Mixing Time of Open Quantum Systems via Hypocoercivity

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Join work with
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arXiv:2404.11503

[1] Initiated @ IPAM long program on Mathematical and Computational Challenges in Quantum Computing, Fall 2023.

Outline

Mixing Time of Open Quantum Systems

Heisenberg Picture

$$\partial_t A = \mathcal{L}A = \underbrace{i[H, A]}_{=:\mathcal{H}} + \underbrace{\sum_j V_j^\dagger [A, V_j] + [V_j^\dagger, A] V_j}_{=:\mathcal{D}} .$$

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Why do we care?

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Algorithmic advancement employing Lindblad equations:

- Universal quantum computation, useful in quantum field theories simulation
  [Verstraete-Wolf-Cirac, Nature Physics 2009], [Osborne-Eisert-Verstraete PRL 2010], [Verstraete-Cirac PRL 2010]
- To prepare and sample from thermal states
  [Chen-Kastoryano-Gilyen 2023], [Chen-Kastoryano-Brandao-Gilyen 2023], [Rall-Wang-Wocjan Quantum 2023], [Ding-Li-Lin 2024], [Jiang-Irani 2024], etc
- Ground states preparation
  [Ding-Chen-Lin PRR 2024]
- To find local minima in quantum systems
  [Chen-Huang-Preskill-Zhou STOC 2024]
- Quantum control
  [Li-Wang ICML 2023]
- Classical optimization
  [Chen-Lu-Wang-Liu-Li 2023]

Mixing Time

Quantum Info (target)

Quantum Markov Semigroup

$$\partial_t A = \mathcal{L} A$$

$$t_{\mathrm{mix}}(\epsilon) = \inf\{t \geq 0 : \|e^{s\mathcal{L}^\star}(\rho) - \sigma\|_1 \leq \epsilon, \forall \rho, s \geq t\}.$$

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Probability Viewpoint

(Ergodicity, Detailed Balance, etc)

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Probability Viewpoint
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Dynamical System /
Differential Equation Viewpoint
(Lyapunov functionals)

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Previous Works for Mixing Time Estimate

How to estimate the mixing time? Typical route:

- One starts with a Lindbladian that satisfies detailed balance condition under certain inner product. (If not, consider a symmetrization of $\mathcal{L}$, denote as $\mathcal{L}_H$.)

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- It implies exponential decay with rate g, namely,

$$\|A(t)\| \leq \|A(0)\| e^{-gt}.$$

Then by duality, one can get an estimate of the mixing time. In particular, $g \sim 1/\text{poly}(N)$ implies $t_{\text{mix}} \sim \text{poly}(N)$.

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  Then by duality, one can get an estimate of the mixing time. In particular, $g \sim 1/\mathrm{poly}(N)$ implies $t_{\mathrm{mix}} \sim \mathrm{poly}(N)$.
- For some g, e.g., $g = \Omega(1)$, modified logarithmic Sobolev inequality can tighten the bound $\Rightarrow t_{\mathrm{mix}} \sim \mathrm{polylog}(N)$. [2]

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Even when H and $\mathcal{D}$ are both simple, $\mathcal{L}$ can still be hard.

Questions:

- Can we use information about the dissipative part $\mathcal{D}$ and the Hamiltonian part $\mathcal{H}$ separately to yield a mixing time estimation?
- What if $\mathcal{L}$ is not detailed balance? Are there still some cases that we can estimate?

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- So what? Applications? We provide a number of physical examples where our conditions can be easily verified, including the transverse field Ising model, Heisenberg model, and quantum walk, with some Pauli noise.
- The technique is based on the construction of an energy functional inspired by the hypocoercivity of (classical) kinetic theory.

