LECTURE NOTES ON "LOWER BOUNDS TO THE SPECTRAL GAP OF DAVIES GENERATORS" BY K. TEMME

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When I started writing this notes, I mostly followed Temme's presentation but as I wrote, I realized it's a bit cleaner to do things from a more general perspective.

1. Introduction

Throughout this note, let $\mathcal{H}$ denote the set of (trace class) linear operators over some separable Hilbert space H. We also let $\mathcal{H}_+ \subset \mathcal{H}$ and $\mathcal{H}_{++} \subset \mathcal{H}$ denote the set of positive semidefinite and positive elements respectively. For any fixed $\sigma \in \mathcal{H}_{++}$ and $s \in [0,1]$, we define

(1) σ-*Weighting Map* For any $\rho \in \mathcal{H}$, define the weighting map $\Gamma_s(\rho) := \sigma^s \rho \sigma^{1-s}$.
(2) σ-*Weighted Inner Product* For any $\rho_1, \rho_2 \in \mathcal{H}$ define the inner product

$$\langle \rho_1, \rho_2 \rangle_s = \langle \Gamma_s(\rho_1), \rho_2 \rangle_{HS} = \operatorname{tr}(\sigma^s \rho_1^\dagger \sigma^{1-s} \rho_2).$$

Note that since $\sigma \succ 0$ we know that $\sigma^\dagger = \sigma$ and it is easily checked that this inner product is non-degenerate (first diagonalize $\sigma = U \Sigma U^\dagger$ then expand in its eigenbasis).

Having the inner σ-weighted inner products, we can now define detailed balance condition

Definition 1 (Detailed Balance)**.** We say a Liouvillian satisfies detailed balance with respect to the inner product $\langle \cdot, \cdot \rangle_s$ for some $s \in [0,1]$ if for all $\hat{O}_1, \hat{O}_2 \in \mathcal{B}(\mathcal{H})$ we have

$$\langle \hat{O}_1, \mathcal{L}^\dagger[\hat{O}_2] \rangle_s = \langle \mathcal{L}^\dagger[\hat{O}_1], \hat{O}_2 \rangle_s.$$

If a state satisfies detailed balance with $s = \frac{1}{2}$ then we say it satisfies the KMS detailed balance condition.

A general Lindblad master equation is defined by a Liouvillian $\mathcal{L}[\cdot] : \mathcal{H} \to \mathcal{H}$ of the following form:

$$\mathcal{L}[\rho] = -i[H, \rho] + \sum_{j=1}^{J} \left(V_j \rho V_j^\dagger - \frac{1}{2} \{ V_j^\dagger V_j, \rho \} \right) \tag{1}$$

While the abstract and title claim you need unique eigenvalues and to use the Davies generator, as far as I can tell, this is not actually the case to do most of the steps. You need to assume that $\mathcal{L}$:

(1) Satisfies KMS detailed balance,
(2) Has a unique, full rank stationary state $\sigma \in \mathcal{H}_{++}$,
(3) The stationary state commutes with the system Hamiltonian (i.e. $[H, \sigma] = 0$).

These assumptions are more or less explicit in Temme's paper. To rederive Temme's work, we also need to make the following assumption:

(4) The jump operators V_j satisfy the rotating wave approximation.

Morally speaking, this assumption is not necessary to understand the overall argument so we will ignore it for now. At a high level, the rotating wave approximation forces a specific type of block structure on the jump operators which allows us to divide the problem of finding the mixing time into many small subproblems which are easier to analyze.

2. Mixing Time and the Spectral Gap

Following results from the theory of classical Markov chains, we might expect that the mixing time of Lindbladian dynamics depends on the spectral gap of its generator. It turns out this is indeed the case, as we can see through the following proposition:

Proposition 2.1 (Trace Norm Convergence for Lindbladian dynamics)**.** *Suppose that $\mathcal{L}$ is a Liouvillian with unique stationary state $\sigma \in \mathcal{H}_{++}$ which satisfies detailed balance. Let $\rho(t)$ be the solution to the evolution equation $\dot{\rho}_t = \mathcal{L}^\dagger(\rho_t)$ with initial conditions ρ_0 then*

$$\|\rho_t - \sigma\|_1^2 \leq \chi^2(\rho_0, \sigma) e^{-2\Delta_{\mathcal{L}} t}$$

where $\chi^2(\rho_0, \sigma)$ denotes the χ^2-divergence

$$\begin{aligned}\chi^2(\rho, \sigma) &= \operatorname{tr}\left[(\rho - \sigma)\sigma^{-\frac{1}{2}}(\rho - \sigma)\sigma^{-\frac{1}{2}}\right] \\ &= \operatorname{tr}\left(\rho\sigma^{-\frac{1}{2}}\rho\sigma^{-\frac{1}{2}}\right) - 1\end{aligned}$$

and $\Delta_{\mathcal{L}}$ denotes the spectral gap of the generator $\mathcal{L}$

$$\Delta_{\mathcal{L}} := 1 - \max\{\lambda : \mathcal{L}[\rho] = \lambda\rho \text{ where } \langle\sigma, \rho\rangle_{HS} = 0, \rho \in \mathcal{H}_+\}$$

Proof. See Lin's notes Section 7 or [3, Lemma 10, Lemma 12] for discrete and continuous time cases respectively. □

Remark 2.2. *Proposition 2.1 is also true even if $\mathcal{L}$ does not satisfy detailed balance although the proof is more complicated (proven in [3]).*

Remark 2.3. *In the worst case, the bound in Proposition 2.1 is fairly pessimistic. If we choose ρ_0 to be the rank one projector on to the smallest singular value of σ, then $\chi^2(\rho_0, \sigma) = \sigma_{\min}^{-1} - 1$ which can be exponentially large in the system size.*

This $O(\sigma_{\min}^{-1})$ dependence in the prefactor can be improved to a $O(\log(\sigma_{\min}^{-1}))$ by establishing a "modified log-Sobolev inequality" for the system in question. However, typically using the modified log-Sobolev inequality tends to degrade the exponential decay rate from $\Delta_{\mathcal{L}}$ to something smaller.

