

Notes on Lindblad equations and Davies generator

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1 Lindblad equation

The canonical form of the Lindblad master equation is [Lin76, GKS76],

$$\frac{d}{dt}\rho = \underbrace{-i[H, \rho]}_{\mathcal{L}_H(\rho)} + \underbrace{\sum_{j=1}^J \left(V_j \rho V_j^\dagger - \frac{1}{2} \{V_j^\dagger V_j, \rho\} \right)}_{\mathcal{L}_V(\rho)} =: \mathcal{L}(\rho). \quad (1)$$

Here $H \in \mathbb{C}^{d \times d}$ is the system Hamiltonian, and $V_j \in \mathbb{C}^{d \times d}$ are known as the jump operators that come from the interactions with the environment. The GKLS theorem [Lin76, GKS76] states that if \mathcal{L} is a Lindbladian (also called the Lindblad generator) with the form given in (1), then $\exp(\mathcal{L}t)$ is a quantum channel, which means it is a completely positive trace-preserving (CPTP) map that transforms one density operator into another. It is also contractive under the trace distance (holds for any CPTP map [NC00, Theorem 9.2]): For any two density operators ρ_1, ρ_2 , and any $t > 0$, it holds that

$$\|\exp(\mathcal{L}t)\rho_1 - \exp(\mathcal{L}t)\rho_2\|_1 \leq \|\rho_1 - \rho_2\|_1. \quad (2)$$

Our interest in this semester includes (but not limited to):

1. Using the Lindblad equation as an *algorithmic tool* to prepare a system state $\rho_S \propto f(H)$, such as thermal state [WT23, CKBG23, CKG23] and ground state [DCL23].
2. Using the Lindblad equation as an *algorithmic tool* to approximate the non-equilibrium system bath coupled dynamics. The main results are a type of equivalence theorems, which roughly states that the system dynamics is only determined by the bath correlation function. [MSHP17, TSHP18, TSL⁺19]
3. Using the Lindblad equation as an *algorithmic tool* for classical optimization [CLW⁺23].
4. Understand the performance of the above algorithms for quasi-free and quadratic Lindblad equations [Pro08, PŽ10, BZ22].
5. Understand some of the aspects of the relaxation (“return-to-equilibrium”) and the mixing time of the Lindblad dynamics for ground state and thermal state preparation [Spo77, Tem13, BCG⁺23].

2 Derivation of Lindblad equation

The main reference of this section is [Lid19]. See e.g., [Lid19, Chapter V, VI] for concepts such as Kraus operators, completely positive maps, quantum channels etc. The lecture notes present four different ways of deriving the Lindblad equation: (1) A specific Kraus operator sum (2) Coarse graining assumption (3) Cumulant expansion and coarse graining (4) “Standard” derivation. The length of the derivation increases in this order, and none of them is very satisfactory or concise (perhaps there is none). Here (1) can be viewed a special example of an algorithm for implementing the Lindblad equation, and (2) (3) contain an Assumption ([Lid19, Eq. (301)]), and “It is an interesting open problem to derive rigorous conditions for this to hold from first principles.”

This section will summarize some steps of (4), given in [Lid19, Chapter XV]. The starting point is the system bath coupled Hamiltonian

$$H = H_S + H_B + H_{SB}, \quad (3)$$

The system bath coupling Hamiltonian takes the form

$$H_{SB} = g \sum_{\alpha} A_{\alpha} \otimes B_{\alpha}, \quad (4)$$

where g is called the coupling constant. For simplicity we assume A_{α}, B_{α} are Hermitian and acts on the system and bath degrees of freedom, respectively.

Define

$$\begin{aligned} H_0 &\equiv H_S \otimes I_B + I_S \otimes H_B, \\ U_0(t) &\equiv \exp(-itH_0) = U_S(t) \otimes U_B(t) = e^{-itH_S} \otimes e^{-itH_B}, \\ \tilde{\rho}_{SB}(t) &\equiv U_0^{\dagger}(t) \rho_{SB}(t) U_0(t), \end{aligned} \quad (5)$$

Then $\tilde{\rho}_{SB}(t)$ is the state in the interaction picture. We have the interaction picture Hamiltonian

$$\tilde{H}(t) = U_0^{\dagger}(t) H_{SB} U_0(t) = g \sum_{\alpha} U_S^{\dagger}(t) A_{\alpha} U_S(t) \otimes U_B^{\dagger}(t) B_{\alpha} U_B(t) \equiv g \sum_{\alpha} A_{\alpha}(t) \otimes B_{\alpha}(t). \quad (6)$$

For a sufficiently large bath that is in particular much larger than the system, it is reasonable to assume that while the system undergoes non-trivial evolution, the bath remains unaffected, and hence that the state of the composite system at time t is

$$\tilde{\rho}_{SB}(t) \approx \tilde{\rho}(t) \otimes \rho_B, \quad (7)$$

This is called the *Born approximation*.

We further assume that first moment of the bath state ρ_B vanishes with respect to the bath coupling operator

$$\langle B_{\alpha} \rangle_B := \text{Tr}[B_{\alpha} \rho_B] = 0. \quad (8)$$

We also assume the bath is stationary, i.e., $[H_B, \rho_B] = 0$. This is satisfied if e.g., $\rho_B \propto e^{-\beta H_B}$ is the Gibbs state corresponding to the bath Hamiltonian.

