i}{\hbar}[H(t),\rho(t)] + \sum_n \frac{1}{2}\left(2C_n\rho(t)C_n^{+} - \rho(t)C_n^{+}C_n - C_n^{+}C_n\rho(t)\right)$$

~~只有一个粒子的情形，~~ $\cancel{\rho(t) = |\psi(t)\rangle\langle\psi(t)|}$ ~~，并且 H(t) 不含时为 H~~

~~令~~ $\cancel{|\varphi(t)\rangle = e^{iHt}|\psi(t)\rangle}$

~~则~~ $\cancel{|\psi(t)\rangle = e^{-iHt}|\varphi(t)\rangle}$

$\cancel{\rho(t) = e^{-iHt}|\varphi(t)\rangle\langle\varphi(t)|e^{iHt}}$

不是纯态

引入 $R(t)$，使 $\rho(t) = e^{-iHt}R(t)e^{iHt}$，$\cancel{R(t) = |\varphi(t)\rangle\langle\varphi(t)|}$

$$\dot{\rho}(t) = \overset{-iH\rho(t)+\rho(t)iH}{\cancel{(-iH+iH)\rho(t)}} + e^{-iHt}\dot{R}(t)e^{iHt}$$

$$= e^{-iHt}\dot{R}(t)e^{iHt} + -iH\rho(t)+\rho(t)iH$$

$$e^{-iHt}\dot{R}(t)e^{iHt} = -\frac{i}{\hbar}\left(He^{-iHt}R(t)e^{iHt} - e^{-iHt}R(t)e^{iHt}H\right)$$

$$+ -iH\rho(t)+\rho(t)iH \quad + \sum_n\frac{1}{2}\left(2C_n e^{-iHt}R(t)e^{iHt}C_n^{+} - e^{-iHt}R(t)e^{iHt}C_n^{+}C_n - C_n^{+}C_n e^{-iHt}R(t)e^{iHt}\right)$$

左乘 e^{iHt} 右乘 e^{-iHt}，则

$$\dot{R}(t) = -\frac{i}{\hbar}\left(HR(t) - R(t)H\right) + \sum_n\frac{1}{2}\left(2e^{iHt}C_n e^{-iHt}R(t)e^{iHt}C_n^{+}e^{-iHt} - R(t)e^{iHt}C_n^{+}C_n e^{-iHt} - e^{iHt}C_n^{+}C_n e^{-iHt}R(t)\right)$$

$$+ -iHR(t)+R(t)iH$$

令 $D_n = e^{iHt}C_n e^{-iHt}$ $\quad D_n^{+} = e^{iHt}C_n^{+}e^{-iHt}$

则 $\dot{R}(t) = -\frac{i}{\hbar}[H, R(t)] + \sum_n\frac{1}{2}\left(2D_nR(t)D_n^{+} - R(t)D_n^{+}D_n - D_n^{+}D_nR(t)\right)$

$+\frac{i}{\hbar}[H,R(t)]$

注意 $D_n = D_n(t)$ 含时　　另外前面其实应为 $e^{iHt/\hbar}$

若 $C_n = \sqrt{\gamma_{mn}}\,|m\rangle\langle n|$

则 $D_n = e^{i(\omega_m-\omega_n)t} C_n$　　　$D_n^+ = e^{-i(\omega_m-\omega_n)t} C_n^+$

那么 $\dot{R}(t) = \cancel{\frac{i}{\hbar}[H,R(t)]} + \sum_n \frac{1}{2}\left(2C_nR(t)C_n^+ - R(t)C_n^+C_n - C_n^+C_nR(t)\right)$

~~与 $\rho(t)$ 的方程相同~~, $R(0)=\rho(0)$

$P = ||\langle 0|\hat{O}(t)|\psi(t)\rangle||^2$　　$\hat{O}(t)$ 为 $\pi/2$ 脉冲

且 $\hat{O}(t) = e^{-iHt}\,\hat{O}\,e^{iHt}$　　$\hat{O}$ 为 $(\pi/2)_y$ 脉冲

则 $P = ||\langle 0|\, e^{-iHt}\,\hat{O}\,e^{iHt}\,e^{-iHt}|\varphi(t)\rangle||^2$

$= ||\langle 0|\, e^{-i\omega_0 t}\,\hat{O}\,|\varphi(t)\rangle||^2$

$= ||\langle 0|\,\hat{O}\,|\varphi(t)\rangle||^2$