The key property which allows us to control the spectral gap $\Delta_{\mathcal{L}}$ involves defining the weighted variance and its corresponding Dirichlet form; both of these have direct analogs in the classical case. In particular, we define the following quantities:

(1) *Weighted Variance* For any $\rho \in \mathcal{H}$ define

$$\operatorname{Var}_\sigma(\rho, \rho) := \langle\rho, \rho\rangle_{\frac{1}{2}} - \langle I, \rho\rangle_{\frac{1}{2}}^2 = \operatorname{tr}\left(\sigma^{\frac{1}{2}}\rho^\dagger\sigma^{\frac{1}{2}}\rho\right) - \operatorname{tr}\left(\sigma\rho\right)^2$$

(2) *Dirichlet form of $\mathcal{L}$* For any $\rho \in \mathcal{H}$ define

$$\mathcal{E}(\rho, \rho) := -\langle\rho, \mathcal{L}[\rho]\rangle_{\frac{1}{2}} = -\operatorname{tr}\left(\sigma^{\frac{1}{2}}\rho^\dagger\sigma^{\frac{1}{2}}\mathcal{L}[\rho]\right)$$

With these definitions, we can characterize the spectral gap of $\mathcal{L}$ variationally:

Lemma 2.4 (Variation Characterization of Spectral Gap)**.** *Suppose that $\mathcal{L}$ is a Liouvillian with unique stationary state $\sigma \in \mathcal{H}_{++}$ which satisfies KMS-detailed balance and has spectral gap $\Delta_{\mathcal{L}}$. Then we have the following characterization of the spectral gap:*

$$\Delta_{\mathcal{L}} := \inf_{\rho \in \mathcal{H}_+} \frac{\mathcal{E}(\rho, \rho)}{\mathrm{Var}_\sigma(\rho, \rho)}$$

Proof. See Lin's note Proposition 17. □

We're now able to outline the strategy of the proof.

3. Proof Strategy

Proof (Short version). Vectorization. □

The "long version" of the proof, will be the remainder of the talk. Notice that both $\mathcal{E}(\cdot, \cdot)$ and $\mathrm{Var}_\sigma(\cdot, \cdot)$ are sesquilinear forms on $\mathcal{H} \times \mathcal{H}$. Therefore, we can find matrices[1] $\hat{\mathcal{E}}$ and $\hat{V}_\sigma$ so that

$$\mathcal{E}(\rho, \rho) = \langle \rho | \hat{\mathcal{E}} | \rho \rangle \qquad \hat{V}_\sigma(\rho, \rho) = \langle \rho | \hat{V}_\sigma | \rho \rangle$$

where $|\rho\rangle$ denotes a vectorization of ρ.

Let's suppose for a moment that we have calculated the matrices $\hat{\mathcal{E}}$ and $\hat{V}_\sigma$ and see how we can they connect to the spectral gap. By the variational characterization of the spectral gap (Lemma 2.4), we know that the spectral gap is the largest real scalar λ such that for all $\rho \in \mathcal{H}_+$

$$\begin{aligned} &\lambda \,\mathrm{Var}_\sigma(\rho, \rho) \leq \mathcal{E}(\rho, \rho) \\ &\implies \lambda \langle \rho | \hat{V}_\sigma | \rho \rangle \leq \langle \rho | \hat{\mathcal{E}} | \rho \rangle \\ &\implies 0 \leq \langle \rho | \hat{\mathcal{E}} - \lambda \hat{V}_\sigma | \rho \rangle \end{aligned}$$

Hence, $\lambda \leq \Delta_{\mathcal{L}}$ if and only $\hat{\mathcal{E}} - \lambda \hat{V}_\sigma$ is positive semidefinite. Since the gap is strictly positive by assumption, if we set $\tau = \lambda^{-1}$, then we can reduce the problem of finding the largest λ so that $\hat{\mathcal{E}} - \lambda \hat{V}_\sigma \succeq 0$ to finding the smallest τ so that $\tau \hat{\mathcal{E}} - \hat{V}_\sigma \succeq 0$. Hence, any upper bound on τ immediately implies a lower bound on λ.

It turns out operators of the form $\tau B - A$ have been considered in the matrix pencil literature and the quantity τ is known as the *support number* of a pair of matrices [1]

$$\tau(A, B) := \inf\{t \in \mathbb{R} \mid rB - A \succeq 0, \ \forall r \geq t\}.$$

The following lemma on the support number and block decompositions plays an important role in what follows:

Lemma 3.1. *Let A, B be positive semidefinite matrices and suppose $A = \sum_{i=1}^q A_i$ and $B = \sum_{i=1}^q B_i$ where $A_i \succeq 0$, $B_i \succeq 0$, then*

$$\tau(A, B) \leq \max_i \tau(A_i, B_i)$$

[1]Minor technical point, in infinite dimensions we don't get this for free, but it's probably ok because everything is assumed to be trace class.

Moreover, if the non-zero entries of A_i, B_i form a block decomposition of A and B respectively then equality holds.