From the Liouville-von Neumann equation

$$\frac{d}{dt} \tilde{\rho}_{SB}(t) = -i [\tilde{H}(t), \tilde{\rho}_{SB}(t)] \quad (9)$$

we have:

$$\tilde{\rho}_{SB}(t) = \rho_{SB}(0) - i \int_0^t ds \left[\tilde{H}(s), \tilde{\rho}_{SB}(s) \right]. \quad (10)$$

Let us now substitute this solution back into the von Neumann equation and take the partial trace:

$$\frac{d}{dt} \tilde{\rho}(t) = \text{Tr}_B \left\{ \frac{d}{dt} \tilde{\rho}_{SB}(t) \right\} = -i \text{Tr}_B \left\{ \left[\tilde{H}(t), \rho_{SB}(0) \right] \right\} + (-i)^2 \text{Tr}_B \left\{ \left[\tilde{H}(t), \int_0^t ds \left[\tilde{H}(s), \tilde{\rho}_{SB}(s) \right] \right] \right\}. \quad (11)$$

Note that

$$\text{Tr}_B \left\{ \left[\tilde{H}(t), \rho_{SB}(0) \right] \right\} = g \sum_{\alpha} [A_{\alpha}(t), \rho_S(0)] \langle B_{\alpha}(t) \rangle_B, \quad (12)$$

and

$$\langle B_{\alpha}(t) \rangle_B = \text{Tr}[U_B^{\dagger}(t) B_{\alpha} U_B(t) \rho_B] = \langle B_{\alpha} \rangle_B = 0. \quad (13)$$

Therefore with a change of variable $\tau = t - s$, and use the Born approximation, the equation of motion of the system density operator becomes

$$\frac{d}{dt} \tilde{\rho}(t) = - \text{Tr}_B \left\{ \left[\tilde{H}(t), \int_0^t d\tau \left[\tilde{H}(t-\tau), \tilde{\rho}(t-\tau) \otimes \rho_B \right] \right] \right\}. \quad (14)$$

Expanding the double commutator, the equation simplifies to

$$\frac{d\tilde{\rho}(t)}{dt} = -g^2 \sum_{\alpha\beta} \int_0^t d\tau \{ \mathcal{B}_{\alpha\beta}(\tau) [A_{\alpha}(t), A_{\beta}(t-\tau) \tilde{\rho}(t-\tau)] + \text{h.c.} \}. \quad (15)$$

Here $\mathcal{B}_{\alpha\beta}(\tau) = \langle B_{\alpha}(\tau) B_{\beta} \rangle_B$ satisfies

$$\mathcal{B}_{\alpha\beta}(-\tau) = \mathcal{B}_{\beta\alpha}^*(\tau). \quad (16)$$

The *Markov approximation* states that the bath has a very short correlation time τ_B , i.e., that the correlation function $\mathcal{B}_{\alpha\beta}(\tau)$ decays rapidly with some characteristic timescale τ_B , e.g., $|\mathcal{B}_{\alpha\beta}(\tau)| \sim e^{-\tau/\tau_B}$. When the simulation time of interest t is much larger than τ_B , we do not need to distinguish $\tilde{\rho}(t-\tau)$ and $\tilde{\rho}(t)$, and can replace the integration range from $[0, t]$ to $[0, \infty)$. This leads to the (interaction picture) *Redfield equation*.

$$\frac{d\tilde{\rho}(t)}{dt} = -g^2 \sum_{\alpha,\beta} \int_0^{\infty} d\tau \{ \mathcal{B}_{\alpha\beta}(\tau) [A_{\alpha}(t), A_{\beta}(t-\tau) \tilde{\rho}(t)] + \text{h.c.} \}. \quad (17)$$

Now we go to the frequency domain by expressing quantities in the system in the eigenbasis of H_S , i.e., $H_S = \sum_a \varepsilon_a |\varepsilon_a\rangle\langle\varepsilon_a|$, then

$$A_{\alpha}(t) = U_S^{\dagger}(t) A_{\alpha} U_S(t) = \sum_{a,b} e^{-i(\varepsilon_b - \varepsilon_a)t} |\varepsilon_a\rangle \langle\varepsilon_a| A_{\alpha} |\varepsilon_b\rangle \langle\varepsilon_b| =: \sum_{\omega = \varepsilon_b - \varepsilon_a} A_{\alpha}(\omega) e^{-i\omega t}. \quad (18)$$

Here $\omega := \varepsilon_b - \varepsilon_a$ is called a *Bohr frequency*, and \sum_{ω} should always be understood as a discrete sum over the Bohr frequencies. Note that for small systems, H_S can be exactly diagonalized, and all Bohr frequencies are known. This is extensively used in the context of e.g., molecular control.

Expressing the commutator in the frequency representation, and define

$$\Gamma_{\alpha\beta}(\omega) := \int_0^\infty d\tau e^{i\omega\tau} \mathcal{B}_{\alpha\beta}(\tau), \quad (19)$$

the Redfield equation becomes

$$\frac{d\tilde{\rho}(t)}{dt} = -g^2 \sum_{\alpha,\beta} \sum_{\omega,\omega'} \left\{ \Gamma_{\alpha\beta}(\omega) e^{i(\omega' - \omega)t} [A_\alpha^\dagger(\omega'), A_\beta(\omega) \tilde{\rho}(t)] + \text{h.c.} \right\}. \quad (20)$$

The Cartesian decomposition of Γ reads

$$\Gamma_{\alpha\beta}(\omega) = \frac{1}{2} \gamma_{\alpha\beta}(\omega) + i S_{\alpha\beta}(\omega), \quad (21)$$

where

$$\gamma_{\alpha\beta}(\omega) = \Gamma_{\alpha\beta}(\omega) + \Gamma_{\beta\alpha}^*(\omega), \quad S_{\alpha\beta}(\omega) = \frac{1}{2i} (\Gamma_{\alpha\beta}(\omega) - \Gamma_{\beta\alpha}^*(\omega)) \quad (22)$$

are Hermitian matrices. This also gives the expression

$$\gamma_{\alpha\beta}(\omega) = \int_0^\infty e^{i\omega\tau} \mathcal{B}_{\alpha\beta}(\tau) d\tau + \int_0^\infty e^{i\omega\tau} \mathcal{B}_{\beta\alpha}^*(\tau) d\tau = \int_{-\infty}^\infty e^{i\omega\tau} \mathcal{B}_{\alpha\beta}(\tau) d\tau, \quad (23)$$

and the inverse Fourier transform is

$$\mathcal{B}_{\alpha\beta}(\tau) = \frac{1}{2\pi} \int_{-\infty}^\infty e^{-i\omega'\tau} \gamma_{\alpha\beta}(\omega') d\omega'. \quad (24)$$

The matrices γ, S are related to each other via the Hilbert transform

$$S_{\alpha\beta}(\omega) = \frac{1}{2\pi} \int_{-\infty}^\infty \gamma_{\alpha\beta}(\omega') \mathcal{P} \left(\frac{1}{\omega - \omega'} \right) d\omega'. \quad (25)$$

