On quantum to classical comparison for Davies generator

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QIP 2026

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Quantum Markov processes

Hamiltonian $H \in \mathbb{C}^{2^n \times 2^n}$, H Hermitian
Quantum Gibbs state of H at inverse temperature β: $\rho_\beta = \frac{\exp(-\beta H)}{\mathrm{tr}(\exp(-\beta H))}$

Understand & predict how open quantum systems behave:

- Physics: simulates system coupled to a heat-bath
- Quantum computing: prepare quantum Gibbs state → optimization, quantum ML, candidate quantum to classical speedup

Davies generator

$$\mathcal{L}(f) = \underbrace{i\,[H,f]}_{\text{coherent}} + \sum \underbrace{G(\omega)\left(S(\omega)^\dagger f S(\omega) - \frac{1}{2}\{S(\omega)^\dagger S(\omega), f\}\right)}_{\text{dissipative}}$$

$[A,B] = AB - BA$

$\{A,B\} = AB + BA$

$$S(\omega) := \sum_{\lambda_1,\lambda_2:\lambda_1-\lambda_2=\omega} \Pi_{\lambda_1} S \Pi_{\lambda_2}$$

Π_λ : *projector to the eigenspace of H of eigenvalue λ*

- Linbladian dynamics $\sigma_t = e^{t\mathcal{L}^+}\sigma_0 \xrightarrow{t\to+\infty} \rho \equiv \rho_\beta = \frac{\exp(-\beta H)}{\mathrm{tr}(\exp(-\beta H))}$
- Hamiltonian H: describes the internal quantum system
- Jump operators $\mathcal{S} = \{S\}$
- Transition rate $G: \underbrace{B_H}_{\text{Bohr frequency}} \to \mathbb{R}_{\geq 0}$

model interactions with the environment

Bohr frequency:

$B_H = \{\lambda_1 - \lambda_2 : \lambda_1, \lambda_2 \in Spec(H)\}$

Davies generator

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Bohr frequency:

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Central question: Rate of convergence

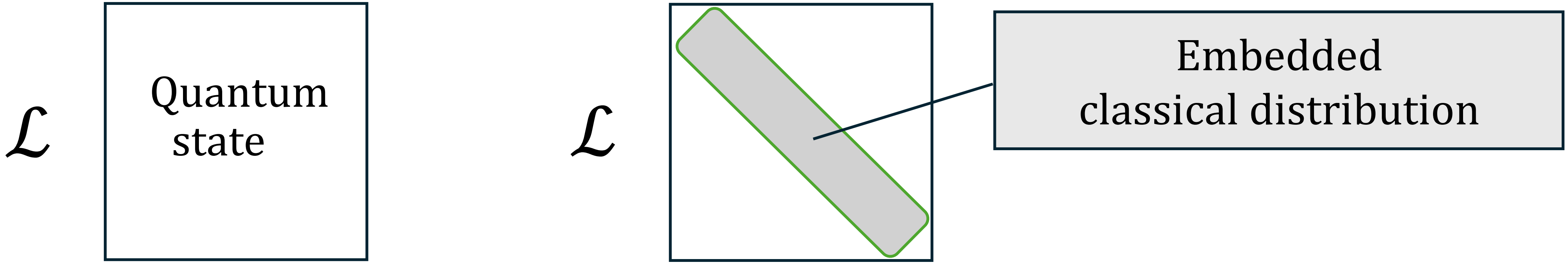
Rate of convergence is controlled by the generator's spectral gap

$$\lambda(\mathcal{L}) = E_1 - E_2 = |E_2|$$

Eigenvalues of generator $\mathcal{L}$: $0 = E_1 \geq E_2 \geq \cdots$

$$\mathcal{L}(id) = 0$$

Quantum vs classical walks



- $\mathcal{L}$: quantum random walk/linear operator on space of quantum states
- V_0: subspace of operators that commute with H. $\mathcal{L}(V_0) \subseteq V_0$
- $\mathcal{L}_{|V_0}$: isomorphic to classical random walk