Proof. By definition, for all $i \in [q]$ $0 \preceq \tau(A_i, B_i)B_i - A_i$ Therefore, summing over i, we have

$$\begin{aligned} 0 &\preceq \sum_{i=1}^{q} \tau(A_i, B_i)B_i - A_i \\ &\preceq (\max_i \tau(A_i, B_i)) \sum_{i=1}^{q} B_i - \sum_{i=1}^{q} A_i \\ &= (\max_i \tau(A_i, B_i))B - A \end{aligned}$$

which proves the first part of the result. To see equality, notice that if A and B can be written as a direct sum of A_i and B_i respectively then if we take $\tau < \max_i \tau(A_i, B_i)$, there must exist an i^* so that $\tau B_{i^*} - A_{i^*} \prec 0$ which is a contradiction. □

The overall idea of the proof is to write $\hat{\mathcal{E}}$ and $\hat{V}_\sigma$ into a block diagonal form and the apply Lemma 3.1 to get a sharp characterization of the spectral gap in terms of the blockwise support numbers $\tau(A_i, B_i)$. By the above argument, upper bounding these support numbers immediately implies a lower bound of the spectral gap. We'll now setup some notation for vectorization.

3.1. **Vectorization Setup.** We start by fixing a choice of orthonormal basis $\{|\alpha\rangle : \alpha \in \mathcal{I}\}$ where $\mathcal{I}$ is some countable indexing set. Vectorization is a basis dependent notion so while the specific choice of orthonormal basis is unimportant, consistently choosing the same basis is critical. Given this choice of basis and $A \in \mathcal{H}$, we define its vectorization as follows:

$$A = \sum_{\alpha\beta} \langle\alpha|A|\beta\rangle |\alpha\rangle \langle\beta| \xrightarrow{\text{vec.}} |A\rangle = \sum_{\alpha\beta} \langle\alpha|A|\beta\rangle |\alpha, \beta\rangle$$

where we recall $|\alpha, \beta\rangle := |\alpha\rangle \otimes |\beta\rangle$.

To see why the vectorization map depends on the choice of basis, suppose that $|\alpha'\rangle$ is a different orthonormal basis and consider the following calculation:

$$\begin{aligned} |\alpha'\rangle \langle\beta'| &= \left(\sum_{\alpha} \langle\alpha|\alpha'\rangle |\alpha\rangle \right) \left(\sum_{\beta} \overline{\langle\beta|\beta'\rangle} \langle\beta| \right) \\ &= \sum_{\alpha\beta} \langle\alpha|\alpha'\rangle \overline{\langle\beta|\beta\rangle} |\alpha\rangle \langle\beta| \\ &\xrightarrow{\text{vec.}} \sum_{\alpha\beta} \langle\alpha|\alpha'\rangle \overline{\langle\beta|\beta'\rangle} |\alpha, \beta\rangle \\ &= \left(\sum_{\alpha} \langle\alpha|\alpha'\rangle |\alpha\rangle \right) \otimes \left(\sum_{\beta} \overline{\langle\beta|\beta'\rangle} |\beta\rangle \right). \end{aligned}$$

While the first term in the tensor product equals $|\alpha'\rangle$, the second term differs from $|\beta'\rangle$ by a complex conjugate. Henceforth, we use $|\overline{\beta'}\rangle$ to denote $|\beta'\rangle$ with its entries in the original basis complex conjugated. With this convention for any orthonormal basis we have $|\alpha'\rangle\langle\beta'| \xrightarrow{\text{vec.}} |\alpha'\overline{\beta'}\rangle$.

Lemma 3.2. *Let $A, B, \rho, \sigma \in \mathcal{H}$ and let $|\Omega\rangle := \sum_\alpha |\alpha\alpha\rangle \in \mathcal{H}\times\mathcal{H}$ be the maximally mixed state. Then the following identities hold*

(1) $\operatorname{tr}(A) = \langle\Omega|A\rangle$,

(2) $\operatorname{tr}(A^\dagger B) = \langle A|B\rangle$,

(3) $|A\rangle = (A\otimes\mathbb{1})|\Omega\rangle$,

(4) $|A\rho B\rangle = (A\otimes B^\top)|\rho\rangle$.

(5) $\operatorname{tr}(\rho^\dagger A\sigma B) = \langle\rho|(A\otimes B^\top)|\sigma\rangle$

Proof. Exercise. □

We're now ready to construct the matrices $\hat{\mathcal{E}}$ and $\hat{V}_\sigma$.

3.2. **Construction of $\hat{\mathcal{E}}$ and $\hat{V}_\sigma$.** By definition of the Dirichlet form we have for any $\rho\in\mathcal{H}_+$

$$\begin{aligned}\mathcal{E}(\rho,\rho) = -\langle\rho,\mathcal{L}[\rho]\rangle_{\frac12} =& i\operatorname{tr}\Big(\Gamma_{\frac12}(\rho)[H,\rho]\Big)\\ &-\sum_j \operatorname{tr}\left(\Gamma_{\frac12}(\rho)\Big(V_j^\dagger\rho V_j - \frac12\Big\{V_j^\dagger V_j,\rho\Big\}\Big)\right)\end{aligned}$$

We can ignore the term involving the system Hamiltonian H since:

$$\begin{aligned}\operatorname{tr}\Big(\Gamma_{\frac12}(\rho)[H,\rho]\Big) &= \operatorname{tr}\left(\sigma^{\frac12}\rho\sigma^{\frac12}[H,\rho]\right)\\ &= \operatorname{tr}\Big(\sigma^{\frac12}\rho\sigma^{\frac12}H\rho - \sigma^{\frac12}\rho\sigma^{\frac12}\rho H\Big) = 0\end{aligned}$$

where the last equality is due to the fact that by assumption $[\sigma,H]=0$ and hence by spectral calculus $[\sigma^{\frac12},H]=0$.