We make the final approximation called the *rotating wave approximation* (also called the *secular approximation*), which states that the off-diagonal term in frequency $\omega \neq \omega'$ can be neglected. We arrive at the interaction picture Lindblad equation

$$\frac{d\tilde{\rho}(t)}{dt} = -i [H_{\text{LS}}, \tilde{\rho}(t)] + g^2 \sum_{\omega} \sum_{\alpha\beta} \gamma_{\alpha\beta}(\omega) \left(A_\beta(\omega) \tilde{\rho}(t) A_\alpha^\dagger(\omega) - \frac{1}{2} \{ A_\alpha^\dagger(\omega) A_\beta(\omega), \tilde{\rho}(t) \} \right) := \tilde{\mathcal{L}}[\rho]. \quad (26)$$

Here

$$H_{\text{LS}} \equiv g^2 \sum_{\omega} \sum_{\alpha\beta} S_{\alpha\beta}(\omega) A_\alpha^\dagger(\omega) A_\beta(\omega) \quad (27)$$

is called the Lamb shift. The Lamb shift is Hermitian. $\tilde{\mathcal{L}}$ is the Lindblad generator in the interaction picture.

Transform back to Schrödinger picture via $\rho(t) = U_S(t) \tilde{\rho}(t) U_S^\dagger(t)$, we obtain

$$\frac{d\rho}{dt} = -i [H_S + H_{\text{LS}}, \rho] + g^2 \sum_{\omega} \sum_{\alpha\beta} \gamma_{\alpha\beta}(\omega) \left(A_\beta(\omega) \rho A_\alpha^\dagger(\omega) - \frac{1}{2} \{ A_\alpha^\dagger(\omega) A_\beta(\omega), \rho \} \right) := \mathcal{L}[\rho]. \quad (28)$$

Here \mathcal{L} is the Lindblad generator.

The following two facts hold.

Fact 1. *The Lamb shift commutes with the system Hamiltonian.*

$$[H_{\text{LS}}, H_S] = 0. \quad (29)$$

Fact 2. *The Lindblad coupling coefficient matrix is positive semidefinite:*

$$\gamma(\omega) \succeq 0. \quad (30)$$

Eq. (30) allows us to orthogonally $\gamma(\omega) = W(\omega)W(\omega)^\dagger$. Then define $V_i(\omega) = \sum_\alpha A_\alpha(\omega)W(\omega)_{\alpha i}^*$, the Lindblad equation becomes

$$\frac{d\rho}{dt} = -i[H_S + H_{\text{LS}}, \rho] + g^2 \sum_\omega \sum_i \left(V_i(\omega) \rho V_i^\dagger(\omega) - \frac{1}{2} \{ V_i^\dagger(\omega) V_i(\omega), \rho \} \right), \quad (31)$$

which takes the canonical form in Eq. (1).

Remark 3. *For all the approximations to hold, physical intuition suggests that the coupling constant needs to be sufficiently small:*

$$g \ll 1/\tau_B < \min_{\omega \neq \omega'} |\omega - \omega'|. \quad (32)$$

We will not go into the justification of this assumption. However, $\min_{\omega \neq \omega'} |\omega - \omega'|$ can vanishing exponentially with respect to the system size, and hence this is a very strong assumption for large systems.

Remark 4. *The derivation above is perturbatively valid for any bath and system-bath coupling operator. However, if the bath Hamiltonian is quadratic, the coupling (bath part) is linear, and the initial state in the bath $\rho_B(0)$ is a Gaussian state, then the system dynamics is fully determined by bath correlation functions (a time-dependent matrix). This allows us to design Lindblad operators to match the bath correlation function to yield exact dynamics in the system. Such non-perturbative equivalence theorems are shown in e.g. [TSHP18].*

3 Davies generator

The folklore theorem in physics is that if $\rho_B \propto e^{-\beta H_B}$ is a Gibbs state, then the system tends to equilibrate to a Gibbs state

$$\rho_G \propto e^{-\beta H_S} \quad (33)$$

By putting the system “in a fridge”, i.e., $\beta \gg 1$ for the bath, we will show that the fixed point of the Lindblad dynamics with a Davies generator is ρ_G with the same inverse temperature. The speed for the cooling process is still an ongoing research direction with many recent progresses.

When ρ_B is a Gibbs state, the bath correlation function satisfies

$$\begin{aligned} \langle B_a(\tau) B_b \rangle &= \text{Tr} \left[\rho_B U_B^\dagger(\tau) B_a U_B(\tau) B_b \right] = \frac{1}{Z} \text{Tr} \left[B_b e^{-(\beta - i\tau) H_B} B_a e^{-i\tau H_B} \right] \\ &= \frac{1}{Z} \text{Tr} \left[B_b e^{i(\tau + i\beta) H_B} B_a e^{-i(\tau + i\beta) H_B} e^{-\beta H_B} \right] = \text{Tr} \left[\rho_B B_b U_B^\dagger(\tau + i\beta) B_a U_B(\tau + i\beta) \right] \\ &= \langle B_b B_a(\tau + i\beta) \rangle_B. \end{aligned} \quad (34)$$

Similarly

$$\langle B_a(\tau)B_b \rangle_B = \langle B_b(-\tau - i\beta)B_a \rangle_B. \quad (35)$$

These conditions are called the *Kubo-Martin-Schwinger* (KMS) condition.

From the KMS condition

$$\gamma_{ab}(\omega) = \int_{-\infty}^{\infty} d\tau e^{i\omega\tau} \langle B_a(\tau)B_b(0) \rangle_B = \int_{-\infty}^{\infty} d\tau e^{i\omega\tau} \langle B_b(-\tau - i\beta)B_a(0) \rangle_B \quad (36)$$

If in addition the correlation function is analytic in the strip between $\tau = -i\beta$ and $\tau = 0$, we can perform a contour deformation, the Fourier transform of the bath correlation function satisfies the frequency domain KMS condition:

$$\gamma_{ab}(-\omega) = e^{-\beta\omega} \gamma_{ba}(\omega). \quad (37)$$

A Lindblad generator $\mathcal{L}[\rho]$ in Eq. (31) satisfying the KMS condition Eq. (37) is called a *Davies generator*.