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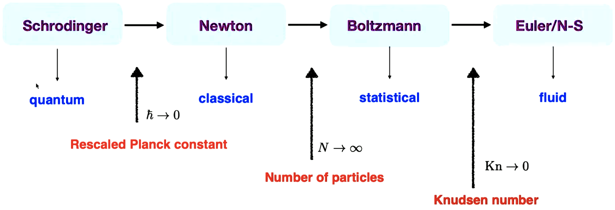

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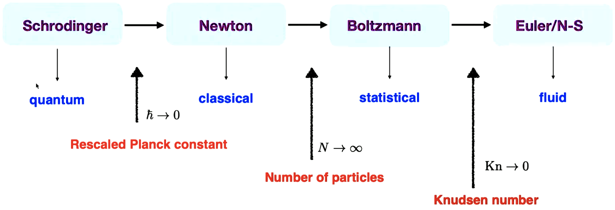

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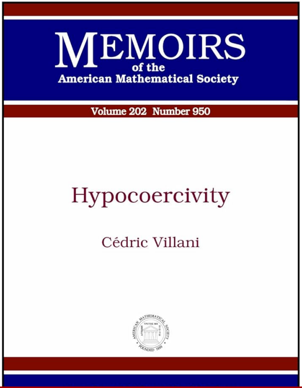

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Quantum!

Minimal Example – Coercivity v.s. Hypocoercivity

Consider a n-dimensional real-valued ODE of:

$$\frac{d}{dt}x = -Ax, \quad t \geq 0.$$

From **Arnold**'s talk that DF attended in 2017. Similar ODE examples, see standard ODE textbook, e.g., [Teschl Page 203], [Brauer-Nohel Page194]

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$$\langle A_H x, x \rangle = x^T A_H x \geq g \left\| x \right\|^2, \quad \forall x.$$

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$$A = \begin{pmatrix} 0 & -1 \\ 1 & 1 \end{pmatrix} \rightarrow \text{ e-vals are } \frac{1}{2} \pm i\frac{\sqrt{3}}{2}.$$

From ODE basics, the solution decays with a rate $\frac{1}{2}$. But the vanilla energy method no longer works! $\frac{d}{dt}\|x(t)\| \leq 0$ (instead of $-g\|x(t)\|$).

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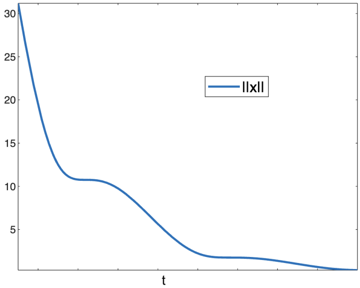

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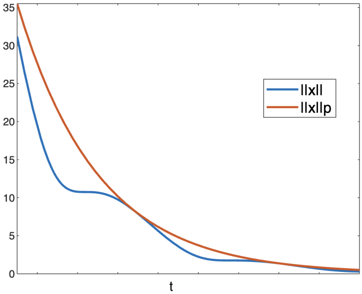

Instead of $x^2 + y^2$, the Lyapunov function is now $x^2+y^2+xy \propto \|x\|_P^2$.

$$\frac{d}{dt}\|x\|_P \leq -\frac{1}{2}\|x\|_P$$

$\|x\|_P$ and $\|x\|$ are equivalent.

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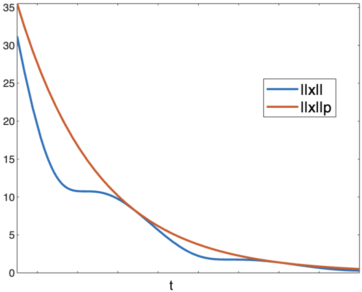

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For e^{-tA} that decays yet A not coercive, it is "hypocoercive".

Our Results – Preparation

For Lindblad Equation (Heisenberg picture)

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Denote the global equilib. state as σ. We consider GNS inner product

$$\langle A, B \rangle = \mathrm{tr}(\sigma A^\dagger B).$$

Remark: Other inner products $\langle A, B\rangle_\alpha = \mathrm{tr}(\sigma^\alpha A^\dagger \sigma^{1-\alpha} B)$ are also ok.