Therefore, to calculate $\hat{\mathcal{E}}$ we simply need to vectorize the following for all j:

$$-\operatorname{tr}\left(\sigma^{\frac12}\rho\sigma^{\frac12}V_j^\dagger\rho V_j - \frac12\left(\sigma^{\frac12}\rho\sigma^{\frac12}V_j^\dagger V_j\rho - \sigma^{\frac12}\rho\sigma^{\frac12}\rho V_j^\dagger V_j\right)\right).$$

Using the cyclic property of trace along with Lemma 3.2 gives us

$$\begin{aligned}\hat{\mathcal{E}} &= -\sum_j (\sigma^{\frac12}V_j^\dagger)\otimes(V_j\sigma^{\frac12})^\top - \frac12(\sigma^{\frac12}V_j^\dagger V_j)\otimes(\sigma^{\frac12})^\top - \frac12\sigma^{\frac12}\otimes(V_j^\dagger V_j\sigma^{\frac12})^\top\\ &= \left(\sigma^{\frac12}\otimes(\sigma^{\frac12})^\top\right)\left(\sum_j \frac12(V_j^\dagger V_j)\otimes\mathbb{1} + \frac12\mathbb{1}\otimes(V_j^\dagger V_j)^\top - V_j^\dagger\otimes V_j^\top\right)\end{aligned}$$

For the variance, using vectorization, we have

$$\begin{aligned}\operatorname{tr}(\sigma^{\frac{1}{2}}\rho\sigma^{\frac{1}{2}}\rho) &= \langle\rho|\sigma^{\frac{1}{2}}\otimes(\sigma^{\frac{1}{2}})^{\top}|\rho\rangle\\ \operatorname{tr}(\sigma^{\frac{1}{2}}\rho\sigma^{\frac{1}{2}}) &= \langle\Omega|\sigma^{\frac{1}{2}}\otimes(\sigma^{\frac{1}{2}})^{\top}|\rho\rangle\end{aligned}$$

Hence

$$\begin{aligned}\hat{V}_{\sigma} &= \sigma^{\frac{1}{2}}\otimes(\sigma^{\frac{1}{2}})^{\top} - \sigma^{\frac{1}{2}}\otimes(\sigma^{\frac{1}{2}})^{\top}|\Omega\rangle\langle\Omega|\,\sigma^{\frac{1}{2}}\otimes(\sigma^{\frac{1}{2}})^{\top}\\ &= \left(\sigma^{\frac{1}{2}}\otimes(\sigma^{\frac{1}{2}})^{\top}\right)\left(\mathbb{1}\otimes\mathbb{1} - |\Omega\rangle\langle\Omega|\,\sigma^{\frac{1}{2}}\otimes(\sigma^{\frac{1}{2}})^{\top}\right)\end{aligned}$$

It's not super clear that these formulae are actually useful in practice; the rotating wave approximation let's you simplify somewhat.

3.3. **Simplification with Rotating Wave Approximation.** The rotating wave approximation is key step in deriving the original Lindblad equation Eq. (1) which our general presentation hasn't accounted for yet.

Remark 3.3. *Applying the rotating wave approximation is equivalent to assuming the Lindblad master equation is given by a Davies generator.*

We start by performing an eigendecomposition of system Hamiltonian H

$$H = \sum_{m}\sum_{i=1}^{N_m}\epsilon_m\,|m(i)\rangle\langle m(i)|$$

where ϵ_m are the eigenvalues, N_m is the degeneracy of the eigenvalue m, $|m(i)\rangle$ is an orthonormal basis for the ϵ_m eigenspace. We also define the spectral projector for the ϵ_m eigenspace

$$\Pi_m := \sum_{i=1}^{N_m}|m(i)\rangle\langle m(i)|$$

and the set of Bohr frequencies

$$\Omega_{\text{Bohr}} := \{\epsilon_m - \epsilon_n : \epsilon_m, \epsilon_n \in \sigma(H)\}.$$

Since $[H,\sigma]=0$ by assumption, we can furthermore choose the eigenfunctions $|m(i)\rangle$ so they are also eigenfunctions of σ.

Since the eigenfunctions of H are complete, we have the property that $\mathbb{1}\otimes\mathbb{1} = \sum_{m,n}\Pi_m\otimes(\Pi_n)^{\top}$. In our vectorized notation, the rotating wave approximation corresponds to the following three properties

$$\left.\begin{aligned}&(\Pi_m\otimes\Pi_n^{\top})(V_j^{\dagger}\otimes V_j^{\top})(\Pi_{m'}\otimes\Pi_{n'}^{\top})\neq 0\\ &(\Pi_m\otimes\Pi_n^{\top})(V_j^{\dagger}V_j\otimes\mathbb{1})(\Pi_{m'}\otimes\Pi_{n'}^{\top})\neq 0\\ &(\Pi_m\otimes\Pi_n^{\top})(\mathbb{1}\otimes V_j^{\dagger}V_j)(\Pi_{m'}\otimes\Pi_{n'}^{\top})\neq 0\end{aligned}\right\}\quad\text{if and only}\quad \epsilon_m-\epsilon_n=\epsilon_{m'}-\epsilon_{n'}.$$

Inspired by this condition, for each $\nu\in\Omega_{\text{Bohr}}$, we define the set of energies whose difference is ν:

$$\mathcal{N}(\nu) := \{(n_1,n_2) : \epsilon_{n_1}-\epsilon_{n_2}=\nu\}.$$

Inserting a two resolutions of the identity we have that

$$\hat{\mathcal{E}} = \sum_{m,n} \sum_{m',n'} (\Pi_m \otimes \Pi_n^\top) \hat{\mathcal{E}} (\Pi_{m'} \otimes \Pi_{n'})$$

but due to the rotating wave approximation, we know that the terms in the sum vanish unless $(m, m') \in \mathcal{N}(\nu)$ and $(n, n') \in \mathcal{N}(\nu)$ for some $\nu \in \Omega_{\text{Bohr}}$.