Example 5. Let $\gamma(\omega)$ be a scalar. Then the choice

$$\gamma(\omega) = \frac{1}{1 + e^{-\beta\omega}} \quad (38)$$

is called Glauber, and the choice

$$\gamma(\omega) = \min\{1, e^{-\beta\omega}\} \quad (39)$$

is called Metropolis–Hastings. \diamond

Remark 6. *From the literature it is unclear to me whether Davies generator must involve the Lamb shift term specified in Eq. (27).*

Direct calculation shows that the frequency dependent system coupling operator satisfies.

$$A_\alpha(\omega)\rho_G = e^{-\beta\omega}\rho_G A_\alpha(\omega), \quad A_\alpha^\dagger(\omega)\rho_G = e^{\beta\omega}\rho_G A_\alpha^\dagger(\omega), \quad [A_\alpha^\dagger(\omega)A_\beta(\omega), \rho_G] = 0. \quad (40)$$

This is important for showing the following fact:

Fact 7. *The Gibbs state is stationary with respect to the Davies generator, i.e.,*

$$\mathcal{L}[\rho_G] = 0. \quad (41)$$

4 Pauli master equation and quantum detailed balance condition

The population in the a th energy eigenbasis state is:

$$p_a(t) = \langle \varepsilon_a | \rho(t) | \varepsilon_a \rangle = \rho_{aa}(t) = \text{Tr} [\Pi_a \rho]. \quad (42)$$

It turns out that the populations in the energy eigenbasis are decoupled from the coherences (off diagonal elements) in the same eigenbasis. The resulting equation is called the *Pauli master*

equation. It shows that viewed in the eigenbasis of H_S , Lindblad equation with a Davies generator has a fundamentally classical and Monte-Carlo nature.

From Eq. (29), the coherent term $H_S + H_{LS}$ can be diagonalized in the energy eigenbasis. Therefore

$$\langle \varepsilon_a | [H_S + H_{LS}, \rho] | \varepsilon_a \rangle = 0. \quad (43)$$

Then

$$\dot{p}_a = g^2 \sum_{\alpha\beta} \sum_{\omega} \gamma_{\alpha\beta}(\omega) \left\langle \varepsilon_a \left| A_{\beta}(\omega) \rho A_{\alpha}^{\dagger}(\omega) - \frac{1}{2} \{A_{\alpha}^{\dagger}(\omega) A_{\beta}(\omega), \rho\} \right| \varepsilon_a \right\rangle. \quad (44)$$

Recall that

$$A_{\beta}(\omega) = \sum_{\omega=\varepsilon_b-\varepsilon_a} A_{ab,\beta} |\varepsilon_a\rangle\langle\varepsilon_b|, \quad A_{\alpha}^{\dagger}(\omega) = \sum_{\omega=\varepsilon_b-\varepsilon_a} A_{ab,\alpha}^* |\varepsilon_b\rangle\langle\varepsilon_a| = \sum_{\omega=\varepsilon_b-\varepsilon_a} A_{ba,\alpha} |\varepsilon_b\rangle\langle\varepsilon_a|. \quad (45)$$

Direct computation shows

$$\begin{aligned} & \langle \varepsilon_a | A_{\beta}(\omega) \rho A_{\alpha}^{\dagger}(\omega) | \varepsilon_a \rangle \\ &= \sum_{\omega=\varepsilon_{a'}-\varepsilon_a} A_{aa',\beta} \rho_{a'b'} \sum_{\omega=\varepsilon_{b'}-\varepsilon_a} A_{b'a,\alpha} \\ &= \sum_{\omega=\varepsilon_{a'}-\varepsilon_a} A_{aa',\beta} p_{a'} A_{a'a,\alpha}. \end{aligned} \quad (46)$$

Here the crucial fact is that the double sum of the Bohr frequencies reduces to a single sum, which means that it only depends on the diagonal entries of the density matrix $p_{a'}$. We have also used that A is Hermitian. Similarly

$$\frac{1}{2} \langle \varepsilon_a | \{A_{\alpha}^{\dagger}(\omega) A_{\beta}(\omega), \rho\} | \varepsilon_a \rangle = \sum_{\omega=\varepsilon_a-\varepsilon_{a'}} A_{aa',\alpha} A_{a'a,\beta} p_a. \quad (47)$$

Now define a transition matrix P as

$$W(a, a') := \sum_{\alpha\beta} \gamma_{\alpha\beta}(\varepsilon_{a'} - \varepsilon_a) A_{a'a,\alpha} A_{aa',\beta} \quad (48)$$

This gives the Pauli master equation

$$\begin{aligned} \dot{p}_a &= \sum_{\alpha\beta} \sum_{a'} \gamma_{\alpha\beta}(\varepsilon_{a'} - \varepsilon_a) A_{a'a,\alpha} A_{aa',\beta} p_{a'} - \gamma_{\alpha\beta}(\varepsilon_a - \varepsilon_{a'}) A_{aa',\alpha} A_{a'a,\beta} p_a \\ &= \sum_{a'} W(a, a') p_{a'} - W(a', a) p_a. \end{aligned} \quad (49)$$

This is a closed set of rate equations for the populations. Since $\gamma(\omega) \succeq 0$, we have $W(a, a') \geq 0$ for any a, a' . So the Pauli master equation describes a continuous-time Markov chain.

Now from the KMS condition, the transition matrix satisfies

$$W(a, a') = \sum_{\alpha\beta} e^{-\beta(\varepsilon_a - \varepsilon_{a'})} \gamma_{\beta\alpha}(\varepsilon_a - \varepsilon_{a'}) A_{a'a,\alpha} A_{aa',\beta} = e^{-\beta(\varepsilon_a - \varepsilon_{a'})} W(a', a). \quad (50)$$

This is a *detailed balance condition*. This immediately shows that the Gibbs state

$$p_a = \pi_a = \frac{e^{-\beta\varepsilon_a}}{Z} \quad (51)$$

is a stationary point of the Pauli master equation, and

$$W(a, a')\pi_{a'} = W(a', a)\pi_a. \quad (52)$$

The Pauli master equation can be written more compactly as

$$\partial_t p(t) = Lp(t), \quad L_{ab} = W(a, b) - \delta_{ab} \sum_{b'} W(b', a). \quad (53)$$