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Lindblad equation is linear $\Rightarrow$ consider the "difference" between a Hermitian A and the fixed point of $\mathcal{L}$ starting from A, i.e. the fluctuation around the global equilibrium, can be defined as

$$A - \frac{\langle I, A \rangle}{\langle I, I \rangle} I = A - \mathrm{tr}[\sigma A] I,$$

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If $\mathcal{D}$ is degenerate, $\dim \ker D > 1$. The energy method fails!

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Consider Trotterization viewpoint:

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By dissipative nature of $\mathcal{D} \Rightarrow$ dynamics exp. damps $(\mathcal{I} - \mathcal{P})A$.

Our Results – Intuition

Consider Trotterization viewpoint:

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For $\mathcal{P}A$, we observe that

$$\begin{aligned} e^{t\mathcal{H}/L}\mathcal{P}A =& \mathcal{P}A + \mathcal{H}\mathcal{P}At/L + \mathcal{O}(t^2/L^2) \\ =& \mathcal{P}A + (\mathcal{I} - \mathcal{P})\mathcal{H}\mathcal{P}At/L + \mathcal{P}\mathcal{H}\mathcal{P}At/L + \mathcal{O}(t^2/L^2) \end{aligned}$$

If $\mathcal{P}\mathcal{H}\mathcal{P} = 0$, the $\mathcal{P}A$ part is being driven to the image of $\mathcal{I} - \mathcal{P}$, i.e., the orthogonal complement of $\ker\mathcal{D}$, which will then be damped by $\mathcal{D}$ in the next step.

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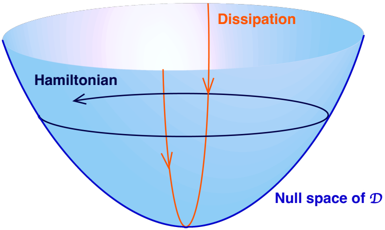

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Notethat $\mathcal{H}$ transforms a diagonal matrix into an off-diagonal one, so that $\mathcal{P}\mathcal{H}\mathcal{P} = 0$. We can also compute that

$$e^{t\mathcal{D}}A = \begin{pmatrix} a & e^{-t}b \\ e^{-t}c & d \end{pmatrix},$$

where everything outside of $\ker \mathcal{D}$ is damped exponentially, while the dynamics governed by $\mathcal{H}$ mixes the terms.

Our Results – Conditions

Condition 1: The operator $\mathcal{D}$ is symmetric and satisfies

$$-\langle \mathcal{D}A, A\rangle \geq \lambda_m \left\|(\mathcal{I}-\mathcal{P})A\right\|^2 ,$$

with some positive λ_m, for all A such that $\mathrm{tr}[\sigma A] = 0$.

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Condition 4: $\|\mathcal{H}(\mathcal{I}-\mathcal{P})A\| + \|\mathcal{D}A\| \leq C'_M \|(\mathcal{I}-\mathcal{P})A\|$, for all Hermitian A.

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Theorem (Main result)

Under conditions 1-4, there exist positive constants λ and C, explicitly computable in terms of λ_m, λ_M and C_M such that

$$\left\| e^{t(\mathcal{H}+\mathcal{D})} A \right\| \leq C e^{-\lambda t} \|A\|, \qquad \forall t \geq 0.$$

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$$C = \left(\frac{1+\varepsilon}{1-\varepsilon}\right)^{1/2}, \quad \lambda = \min\left\{\frac{1}{4}\frac{\lambda_m}{1+\varepsilon}, \frac{1}{3}\frac{\varepsilon}{1+\varepsilon}\frac{\lambda_M}{\alpha+\lambda_M}\right\},$$

where ε are defined in

$$\varepsilon = \frac{1}{2}\min\left\{\frac{\lambda_m \lambda_M}{(\alpha+\lambda_M)(1+C'_M/(2\sqrt{\alpha}))^2}, 1\right\}.$$