Now we can define the matrix $\hat{\mathcal{E}}^\nu$ as follows

$$\begin{aligned}\hat{\mathcal{E}}^\nu &:= \sum_{\boldsymbol{m},\boldsymbol{n} \in \mathcal{N}(\nu)} (\Pi_{m_1} \otimes \Pi_{n_1}) \hat{\mathcal{E}} (\Pi_{m_2} \otimes \Pi_{n_2}^\top) \\ &= \sum_{\boldsymbol{m},\boldsymbol{n} \in \mathcal{N}(\nu)} \left(\sigma^{\frac{1}{2}} \otimes (\sigma^{\frac{1}{2}})^\top \right) (\Pi_{m_1} \otimes \Pi_{n_1}^\top) \left(\sum_j \frac{1}{2} (V_j^\dagger V_j) \otimes \mathbb{1} + \frac{1}{2} \mathbb{1} \otimes (V_j^\dagger V_j)^\top - V_j^\dagger \otimes V_j^\top \right) (\Pi_{m_2} \otimes \Pi_{n_2}^\top).\end{aligned}$$

We can perform a similar decomposition for the variance matrix $\hat{V}_\sigma$. In particular, inserting a resolution of the identity

$$\begin{aligned}\hat{V}_\sigma &= \sum_{m,n} \sum_{m',n'} (\Pi_m \otimes \Pi_n^\top) \hat{V}_\sigma (\Pi_{m'} \otimes \Pi_{n'}^\top) \\ &= \sum_{m,n} \sum_{m',n'} \left(\sigma^{\frac{1}{2}} \otimes (\sigma^{\frac{1}{2}})^\top \right) (\Pi_m \otimes \Pi_n^\top) \left(\mathbb{1} \otimes \mathbb{1} - |\Omega\rangle \langle\Omega| \, \sigma^{\frac{1}{2}} \otimes (\sigma^{\frac{1}{2}})^\top \right) (\Pi_{m'} \otimes \Pi_{n'}^\top)\end{aligned}$$

Now notice that for any $A \in \mathcal{H}$ we have

$$\langle A| \, (\Pi_{m_1} \otimes \Pi_{m_2}^\top) \, |\Omega\rangle = \operatorname{tr} (A^\dagger \Pi_{m_1} \Pi_{m_2}) = \begin{cases} \operatorname{tr} (A \Pi_{m_1}) & m_1 = m_2 \\ 0 & m_1 \neq m_2. \end{cases}$$

which gives us two cases, $\nu = 0$

$$\begin{aligned}\hat{V}_\sigma^{\nu=0} = &\sum_m \left(\sigma^{\frac{1}{2}} \otimes (\sigma^{\frac{1}{2}})^\top \right) (\Pi_m \otimes \Pi_m^\top) \\ &- \sum_{m,m'} (\Pi_m \otimes \Pi_m^\top) \left(\sigma^{\frac{1}{2}} \otimes (\sigma^{\frac{1}{2}})^\top \right) |\Omega\rangle \langle\Omega| \left(\sigma^{\frac{1}{2}} \otimes (\sigma^{\frac{1}{2}})^\top \right) (\Pi_{m'} \otimes \Pi_{m'}^\top)\end{aligned}$$

and $\nu \neq 0$

$$\hat{V}_\sigma^{\nu \neq 0} = \sum_{\boldsymbol{m} \in \mathcal{N}(\nu)} \left(\sigma^{\frac{1}{2}} \otimes (\sigma^{\frac{1}{2}})^\top \right) (\Pi_{m_1} \otimes \Pi_{m_2}^\top).$$

Hence, we can write

$$\hat{\mathcal{E}} = \bigoplus_{\nu \in \Omega_{\text{Bohr}}} \hat{\mathcal{E}}^\nu \qquad \hat{V}_\sigma = \bigoplus_{\nu \in \Omega_{\text{Bohr}}} \hat{V}_\sigma^\nu.$$

where $\hat{\mathcal{E}}^\nu$ and $\hat{V}_\sigma^\nu$ are block diagonal the same basis.

One important special case of is when $\nu = 0$. In this case, we are effectively the projecting the dynamics into an eigenbasis of the system Hamiltonian H and we recover the Pauli master equation. Based on the previous discussion, the main result of Temme's paper now follow immediately from Lemma 3.1

Theorem 1 (Main Theorem)**.** *In the above setup, the mixing time λ is equal to*

$$\lambda := \min\{\lambda_{cl}, \lambda_{QM}\}$$

where $\lambda_{cl} := \tau(\hat{V}_\sigma^{\nu=0}, \hat{\mathcal{E}}^{\nu=0})^{-1}$ and $\lambda_{QM} := \min_{\nu\neq 0} \tau(\hat{V}_\sigma^{\nu}, \hat{\mathcal{E}}^{\nu})^{-1}$

The above result applies any system which uses a Davies generator however one can get a cleaner theoretical result if you additionally assume that the eigenvalues of the system Hamiltonian are unique[2].