The matrix L is called a generator or the Q matrix. Then $p(t) = e^{Lt}p(0)$. If we are interested in an observable O with its average $\sum_a O_a p_a(t)$, we can equivalently evolve the operator as

$$\sum_a O_a p_a(t) = O^\top e^{Lt} p = (e^{L^\top t} O)^\top p(0) =: O(t)^\top p(0). \quad (54)$$

So $O(t)$ satisfies the equation

$$\partial_t O(t) = L^\top O(t). \quad (55)$$

Define the π -inner product $\langle f, g \rangle_\pi = \sum_a f_a g_a \pi_a$, then

$$\langle f, L^\top g \rangle_\pi = \sum_{a, a'} f_a \pi_a W(a', a) g(a') - \sum_{ab'} f_a \pi_a g_a \sum_{b'} W(b', a), \quad (56)$$

and

$$\langle L^\top f, g \rangle_\pi = \sum_{a, a'} W(a, a') f_a \pi_{a'} g(a') - \sum_{ab'} f_a \pi_a g_a \sum_{b'} W(b', a) \quad (57)$$

Therefore the detailed balance condition is satisfied if and only if L^\top is symmetric with respect to the π -inner product. The mapping $(f, g) \mapsto \langle f, L^\top g \rangle_\pi$ is called a *Dirichlet form*.

When $\pi_a > 0$ for any a , we can define an invertible mapping $[T(f)]_a = \sqrt{\pi_a} f_a$. Then

$$D = TL^\top T^{-1} \quad (58)$$

is called the *discriminate matrix* or *discriminant*. Then for any $f, g \in \mathbb{R}^N$,

$$\langle Tf, DTg \rangle = \langle f, T^2 L^\top g \rangle = \langle f, L^\top g \rangle_\pi = \langle L^\top f, g \rangle_\pi = \langle DTf, Tg \rangle. \quad (59)$$

Since T is invertible, D is symmetric with respect to the ℓ^2 inner product. Hence all eigenvalues of L, L^\top are real.

5 Relaxation and mixing time

The Lindblad dynamics has an attractor

$$\lim_{t \rightarrow \infty} \rho(t) = e^{\mathcal{L}t} \rho(0) = \sigma, \quad \forall \rho(0), \quad (60)$$

then the system is *relaxing*. By uniqueness, for Davies generator, $\sigma = \rho_G$.

If a system is relaxing, then the *relaxation time*, or *mixing time* t_{mix} is the time to reach ϵ -close to its stationary distribution:

$$t_{\text{mix}}(\epsilon) = \inf \{t \geq 0 \mid \|e^{\mathcal{L}t}(\rho) - \sigma\|_1 \leq \epsilon, \quad \forall \rho \in \mathcal{D}(\mathcal{H})\}. \quad (61)$$

The Lindblad generator acts linearly on ρ and can be identified with a matrix when choosing a proper basis. Here $\|A\|_1 = \text{Tr}|A| = \text{Tr}[\sqrt{A^\dagger A}]$ is the trace norm.

The spectral gap of the vectorized Lindbladian denoted by \mathbf{L} is defined to be the negative real part of the 2nd largest eigenvalue,

$$\Delta_{\mathcal{L}} = -\text{Re}[\lambda_1(\mathbf{L})]. \quad (62)$$

Since the Lindbladian dynamics is contractive, the spectral gap must be non-negative. However, assuming the system is relaxing, then the spectral gap is positive (this rules out purely imaginary eigenvalues. In fact, later we will see that for detailed balanced Lindbladian dynamics, all eigenvalues are real). Then the mixing time is $\mathcal{O}(\log(1/\epsilon)/\Delta_{\mathcal{L}})$.

Can we study the convergence of the Lindblad equation with a Davies generator in terms of the convergence of the Pauli master equation? Unfortunately, Pauli master equation provides some hints but the gap between the convergence of the quantum versus classical setting can be arbitrarily large (Remark 18).

6 Detailed balanced Lindbladian

A more intrinsic definition of the quantum detailed balance condition for Lindbladians can be formulated using the quantum version of the Dirichlet form. The following discussion follows [WT23, Section 2], which summarizes a number of recent progresses, e.g., by Carlen and Maas [CM20].

Given an invertible density operator $\sigma \in L(\mathcal{H})$, for any $s \in [0, 1]$ one can define a σ^s -inner product by

$$\langle A, B \rangle_s = \langle A, \sigma^{1-s} B \sigma^s \rangle. \quad (63)$$

Here $\langle A, B \rangle$ denotes the Hilbert-Schmidt (HS) inner product. As special cases, when $s = 1$,

$$\langle A, B \rangle_1 = \langle A, B \sigma \rangle \quad (64)$$

is called the Gelfand-Naimark-Segal (GNS) inner product. When $s = \frac{1}{2}$,

$$\langle A, B \rangle_{\frac{1}{2}} = \left\langle A, \sigma^{\frac{1}{2}} B \sigma^{\frac{1}{2}} \right\rangle \quad (65)$$

is called the Kubo-Martin-Schwinger (KMS) inner product (should be distinguished from the KMS condition, which is a periodic type boundary condition for the correlation function of a thermal bath).

Let $\mathcal{L} : L(\mathcal{H}) \rightarrow L(\mathcal{H})$ be any linear operator and \mathcal{L}^\dagger be its adjoint with respect to the HS inner product. Then

$$\langle A, \mathcal{L}^\dagger[B] \rangle_s = \langle \sigma^{1-s} A \sigma^s, \mathcal{L}^\dagger[B] \rangle = \langle \mathcal{L}[\sigma^{1-s} A \sigma^s], B \rangle. \quad (66)$$

Define a mapping $\Delta_s[A] = \sigma^{1-s} A \sigma^s$. Then

$$\mathcal{L}[\sigma^{1-s} A \sigma^s] = \sigma^{1-s} \mathcal{L}^\dagger[A] \sigma^s, \quad (67)$$

or

$$\mathcal{L} \circ \Delta_s = \Delta_s \circ \mathcal{L}^\dagger. \quad (68)$$

if and only if

$$\langle A, \mathcal{L}^\dagger[B] \rangle_s = \langle \mathcal{L}[\sigma^{1-s} A \sigma^s], B \rangle = \langle \mathcal{L}^\dagger[A], \sigma^{1-s} B \sigma^s \rangle = \langle \mathcal{L}^\dagger[A], B \rangle_s. \quad (69)$$

The condition Eq. (68) is called the σ^s -detailed balance condition.