Hamiltonians with simple spectrum: Temme'13

Any Hamiltonian: Our work

Classical walks

$\mathcal{L}_{|V_0}$: isomorphic to classical random walk

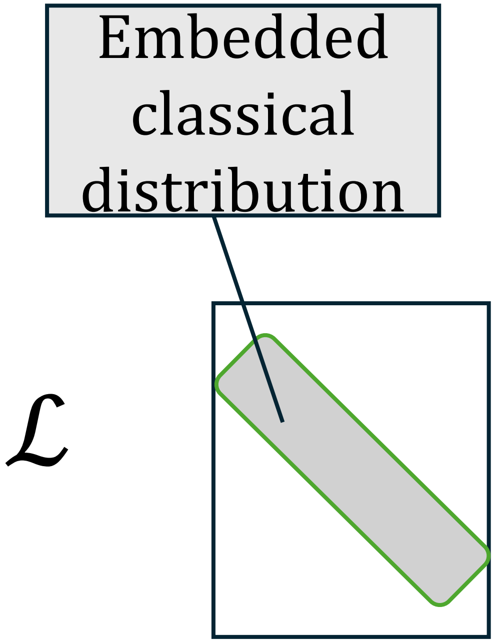
For $eigenbasis\ U = \{u_i\}_{i=1}^N$ of H $\quad\quad \rho = \rho_\beta = \frac{\exp(-\beta H)}{\mathrm{tr}(\exp(-\beta H))}$

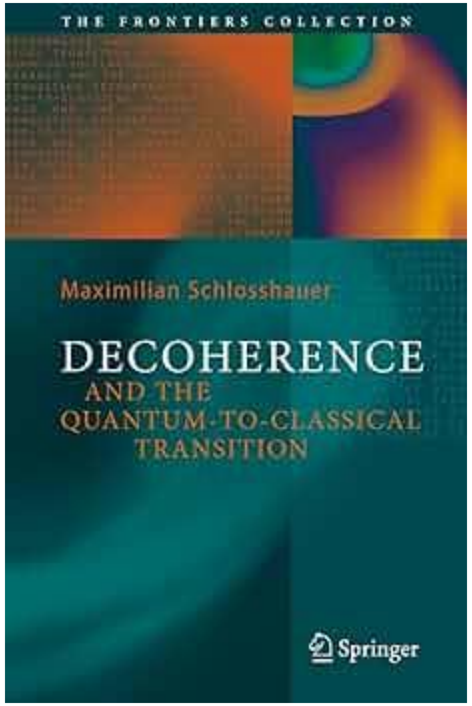
- Stationary distribution: $\pi : U \to \mathbb{R}_{\geq 0} \quad \pi(u_i) := \langle u_i|\rho|u_i\rangle$
- Transition matrix: $P_{\mathcal{L},U}[u_i \to u_j] = \langle \mathcal{L}(|u_j\rangle\langle u_j|), |u_i\rangle\langle u_i|\rangle$

<u>Prop</u>: There exists $eigenbasis\ U^*\ of\ H$

s.t. $\lambda(\mathcal{L}_{|V_0}) =$ spectral gap of classical Markov generator wrt U^*