4. Simplification for Distinct Eigenvalues

In the case that H has distinct eigenvalues, we can uniquely define a basis of eigenvalues $\{|m\rangle\}$ as well as the set $\mathcal{N}(\nu)$ for each $\nu \in \Omega_{\text{Bohr}}$. In this basis, we can write each $\hat{\mathcal{E}}^\nu$ as

$$\begin{aligned}\hat{\mathcal{E}}^\nu =& \sum_j \sum_{\boldsymbol{m}\in\mathcal{N}(\nu)} \frac{1}{2}\sqrt{\sigma_{m_1}\sigma_{m_2}} \left(\langle m_1|V_j^\dagger V_j|m_1\rangle + \langle m_2|V_j^\dagger V_j|m_2\rangle\right) |m_1\overline{m_2}\rangle \langle m_1\overline{m_2}| \\ &- \sum_j \sum_{\boldsymbol{m},\boldsymbol{n}\in\mathcal{N}(\nu)} \sqrt{\sigma_{m_1}\sigma_{m_2}} \langle m_1|V_j^\dagger|n_1\rangle \langle m_2|V_j|n_2\rangle |m_1\overline{m_2}\rangle \langle n_1\overline{n_2}|\end{aligned}$$

where we recall the notation $|\alpha\overline{\beta}\rangle$ introduced as part of our vectorization step (Section 3.1). Similarly, for $\hat{V}_\sigma^\nu$ we can write

$$\hat{V}_\sigma^{\nu=0} = \sum_{m_1} \sigma_{m_1} |m_1\overline{m_1}\rangle \langle m_1\overline{m_1}| - \sum_{m_1,m_2} \sigma_{m_1}\sigma_{m_2} |m_2\overline{m_2}\rangle \langle m_1\overline{m_1}| .$$

For $\nu \neq 0$, we have

$$\hat{V}_\sigma^{\nu\neq 0} = \sum_{\boldsymbol{m}\in\mathcal{N}(\nu)} \sqrt{\sigma_{m_1}\sigma_{m_2}} |m_1\overline{m_2}\rangle \langle m_1\overline{m_2}|$$

Remark 4.1. *In more standard notations, the jump operators V_j are decomposed as $V_j = \sum_{\omega\in\Omega_{\text{Bohr}}} V_j(\omega)$, where*

$$V_j(\omega) := \sum_{\boldsymbol{m}\in\mathcal{N}(\omega)} \langle m_1|V_j|m_2\rangle |m_1\rangle \langle m_2| .$$

For the later calculations, I think avoiding this ω dependence is a little cleaner.

[2]As mentioned in Lin's notes, there's a bit of ambiguity here about whether the system Hamiltonian should include the Lamb shift term or not. Based on the derivation, we can see that what's important is how the eigenspaces of the Hamiltonian related to the jump operators.

4.1. **Simplification for $\nu = 0$.** To better understand the $\nu = 0$ case, we recall the definition of the graph Laplacian for a weighted graph:

Definition 2. Given a weighted graph $G = (V, E)$ with edge weights $\{w_{v,w} : v, w \in V\}$, the *graph Laplacian*, L, is defined as the $\#|V| \times \#|V|$ matrix

$$L_{v,w} = \begin{cases} \sum_{w' \in N(v)} w_{v,w'} & v = w \\ -w_{v,w} & w \in N(v) \\ 0 & \text{otherwise} \end{cases}$$

where $N(v)$ denotes the neighbors of $v \in V$.

Since σ is a quantum state $\operatorname{tr}(\sigma) = 1$ and hence $\sum_{m_2} \sigma_{m_2} = 1$. Therefore, we can immediately see that $\hat{V}_\sigma^{\nu=0}$ is a graph Laplacian for the complete graph whose vertices are indexed by the eigenfunctions of H where the weight of the edge between $|m\rangle$ and $|n\rangle$ is $\sigma_m \sigma_n$. It turns out $\hat{\mathcal{E}}^{\nu=0}$ also can be viewed as a graph Laplacian.

For $\nu = 0$, the sums over $\mathcal{N}(\nu)$ reduce to summing over the eigenfunctions of H hence we have

$$\begin{aligned} \hat{\mathcal{E}}^{\nu=0} &= \sum_j \sum_m \sigma_m \langle m|V_j^\dagger V_j|m\rangle \, |m\overline{m}\rangle \langle m\overline{m}| - \sum_j \sum_{m,n} \sigma_m \langle m|V_j^\dagger|n\rangle \langle m|V_j|n\rangle \, |m\overline{m}\rangle \langle n\overline{n}| \\ &= \sum_j \sum_m \sigma_m \| V_j |m\rangle \|^2 \, |m\overline{m}\rangle \langle m\overline{m}| - \sum_j \sum_{m,n} \sigma_m |\langle n|V_j|m\rangle|^2 \, |m\overline{m}\rangle \langle n\overline{n}| \end{aligned}$$

which is again a weighted graph Laplacian on the eigenstates of H since $\sum_n |\langle n|V_j|m\rangle|^2 = \| V_j |m\rangle \|^2$.

Using this connection with graph Laplacians, one can appeal to known results for the mixing time of Markov chains and graph theory[3]:

$$\tau^{\nu=0} = \max_{(m,n)\in K} \frac{1}{P(m,n)} \sum_{\gamma_{ab} \ni (m,n)} \sigma_a \sigma_b |\gamma_{ab}| \tag{2}$$

where K the graph induced by the hops between different eigenstates of H and $P(m,n) := \sum_j |\langle m|V_j|n\rangle|^2$. The sum is taken over a set of paths $\{\gamma_{ab}\}$ chosen to connect all pairs of vertices (a, b) through edges in K. The sum $\gamma_{ab} \ni (m, n)$ is taken over all paths that contain the link (m, n) and $|\gamma_{ab}|$ denotes the length of the path traversed from a to b.