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Under conditions 1-4, for $\lambda_m, \lambda_M \leq \mathcal{O}(1)$, $C'_M \geq \Omega(1)$, if σ is full-rank, the mixing time $t_{\mathrm{mix}}(\epsilon)$ satisfies

$$t_{\mathrm{mix}}(\epsilon) = \mathcal{O}\left(\frac{C_M'^2}{\lambda_m \lambda_M} \log(\|\sigma^{-1}\|_\infty / \epsilon) \right).$$

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Remark: 1. $\mathcal{L}$ does NOT need to satisfy detailed balanced conditions.
2. Take-home message: Hamiltonian enhances mixing.

Applications to Physical Examples – Single Qutrit

Example 1: **Single Qutrit**. Hilbert sp. is spanned by $\{|0\rangle, |1\rangle, |2\rangle\}$.

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$$H = \omega(|1\rangle\langle 2| + |2\rangle\langle 1|)$$

$$V_1 = \sqrt{\gamma}\sigma^-, \quad V_2 = \sqrt{\gamma}\sigma^+,$$

where $\sigma^- = |0\rangle\langle 1|$ is the lowering operator, and $\sigma^+ = |1\rangle\langle 0|$ is the raising operator. $\mathcal{H}A = i[H, A]$, $\mathcal{D}A = \sum_j V_j^\dagger[A, V_j] + [V_j^\dagger, A]V_j$.

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$$\sigma = \frac{1}{2}|0\rangle\langle 0| + \frac{1}{4}|1\rangle\langle 1| + \frac{1}{4}|2\rangle\langle 2|.$$

One can verify all conditions with $\lambda_m = (3/2)\gamma$, $\lambda_M = \omega^2$, and $C'_M = \mathcal{O}(|\omega| + \gamma)$. Our theorem yields:

$$t_{\text{mix}}(\epsilon) = \mathcal{O}((\omega^2 + \gamma^2)\omega^{-2}\gamma^{-1}\log(1/\epsilon))$$

Applications to Physical Examples – N-body systems

Dephasing noise:

$$\mathcal{D}A = \gamma \sum_i (Z_i A Z_i - A).$$

The kernel of $\mathcal{D}$ is spanned by $\{Z^{\otimes \vec{b}} : \vec{b} \in \{0,1\}^N\}$.
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$$t_{\text{mix}}(\epsilon) = \mathcal{O}\left(\frac{N^2(1+\gamma)^2}{\gamma h^2}(N + \log(1/\epsilon))\right).$$

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$$H = -\sum_{i=1}^{N-1} (J_x X_i X_{i+1} + J_y Y_i Y_{i+1} + J_z Z_i Z_{i+1}) + h \sum_{i=1}^{N} X_i.$$

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On a d-regular connected graph $G = (V, E)$, denote its adjacency matrix as

$$H = \sum_{ij} h_{ij} |i\rangle \langle j| .$$

The smallest eigenvalue of the graph Laplacian $L = dI - H$ is 0. The second smallest eigenvalue is denoted as Δ (i.e. the spectral gap).

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$\lambda_M = 2\Delta$ and $C'_M = \mathcal{O}(d + \gamma N)$. Our theorem yields:

$$t_{\text{mix}}(\epsilon) = \mathcal{O}\left(\frac{(d + \gamma N)^2}{\gamma \Delta} (N + \log(1/\epsilon)) \right) .$$

Our results – Proof Idea

If we consider a naive energy estimate using $\|A\|^2$,

$$\partial_t A = (\mathcal{H} + \mathcal{D})A, \quad \langle A, B \rangle = \mathrm{tr}(\sigma A^\dagger B).$$

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To characterize the convergence we construct a twisted norm, which serves as a Lyapunov functional of the system, as

$$\mathfrak{L}[A] := \frac{1}{2}\|A\|^2 - \varepsilon \Re\langle \mathcal{A}A, A\rangle,$$

with some $\varepsilon \in (0,1)$ to be fixed and

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for some $\alpha > 0$. Importantly, this Lyapunov functional can be shown equivalent to $\|A\|$, namely,

$$\frac{1}{2}(1-\varepsilon)\|A\|^2 \le \mathfrak{L}[A] \le \frac{1}{2}(1+\varepsilon)\|A\|^2.$$