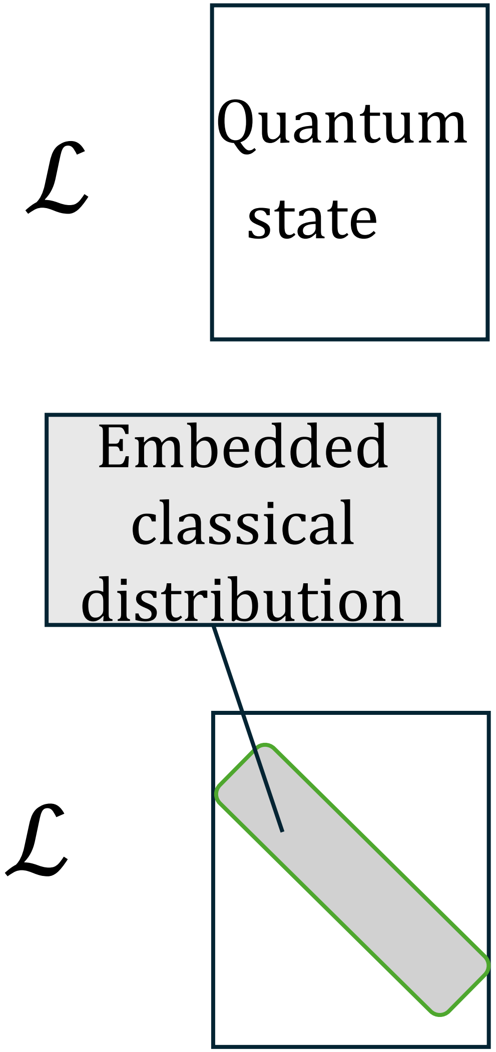
$\mathcal{L}$ Quantum state

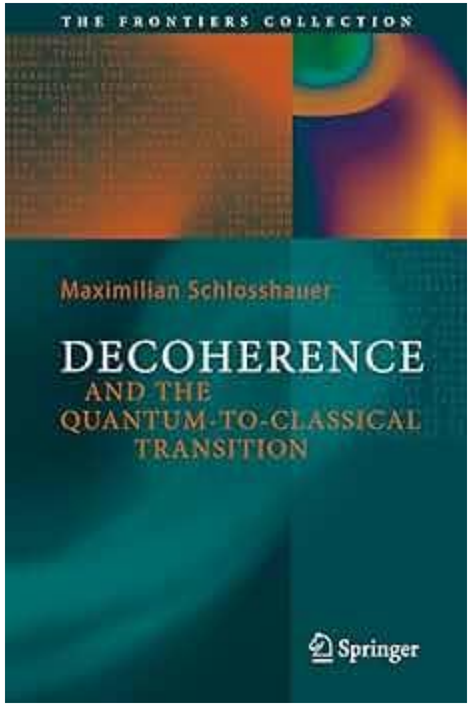




Q: quantum spectral gap comparable to classical spectral gap? $\lambda(\mathcal{L})$ vs. $\lambda(\mathcal{L}_{|V_0})$

- Physicists' belief: yes
- Mathematicians' findings: no, for some(contrived) Hamiltonian [Tem'13]





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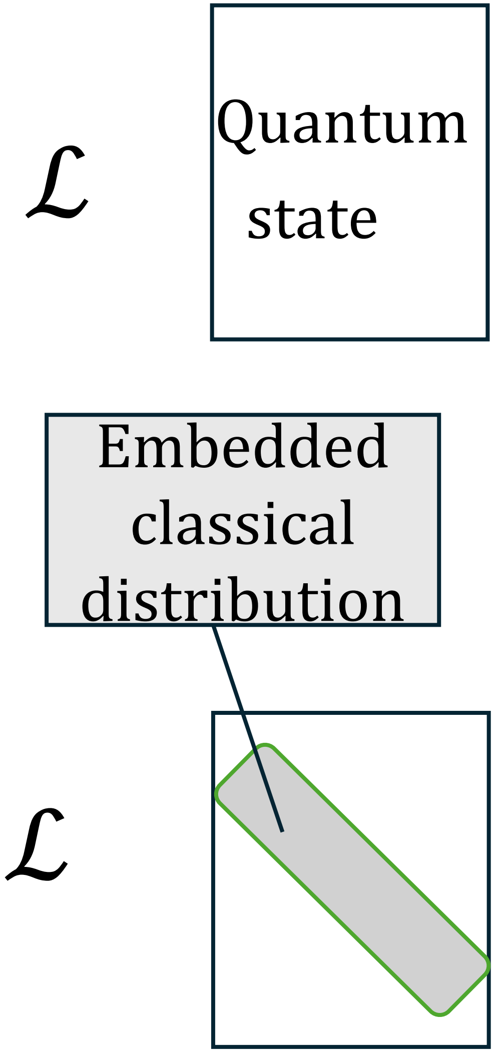
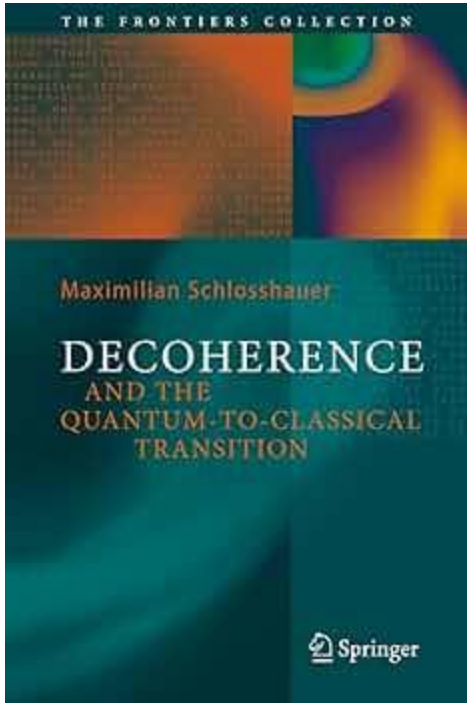
$\exists H, \mathcal{L}$:

$$\lambda(\mathcal{L}) = 2^{-n}\lambda(\mathcal{L}_{|V_0})$$

n: #qubits





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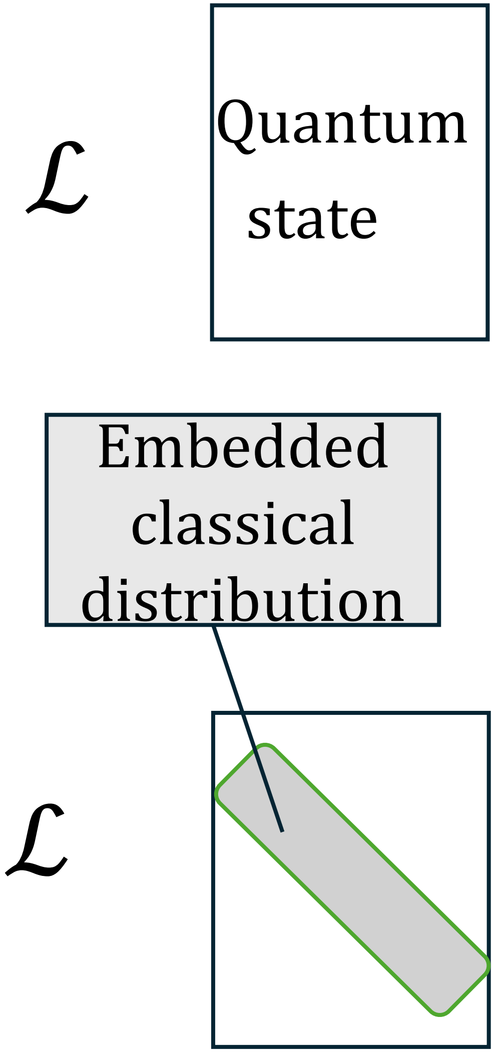
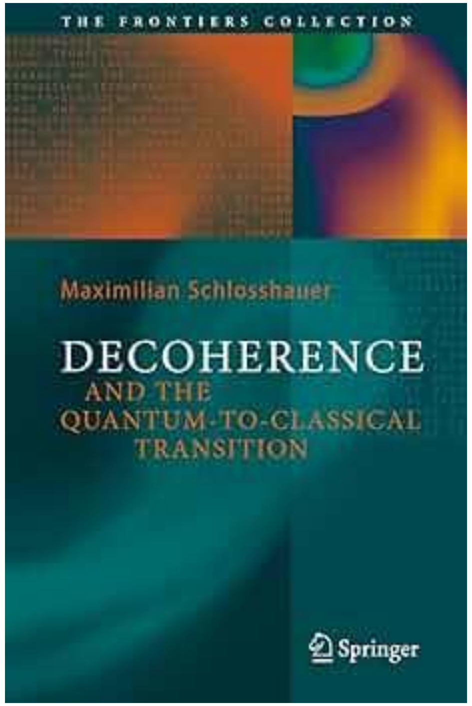
Eigenvalues of H are $1,2,\ldots,2^n$





Q: quantum spectral gap comparable to classical spectral gap? $\lambda(\mathcal{L})$ vs. $\lambda(\mathcal{L}_{|V_0})$

- Physicists' belief: yes
- Mathematicians' findings: no, for some Hamiltonian [Tem'13]
- Our work: yes, for Hamiltonians H where Spec(H) doesn't contain a proper arithmetic progression.
  Example: random perturbation of arbitrary Hamiltonian
- Implication:
  - Open the way to use classical techniques to analyze quantum walk
  - Match physicists' prediction

Proof

Def: Proper Arithmetic Progression of length D:

$$\{a, a+d, a+2d, \cdots, a+d\,(D-1)\} \subseteq Spec(H) \text{ where } d \neq 0$$

Thm 1: If Spec(H) doesn't contain a PAP of length $> D$

$$\lambda(\mathcal{L}_{|V_0}) \geq \lambda(\mathcal{L}) \geq \frac{1}{2D}\,\lambda(\mathcal{L}_{|V_0})$$

Lem 1: $H_{\boldsymbol{h}} = H_0 + \sum h_i Z_i$, $\exists \mathcal{U} \subseteq \mathbb{R}^n$ of Lebesgue measure 1 s.t. $\forall (h_i)_i \in \mathcal{U}$, $Spec(H_{\boldsymbol{h}})$ doesn't contain a PAP with length > 2 or repeated eigenvalues.