4.2. **Simplification for $\nu \neq 0$.** Since $\hat{V}_\sigma^{\nu\neq 0}$ is a diagonal matrix, there's not much we can do in terms of simplification. For $\hat{\mathcal{E}}^{\nu\neq 0}$, we start by inserting a resolution of the identity

$$\begin{aligned} \hat{\mathcal{E}}^\nu = &\sum_j \sum_k \sum_{\boldsymbol{m} \in \mathcal{N}(\nu)} \frac{1}{2} \sqrt{\sigma_{m_1} \sigma_{m_2}} \Big(|\langle k|V_j|m_1\rangle|^2 + |\langle k|V_j|m_2\rangle|^2 \Big) \, |m_1 \overline{m_2}\rangle \langle m_1 \overline{m_2}| \\ &- \sum_j \sum_{\boldsymbol{m},\boldsymbol{n} \in \mathcal{N}(\nu)} \sqrt{\sigma_{m_1} \sigma_{m_2}} \langle m_1|V_j^\dagger|n_1\rangle \langle m_2|V_j|n_2\rangle \, |m_1 \overline{m_2}\rangle \langle n_1 \overline{n_2}| \end{aligned}$$

[3]The reference given in the paper is [2] but I haven't checked it

where the set $\{|k\rangle\}$ is a complete basis of eigenstates of H. Since we are interested in relating $\hat{\mathcal{E}}^{\nu}$ to a positive semidefinite constraint, we would like to compare the terms in the first sum (which is clearly positive semidefinite) to the second sum. Since we sum over all eigenstates in the first sum, there are some terms which will not have matching terms in the second sum. In particular, with regards to k, we have three cases:

(1) $(m_1, k) = (m_1, n_1)$ for some $(m_1, n_1) \in \mathcal{N}(\nu)$

(2) $(k, m_2) = (n_2, m_2)$ for some $(n_2, m_2) \in \mathcal{N}(\nu)$

(3) $(m_1, k) \notin \mathcal{N}(\nu)$ and $(k, m_2) \notin \mathcal{N}(\nu)$.

To handle the last case, we define the index set

$$\mathcal{S}(\nu) := \{(k, m_1, m_2) : (m_1, k) \notin \mathcal{N}(\nu) \text{ and } (k, m_2) \notin \mathcal{N}(\nu)\},$$

and collect the terms which do not have corresponding terms in $\hat{\mathcal{E}}_2^{\nu}$ into a new matrix:

$$\hat{\mathcal{E}}^{\nu}_{\text{no match}} := \frac{1}{2} \sum_j \sum_k \sum_{\boldsymbol{m} \in \mathcal{N}(\nu)} \delta_{(k,m_1,m_2)\in\mathcal{S}} \sqrt{\sigma_{m_1}\sigma_{m_2}} \Big(|\langle k|V_j|m_1\rangle|^2 + |\langle k|V_j|m_2\rangle|^2 \Big) |m_1\overline{m_2}\rangle \langle m_1\overline{m_2}| .$$

The matched terms can be grouped into the matrix:

$$\begin{aligned}\hat{\mathcal{E}}^{\nu}_{\text{match}} := \frac{1}{2} \sum_j \sum_{\boldsymbol{m},\boldsymbol{n} \in \mathcal{N}(\nu)} & \sqrt{\sigma_{m_1}\sigma_{m_2}} \Big(|\langle n_1|V_j|m_1\rangle|^2 + |\langle n_2|V_j|m_2\rangle|^2 \Big) |m_1\overline{m_2}\rangle \langle m_1\overline{m_2}| . \\ & - \sum_j \sum_{\boldsymbol{m},\boldsymbol{n} \in \mathcal{N}(\nu)} \sqrt{\sigma_{m_1}\sigma_{m_2}} \langle m_1|V_j^{\dagger}|n_1\rangle \langle m_2|V_j|n_2\rangle |m_1\overline{m_2}\rangle \langle n_1\overline{n_2}|\end{aligned}$$

By Gershgorin's theorem, we can lower bound the eigenvalues of $\hat{\mathcal{E}}^{\nu}_{\text{match}}$ by the difference

$$\begin{aligned}\min_{\boldsymbol{m} \in \mathcal{N}(\nu)} & \left[\frac{1}{2} \sum_{\boldsymbol{n} \in \mathcal{N}(\nu)} \sqrt{\sigma_{m_1}\sigma_{m_2}} \sum_j \Big(|\langle n_1|V_j|m_1\rangle|^2 + |\langle n_2|V_j|m_2\rangle|^2 \Big) \right] \\ & - \left[\sum_{\boldsymbol{n} \in \mathcal{N}(\nu)} \sqrt{\sigma_{m_1}\sigma_{m_2}} \left| \sum_j \langle m_1|V_j^{\dagger}|n_1\rangle \langle m_2|V_j|n_2\rangle \right| \right] .\end{aligned}$$

This can further be lower bounded by

$$\min_{\boldsymbol{m} \in \mathcal{N}(\nu)} \frac{1}{2} \sum_{\boldsymbol{n} \in \mathcal{N}(\nu)} \sqrt{\sigma_{m_1}\sigma_{m_2}} \sum_j \Big(|\langle n_1|V_j|m_1\rangle| - |\langle n_2|V_j|m_2\rangle| \Big)^2$$

by pulling the absolute values into the subtracted term and completing the square.