This calculation also proves

Proposition 8. *A Lindbladian \mathcal{L} satisfies σ^s -detailed balance condition if and only if \mathcal{L}^\dagger is symmetric with respect to the σ^s -inner product.*

Interestingly, the quantum detailed balance condition for all σ^s -inner products are equivalent. The following theorem is given by a [CM20, Lemma 2.1], which is a special case of [CM17, Theorem 2.9].

Theorem 9. *Let \mathcal{L} be σ^s -detailed balanced for any $s \in [0, 1] \setminus \{\frac{1}{2}\}$, then \mathcal{L} is σ^s -detailed balanced for all $s \in [0, 1]$.*

For instance, the detailed balance condition in [CKG23] corresponds to the KMS inner product with $s = \frac{1}{2}$, which is a weaker version of the detailed balance. The quantum detailed balance condition in the literature is often the stronger version with $s = 1$. This is also called σ -GNS detailed balanced.

Proposition 10. *Let \mathcal{L} be σ^s -detailed balanced for any $s \in [0, 1]$. Then $\mathcal{L}(\sigma) = 0$.*

Proof. The trace preserving condition implies $\mathcal{L}^\dagger(I) = 0$. Then

$$0 = \langle \mathcal{L}^\dagger(I), A \rangle_s = \langle I, \mathcal{L}^\dagger(A) \rangle_s = \text{Tr}(\sigma \mathcal{L}^\dagger(A)) = \text{Tr}(\mathcal{L}(\sigma) A). \quad (70)$$

Since A is arbitrary, we have $\mathcal{L}(\sigma) = 0$. \square

The concept of σ^s -detailed balance can be generalized from generators to quantum channels.

Definition 11. *A quantum channel \mathcal{Q} satisfies the σ^s -detailed balance condition if its Hilbert-Schmidt adjoint \mathcal{Q}^\dagger is symmetric with respect to the σ^s -inner product.*

Proposition 12. *Let \mathcal{Q} be σ^s -detailed balanced quantum channel for any $s \in [0, 1]$. Then $\mathcal{Q}(\sigma) = \sigma$.*

Proof. The trace preserving condition implies $\mathcal{Q}^\dagger(I) = I$. Then

$$\text{Tr}[\sigma A] = \langle \mathcal{Q}^\dagger(I), A \rangle_s = \langle I, \mathcal{Q}^\dagger(A) \rangle_s = \text{Tr}(\sigma \mathcal{Q}^\dagger(A)) = \text{Tr}(\mathcal{Q}(\sigma) A). \quad (71)$$

Since A is arbitrary, we have $\mathcal{Q}(\sigma) = \sigma$. \square

Example 13 (KMS does not imply GNS [TKR⁺10, Section IV]). Consider a channel of Kraus form $\mathcal{Q}[\rho] = \sum_{i=1,2} A_i \rho A_i^\dagger$ with

$$A_1 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 0 & 0 \end{pmatrix}, \quad A_2 = \frac{1}{2} \begin{pmatrix} 1 & -1 \\ 1 & -1 \end{pmatrix}. \quad (72)$$

For

$$\sigma = \frac{1}{6} \begin{pmatrix} 5 & 1 \\ 1 & 1 \end{pmatrix}, \quad (73)$$

direct calculation shows $\mathcal{Q}[\sigma] = \sigma$. Furthermore, σ is the unique fixed point of \mathcal{Q} , and

$$\sqrt{\sigma} = \frac{1}{2\sqrt{15}} \begin{pmatrix} 7 & 1 \\ 1 & 3 \end{pmatrix}. \quad (74)$$

Then

$$\mathcal{T} = \Delta_{\frac{1}{2}} \circ \mathcal{Q}^\dagger \circ (\Delta_{\frac{1}{2}})^{-1} \circ \mathcal{Q} \quad (75)$$

has a Kraus form and is completely positive. To show \mathcal{T} is trace preserving, use $\Delta_{\frac{1}{2}}(I) = \sigma$. Then for any ρ ,

$$\text{Tr}[\mathcal{T}\rho] = \text{Tr}[\Delta_{\frac{1}{2}} \circ \mathcal{Q}^\dagger \circ (\Delta_{\frac{1}{2}})^{-1} \circ \mathcal{Q}[\rho]] = \text{Tr}[\sigma \mathcal{Q}^\dagger \circ (\Delta_{\frac{1}{2}})^{-1} \circ \mathcal{Q}[\rho]] = \text{Tr}[\sigma (\Delta_{\frac{1}{2}})^{-1} \circ \mathcal{Q}[\rho]] = \text{Tr}[\mathcal{Q}[\rho]] = \text{Tr}[\rho]. \quad (76)$$

So \mathcal{T} is a quantum channel.

It is $\sigma^{\frac{1}{2}}$ -detailed balanced by construction, i.e., $\mathcal{T} \circ \Delta_{\frac{1}{2}} = \Delta_{\frac{1}{2}} \circ \mathcal{T}^\dagger$.

Direct calculation shows

$$\mathcal{T} \circ \Delta_1(X) - \Delta_1 \circ \mathcal{T}^\dagger(X) = \frac{1}{300} \begin{pmatrix} 7 X_{12} & 49 X_{21} - 7 X_{11} + 7 X_{22} \\ -49 X_{12} & -7 X_{12} \end{pmatrix} \neq 0. \quad (77)$$

So \mathcal{T} is not σ -detailed balanced. (Interesting to note that $\mathcal{G} = \Delta_1 \circ \mathcal{Q}^\dagger \circ (\Delta_1)^{-1} \circ \mathcal{Q}$ is GNS-symmetric but it is not a quantum channel).

◇

The following theorem shows that a detailed balanced Lindbladian is a Davies generator, i.e., it can be derived from a thermal bath.