Cor 1: $H_{\boldsymbol{h}} = H_0 + \sum h_i Z_i$, H_0 arbitrary, $\exists \mathcal{U} \subseteq \mathbb{R}^n$ of Lebesgue measure 1 s.t. $\forall (h_i)_i \in \mathcal{U}$, Linbladian $\mathcal{L}$ wrt $H_{\boldsymbol{h}}$

$$\lambda(\mathcal{L}) = \Theta(1)\,\lambda(\mathcal{L}_{|V_0})$$

Proof of Lem 2: [inspired by Huang-Harrow'23]

Thm 1: If H doesn't contain a proper arithmetic progression of length $> D$

$$\lambda(\mathcal{L}_{|V_0}) \geq \lambda(\mathcal{L}) \geq \frac{1}{2D}\lambda(\mathcal{L}_{|V_0})$$

$V_0^c = \cup_{\omega \neq 0} \mathrm{V}_\omega$

V_ω: *image of map* $f \to f(\omega)$. *Invariant under* $\mathcal{L}$

$$\lambda(\mathcal{L}) = \min_{\omega} \lambda(\mathcal{L}_{|V_\omega})$$

$$f \mapsto f(\omega) := \sum_{\lambda_1,\lambda_2:\lambda_1-\lambda_2=\omega} \Pi_{\lambda_1} f \Pi_{\lambda_2}$$

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$$\mathrm{Var}(f) := \langle f, f \rangle_\rho - \mathrm{tr}(\rho f)\,\mathrm{tr}(\rho f^\dagger)$$

$$\lambda\big(\mathcal{L}_{|V_\omega}\big) = \min_{f \in V_\omega} \frac{\mathcal{E}_{\mathcal{L}}(f)}{\mathrm{Var}(f)}$$

$$f \in V_\omega \begin{array}{l} \nearrow \\ \searrow \end{array} \left. \begin{array}{l} g := e^{\frac{\beta\omega}{4}}(f f^\dagger)^{1/2} \\[2em] h := e^{-\frac{\beta\omega}{4}}(f^\dagger f)^{1/2} \end{array} \right\} \in V_0$$

$$2\mathcal{E}_{\mathcal{L}}(f) \geq \mathcal{E}_{\mathcal{L}}(g) + \mathcal{E}_{\mathcal{L}}(h)$$

$$\mathrm{Var}(g) + \mathrm{Var}(h) \geq \frac{1}{D}\,\mathrm{Var}(f)$$

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$$2\mathcal{E}_{\mathcal{L}}(f) \geq \mathcal{E}_{\mathcal{L}}(g) + \mathcal{E}_{\mathcal{L}}(h) \geq \lambda(\mathcal{L}_{|V_0})\left(Var(g) + Var(h)\right) \geq \frac{1}{D} Var(f)$$

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$$\mathrm{Var}(g) + \mathrm{Var}(h) \geq \frac{1}{D}\,\mathrm{Var}(f)$$

$$2\mathcal{E}_{\mathcal{L}}(f) - (\mathcal{E}_{\mathcal{L}}(g) + \mathcal{E}_{\mathcal{L}}(h)) = \sum_{\tilde{\omega}} \tilde{G}(\tilde{\omega}) T(\tilde{\omega}) \geq 0$$

$$T(\tilde{\omega}) = \mathrm{tr}(S(\omega)\tilde{g}S(\omega)^{\dagger}\tilde{g}) + \mathrm{tr}(S(\omega)\tilde{h}S(\omega)^{\dagger}\tilde{h}) - \mathrm{tr}(S(\omega)\tilde{f}S(\omega)^{\dagger}\tilde{f}^{\dagger}) - \mathrm{tr}(S(\omega)\tilde{f}^{\dagger}S(\omega)^{\dagger}\tilde{f}) \geq 0$$