Since $\hat{\mathcal{E}}^{\nu}_{\text{no match}}$ is diagonal, repeating an analogous argument lets us conclude that

$$\begin{aligned}\hat{\mathcal{E}}^{\nu} \succeq \min_{\boldsymbol{m} \in \mathcal{N}(\nu)} & \frac{1}{2} \sum_{j,k} \delta_{(k,m_1,m_2)\in\mathcal{S}} \sqrt{\sigma_{m_1}\sigma_{m_2}} \Big(|\langle k|V_j|m_1\rangle|^2 + |\langle k|V_j|m_2\rangle|^2 \Big) \\ & + \frac{1}{2} \sum_{\boldsymbol{n} \in \mathcal{N}(\nu)} \sqrt{\sigma_{m_1}\sigma_{m_2}} \sum_j \Big(|\langle n_1|V_j|m_1\rangle| - |\langle n_2|V_j|m_2\rangle| \Big)^2 .\end{aligned}$$

Now recall that we are interested in finding τ^ν so that $\tau^\nu \hat{\mathcal{E}}^\nu - \hat{V}_\sigma^\nu \succeq 0$. Let's define the constant Λ_{QM}^ν as follows

$$\begin{aligned}\Lambda_{QM}^\nu := \min_{\boldsymbol{m}\in\mathcal{N}(\nu)} \frac{1}{2}\sum_{j,k} \delta_{(k,m_1,m_2)\in\mathcal{S}}\Big(|\,\langle k|V_j|m_1\rangle\,|^2 + |\,\langle k|V_j|m_2\rangle\,|^2\Big) \\ + \frac{1}{2}\sum_j \sum_{\boldsymbol{n}\in\mathcal{N}(\nu)} \left(|\,\langle n_1|V_j|m_1\rangle\,| - |\,\langle n_2|V_j|m_2\rangle\,|\right)^2 .\end{aligned} \tag{3}$$

Since $\hat{V}_\sigma^\nu$ is diagonal for $\nu \neq 0$, we immediately see that $\tau^\nu \leq (\Lambda_{QM}^\nu)^{-1}$. Hence Λ_{QM}^ν is a lower bound for the quantum mechanical mixing time. It's worth noting that this Λ_{QM}^ν is not sharp (due to the application of Gershgorin's theorem) however the steps before that are sharp.

5. An Example: Particle on a Line

We now apply the theory to calculate the mixing time for a single Fermion on a line with Dirichlet boundary conditions (see [4, Section 5, Example 2] for motivation for this model). In particular, let our Hamiltonian be given by:

$$H = -g\sum_{r=1}^{N} |r\rangle\langle r| + \sum_{r=1}^{N-1} |r+1\rangle\langle r| + |r\rangle\langle r-1|$$

Due to the periodic boundary conditions, the eigenpairs of H can be written as $\{(\epsilon_k, |\epsilon_k\rangle) : k \in \{1,\cdots,N\}\}$, where

$$\epsilon_k = 2\cos\left(\frac{k\pi}{N+1}\right) - g$$

$$|\epsilon_k\rangle = \sqrt{\frac{2}{N+1}}\sum_{r=0}^{N} \sin\left(\frac{\pi}{N+1}kr\right)|r\rangle$$

Projected into this eigenbasis the jump operators $\{V_r\}_{r=1}^N$ are written:

$$\langle\epsilon_k|V_r|\epsilon_{k'}\rangle = \frac{2\gamma G(\epsilon_k - \epsilon_{k'})^{\frac{1}{2}}}{N+1}\sin\left(\frac{\pi}{N+1}kr\right)\sin\left(\frac{\pi}{N+1}k'r\right)$$

where γ is a constant and $G(\omega) = (1+e^{\beta\omega})^{-1}$ is a bath function motivated by classical Glauber dynamics.

First, notice that since $\|H\| \leq 2$, we have the lower bound $G(\omega) \geq (1+e^{4\beta})^{-1}$. For $N > 1$, the differences of eigenvalues of H are incommensurate so for any $\nu \in \Omega_{\text{Bohr}}$ there is only one $(n_1, n_2) \in \mathcal{N}(\nu)$. Using Eq. (3) and using the properties of Fourier series it can be easily checked

that

$$\begin{aligned}\Lambda_{QM}^{\nu} &\geq \frac{1}{2}\sum_{j,k}\delta_{(k,m_1,m_2)\in\mathcal{S}}\Big(|\,\langle k|V_j|m_1\rangle\,|^2+|\,\langle k|V_j|m_2\rangle\,|^2\Big)\\ &= \frac{4\gamma^2 G(\nu)}{(N+1)^2}\left((N+1)^2-(N+1)\right)\\ &\geq 2\gamma^2(1+e^{4\beta})^{-1}.\end{aligned}$$

where in the last line we have used that $N>1$. As for the classical mixing time, since all momentum hoppings are possible in this model, Eq. (2) reduces to

$$\tau = \max_{(k,k')} P(k,k')^{-1}\sigma_k$$

where

$$P(k,k') = \sum_r |\,\langle\epsilon_k|V_r|\epsilon_{k'}\rangle\,|^2 = G(\epsilon_k-\epsilon_{k'})\frac{4\gamma^2 N}{(N+1)^2}$$

Since the stationary distribution is known to be $\sigma = Z^{-1}e^{\beta H}$, have the upper bound

$$\sigma_a \leq N^{-1}e^{-\beta(\epsilon_a-\|H\|)} \leq N^{-1}e^{2\beta}e^{-\beta\epsilon_a}$$

and hence we have the upper bound

$$\tau \leq \left(\min_{\omega\in\Omega_{\text{Bohr}}} G(\omega)^{-1}\right)e^{4\beta}\frac{(N+1)^2}{N^2} \leq \frac{e^{4\beta}}{1+e^{4\beta}}\frac{(N+1)^2}{N^2}$$

Since $\frac{x}{1+x^2}\leq\frac{1}{2}$ for all $x\in\mathbb{R}$, we recover the lower bound

$$\lambda_{cl} \geq 2\gamma^2\frac{N^2}{(N+1)^2} \geq \gamma^2$$

which completes the calculation.

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