Theorem 14 ([CM20, Theorem 2.4]). *If a Lindbladian \mathcal{L} is σ -GNS detailed balanced and let $\sigma = e^{-h}$. Then \mathcal{L} is in the following canonical form*

$$\mathcal{L}(\rho) = \sum_{\alpha} c_{\alpha} \mathcal{L}_{\alpha}(\rho), \quad c_{\alpha} > 0. \quad (78)$$

with

$$\mathcal{L}_{\alpha}(\rho) = \sum_{\omega} \gamma_{\alpha}(\omega) \left(A_{\alpha}(\omega) \rho A_{\alpha}^{\dagger}(\omega) - \frac{1}{2} \{ A_{\alpha}^{\dagger}(\omega) A_{\alpha}(\omega), \rho \} \right). \quad (79)$$

For each α , the summation index ω runs over all different Bohr frequencies of h . The operators $A_{\alpha}(\omega)$ and scalars $\gamma_{\alpha}(\omega)$ satisfy

$$\begin{aligned} A_{\alpha}(\omega) &= A_{\alpha}^{\dagger}(-\omega) \\ A_{\alpha}(\omega) \sigma &= e^{-\omega} \sigma A_{\alpha}(\omega) \\ \gamma_{\alpha}(\omega) &\geq 0 \\ \gamma_{\alpha}(-\omega) &= e^{-\omega} \gamma_{\alpha}(\omega). \end{aligned} \quad (80)$$

Due to the canonical form, the Pauli master equation satisfies the detailed balance condition. This also establishes the connection between the quantum σ^s -detailed balance condition and the classical detailed balance condition.

Remark 15. *The structure of a single sum over Bohr frequencies implies that a “secular approximation” has been done. This is sometimes regarded as a theoretical evidence that the GNS detailed balance is an idealized construction and is difficult to be exactly implement in practice. It seems to be an open question whether the KMS detailed balanced Lindbladian can have such a concrete canonical form.*

7 Variational characterization of spectral gap

Vectorization is not the only way for computing the spectral gap of \mathcal{L} . If \mathcal{L} is σ^s -detailed balanced for any $0 \leq s \leq 1$, then Theorem 9 states that it is $\sigma^{\frac{1}{2}}$, or KMS-detailed balanced. Define a shorthand notation $T = \Delta_{\frac{1}{2}}$, which satisfies

$$T(\rho) = \sigma^{\frac{1}{4}} \rho \sigma^{\frac{1}{4}}. \quad (81)$$

The KMS detailed balance condition states

$$\mathcal{L} \circ T^2 = T^2 \circ \mathcal{L}^\dagger, \quad (82)$$

We can then construct

$$\mathcal{K} = \frac{1}{2} (T \circ \mathcal{L}^\dagger \circ T^{-1} + T^{-1} \circ \mathcal{L} \circ T) = T \circ \mathcal{L}^\dagger \circ T^{-1} = T^{-1} \circ \mathcal{L} \circ T, \quad (83)$$

which is similar to \mathcal{L} . Note that $\mathcal{K}(\sqrt{\sigma}) = 0$. Furthermore, \mathcal{K} is self-adjoint with respect to the HS inner product $\langle \cdot, \cdot \rangle$. The mapping $\mathcal{Q} = I + \mathcal{K}$ is called the *quantum discriminate*.

This proves that all eigenvalues of \mathcal{L} are real, and the spectral gap can be characterized variationally by the Courant-Fischer minimax principle

$$\lambda = \min_{f, \langle \sqrt{\sigma}, f \rangle = 0} \frac{-\langle f, \mathcal{K}f \rangle}{\langle f, f \rangle} = \min_{f, \text{Tr}[\sqrt{\sigma}f] = 0} \frac{-\langle f, \mathcal{K}f \rangle}{\langle f, f \rangle - \langle \sqrt{\sigma}, f \rangle^2} \quad (84)$$

Note that both the numerator and the denominator are invariant with respect to the transformation $f \rightarrow f + c\sqrt{\sigma}$. So the orthogonality constraint can be dropped. Finally, letting $f = T(g)$, we find

$$\langle f, \mathcal{K}f \rangle = \langle T(g), T \circ \mathcal{L}^\dagger(g) \rangle = \langle g, \mathcal{L}^\dagger(g) \rangle_{\frac{1}{2}}, \quad (85)$$

and

$$\langle f, f \rangle - \langle \sqrt{\sigma}, f \rangle^2 = \langle g, g \rangle_{\frac{1}{2}} - \text{Tr}[\sigma g]^2 =: \text{Var}(g). \quad (86)$$

So we obtain the following result.

Proposition 16 (Variational characterization of the spectral gap). *The spectral gap of a σ^s -detailed balanced Lindbladian \mathcal{L} can be expressed in terms of the Dirichlet form as*

$$\Delta_{\mathcal{L}} = \inf_f \frac{-\langle f, \mathcal{K}f \rangle}{\langle f, f \rangle - \langle \sqrt{\sigma}, f \rangle^2} = \inf_g \frac{-\langle g, \mathcal{L}^\dagger(g) \rangle_{\frac{1}{2}}}{\text{Var}(g)}. \quad (87)$$

On the other hand, let $g = T^{-2}(\rho - \sigma)$. Then $\text{Tr}[\sigma g] = 0$, and

$$\text{Var}(g) = \text{Tr}[(\rho - \sigma)T^{-2}(\rho - \sigma)] = \text{Tr}[(\rho - \sigma)\Delta_{\frac{1}{2}}^{-1}(\rho - \sigma)] = \text{Tr}[\rho\sigma^{-\frac{1}{2}}\rho\sigma^{-\frac{1}{2}}] - 1 =: \chi^2(\rho, \sigma) \quad (88)$$

is called the χ^2 -divergence.