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Remark. In fact Condition 4, i.e.

$$\|\mathcal{H}(\mathcal{I}-\mathcal{P})A\| + \|\mathcal{D}A\| \le C_M' \|(\mathcal{I}-\mathcal{P})A\|,$$

for all Hermitian A, can be relaxed to

$$\|\mathcal{A}\mathcal{H}(\mathcal{I}-\mathcal{P})A\| + \|\mathcal{A}\mathcal{D}A\| \le C_M(\alpha)\,\|(\mathcal{I}-\mathcal{P})A\|$$

for all Hermitian A.

Conclusion

We propose a new theoretical framework to estimate the mixing time of the Lindblad Equation that treats $\mathcal{H}$ and $\mathcal{D}$ separately via hypocoercivity. It

- thus *circumvents* the need for a priori estimation of the spectral gap of the full Lindbladian generator;
- does *not* require the Lindbladian to satisfy the detailed balance condition;
- can be applied to various physical examples, include Transverse Field Ising Model, Heisenberg Model, and quantum walk.

Future Directions

- More applications?
- Relax the condition of $PHP = 0$?
- There are various different frameworks of hypocoercivity for kinetic theory. What are their quantum analog? Can they yield tighter estimate?

Thank you for your attention!

Reference:
Mixing Time of Open Quantum Systems via Hypocoercivity
Di Fang, Jianfeng Lu, Yu Tong [arXiv:2404.11503]

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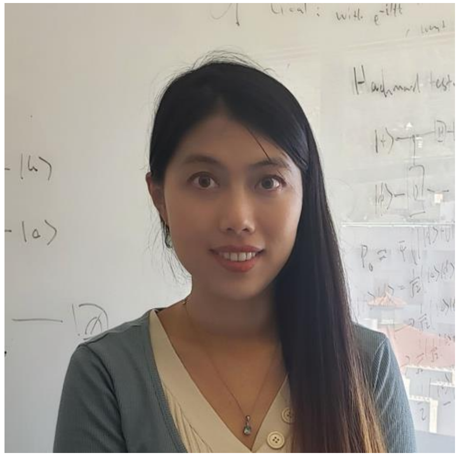

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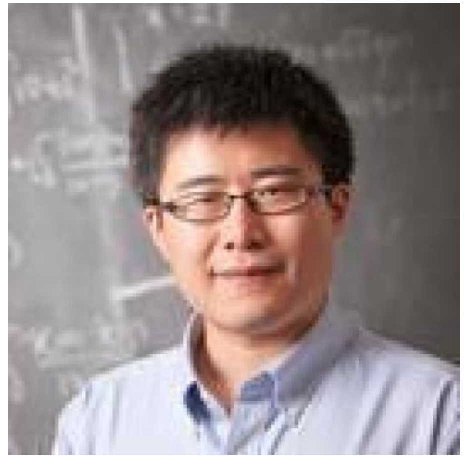

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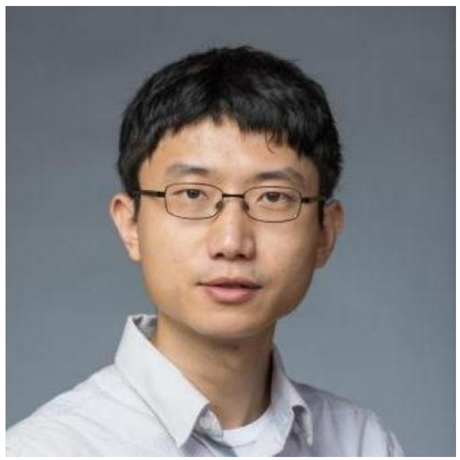

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