Now in the Lindblad dynamics, let $g(t) = T^{-2}(\rho(t) - \sigma)$. Using $L^\dagger \circ T^{-2}(\sigma) = L^\dagger(I) = 0$, the equation of motion for $g(t)$ is

$$\partial_t g(t) = T^{-2}\mathcal{L}(\rho(t)) = \mathcal{L}^\dagger \circ T^{-2}(\rho(t)) = \mathcal{L}^\dagger(g(t)). \quad (89)$$

Then

$$\partial_t \text{Var}(g(t)) = \langle \mathcal{L}^\dagger(g(t)), g(t) \rangle_{\frac{1}{2}} + \langle g(t), \mathcal{L}^\dagger(g(t)) \rangle_{\frac{1}{2}} = 2 \langle g, \mathcal{L}^\dagger(g) \rangle_{\frac{1}{2}}. \quad (90)$$

By the variational characterization,

$$\partial_t \text{Var}(g(t)) \leq -2\Delta_{\mathcal{L}} \partial_t \text{Var}(g(t)). \quad (91)$$

So

$$\chi^2(\rho(t), \sigma) \leq \chi^2(\rho(0), \sigma) e^{-2\Delta_{\mathcal{L}} t}. \quad (92)$$

Proposition 17 ([TKR⁺10, Lemma 5]). *For any density operators ρ, σ ,*

$$\|\rho - \sigma\|_1^2 \leq \chi^2(\rho, \sigma). \quad (93)$$

The value of $\chi^2(\rho, \sigma)$ is maximized when ρ is a projector onto the subspace corresponding to the smallest eigenvalue of σ denoted by σ_{\min} , and the maximal value is $\sigma_{\min}^{-1} - 1$. This proves

$$\|\rho(t) - \sigma\|_1 \leq \sqrt{\chi^2(\rho(0), \sigma)} e^{-\Delta_{\mathcal{L}} t} < \sqrt{1/\sigma_{\min}} e^{-\Delta_{\mathcal{L}} t}. \quad (94)$$

For a finite temperature system, $\sigma_{\min} = e^{-\beta\|H_S\|}/Z_\beta$, and this gives

$$\|\rho_t - \sigma\|_1 \leq Z_\beta e^{\beta\|H_S\|} e^{-\Delta_{\mathcal{L}} t}. \quad (95)$$

So the bound is only meaningful in the high temperature or the asymptotic $t \rightarrow \infty$ regime.

Remark 18 (Spectral gap of classical and quantum evolution). *Recall that the Pauli master equation describes a classical Markov process with spectral gap $\Delta_{\mathcal{L}, \text{cl}}$. Is it possible to show that $\Delta_{\mathcal{L}, \text{cl}} = \Delta_{\mathcal{L}}$, or at least use $\Delta_{\mathcal{L}, \text{cl}}$ to derive a generically useful lower bound for the spectral gap. Unfortunately this is not true. See a counterexample in [Tem13, Section III.A] where $\Delta_{\mathcal{L}} = \Delta_{\mathcal{L}, \text{cl}}/N$ (N is the Hilbert space dimension). This highlights the importance of the decoherence of the off-diagonal terms in the density matrix (in the energy eigenbasis).*

8 Log-Sobolev inequalities

Spectral gap is not the only way of bounding the mixing time. The relative entropy between two quantum states ρ, σ is

$$D(\rho\|\sigma) = \text{Tr}[\rho(\log(\rho) - \log(\sigma))]. \quad (96)$$

The trace norm can be bounded by the relative entropy (called the *quantum Pinsker inequality*) as

$$\|\rho - \sigma\|_1 \leq 2D(\rho\|\sigma). \quad (97)$$

If the following bound can be established for some $\alpha > 0$ (called *modified log-Sobolev inequality* [BCG⁺23]),

$$2\alpha D(\rho_t\|\sigma) \leq -\text{Tr}[\mathcal{L}(\rho_t)(\log(\rho_t) - \log(\sigma))], \quad (98)$$

then compare it with the derivative of the relative entropy (also called the *entropy production*)

$$-\partial_t D(\rho_t\|\sigma) = -\text{Tr}[\mathcal{L}(\rho_t)(\log(\rho_t) - \log(\sigma))] \quad (99)$$

we have

$$\partial_t D(\rho_t\|\sigma) \leq -2\alpha D(\rho_t\|\sigma). \quad (100)$$

This gives the estimate:

$$\|\rho_t - \sigma\|_1 \leq \sqrt{2D(\rho_0\|\sigma)}e^{-\alpha t}. \quad (101)$$

The value of $D(\rho_0\|\sigma)$ is maximized when ρ_0 is a projector onto the subspace corresponding to the smallest eigenvalue of σ denoted by σ_{\min} , and the maximal value is $\log(1/\sigma_{\min})$. Hence

$$\|\rho_t - \sigma\|_1 \leq \sqrt{2\log(1/\sigma_{\min})}e^{-\alpha t}. \quad (102)$$

For a finite temperature system, $\sigma_{\min} = e^{-\beta\|H_S\|}/Z_\beta$, and the modified log-Sobolev inequality states

$$\|\rho_t - \sigma\|_1 \leq \sqrt{2(\log Z_\beta + \beta\|H_S\|)}e^{-\alpha t}, \quad (103)$$

and the preconstant is expected to grow only polynomially in the system size as well as the inverse temperature. This is a significant improvement over the spectral gap bound, if $\alpha = \Delta_{\mathcal{L}}$. However, it is likely that in practice $\alpha < \Delta_{\mathcal{L}}$, then the log-Sobolev estimate becomes asymptotically weaker.

Remark 19. *In the discussion of mixing time, σ^{-1} (or its fractional power) is repeatedly used. So the analysis only holds for a system at the finite temperature. If σ is the ground state, then σ_{\min}^{-1} blows up. No theoretical tools are available except for exactly solvable systems (reaching the low temperature limit is also hard for classical Markov chains).*

Remark 20. *Somewhat confusingly, the log-Sobolev inequality establishes a similar entropy production procedure but for $\text{Ent}_1(f)$ defined as, which is called the L^1 relative entropy, see [KT13].*

$$\text{Ent}_1(f) = \text{Tr}\left[\Delta_{\frac{1}{2}}(f)\left(\log\left(\Delta_{\frac{1}{2}}(f)\right) - \log(\sigma)\right)\right] - \text{tr}\left[\Delta_{\frac{1}{2}}(f)\right]\log\left(\text{Tr}\left[\Delta_{\frac{1}{2}}(f)\right]\right) \quad (104)$$

Note that

$$\text{Ent}_1(\Delta_{\frac{1}{2}}^{-1}f) = D(\rho\|\sigma). \quad (105)$$

The log-Sobolev inequality is of the form

$$\partial_t \text{Ent}_1(\rho_t) \leq 2\alpha D \text{Ent}_1(\rho_t). \quad (106)$$

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