Spectral decomposition then rewritten as Sum-of-Square

$$\tilde{g} = \sum_{i=1}^{k} \sqrt{\lambda_i} u_i u_i^{\dagger}, \quad \tilde{f} = \sum_{i=1}^{k} \sqrt{\lambda_i} u_i \tilde{v}_i^{\dagger}, \quad \tilde{h} = \sum_{i=1}^{k} \sqrt{\lambda_i} \tilde{v}_i \tilde{v}_i^{\dagger}$$

$$T(\tilde{\omega}) = \sum_{i,j} (\lambda_i \lambda_j)^{1/2} |u_i^{\dagger} S(\omega) u_j - \tilde{v}_i^{\dagger} S(\omega) \tilde{v}_j|^2 \geq 0$$

Lem 1': If H doesn't contain a proper arithmetic progression of length $> D$

$$\lambda(\mathcal{L}_{|V_\omega}) \geq \frac{1}{2D} \lambda(\mathcal{L}_{|V_0})$$

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$$\mathcal{E}_{\mathcal{L}}(f) := -\langle \mathcal{L}(f), f \rangle_\rho$$

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$$2\mathcal{E}_{\mathcal{L}}(f) \geq \mathcal{E}_{\mathcal{L}}(g) + \mathcal{E}_{\mathcal{L}}(h)$$

$$\boxed{\mathrm{Var}(g) + \mathrm{Var}(h) \geq \frac{1}{D} \mathrm{Var}(f)}$$

$$\mathrm{Var}(g) + \mathrm{Var}(h) \geq \frac{1}{D}\mathrm{Var}(f)$$

$[g, H] = 0 \Rightarrow$ Spectral decomposition where $\{u_i\}_i$ and $\{v_i\}_i$ are orthonormal eigenbasis of H

$$g = e^{\frac{\beta\omega}{4}} \sum \lambda_i |u_i\rangle\langle u_i|, \; f = \sum \lambda_i |u_i\rangle\langle v_i|, \text{ and } h = e^{-\frac{\beta\omega}{4}} \sum \lambda_i |v_i\rangle\langle v_i|$$

AM-GM inequality: $\rho(u_i), \rho(v_i)$ are eigenvalues of ρ corresponding to u_i, v_i

$$\mathrm{Var}(g) \geq \left(1 - \sum \rho(u_i)\right)\mathrm{Var}(f), \quad \mathrm{Var}(h) \geq \left(1 - \sum \rho(v_i)\right)\mathrm{Var}(f)$$

If $\beta\omega \geq 0$: show $1 - \sum \rho(u_i) \geq 1/D \;\Rightarrow\; \mathrm{Var}(g) \geq \frac{1}{D}\mathrm{Var}(f)$

If $\beta\omega \leq 0$: show $Var(h) \geq \frac{1}{D} Var(f)$

$$\mathrm{Var}(g) + \mathrm{Var}(h) \geq \frac{1}{D}\mathrm{Var}(f)$$

$\{u_i\}_i$ and $\{v_i\}_i$ are orthonormal eigenbasis of H, eigenvalue $H(u_i), H(v_i)$

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Assume $\beta\omega \geq 0$: show $\boxed{1 - \sum \rho(u_i) \geq 1/D} \Rightarrow \mathrm{Var}(g) \geq \frac{1}{D}\mathrm{Var}(f)$

$f \in V_\omega \Rightarrow H(v_i) = H(u_i) - \omega$

Take maximal sequence $u_{i_1}, \ldots, u_{i_k}$, where $H(u_{i_{j+1}}) = H(u_{i_j}) - \omega \forall j$

$H(v_{i_k}) = H(u_{i_k}) - \omega$ is also in $\mathrm{spec}(H)$

$$\mathrm{Var}(g) + \mathrm{Var}(h) \geq \frac{1}{D}\mathrm{Var}(f)$$

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Assume $\beta\omega \geq 0$: show $\boxed{1 - \sum \rho(u_i) \geq 1/D} \Rightarrow \mathrm{Var}(g) \geq \frac{1}{D}\mathrm{Var}(f)$

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but v_{i_k} not in spectral decomposition of g

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Assume $\beta\omega \geq 0$: show $\boxed{1 - \sum \rho(u_i) \geq 1/D} \Rightarrow \mathrm{Var}(g) \geq \frac{1}{D}\mathrm{Var}(f)$

$f \in V_\omega \Rightarrow H(v_i) = H(u_i) - \omega$

Take $\boxed{\text{maximal}}$ sequence $u_{i_1}, \ldots, u_{i_k}$, where $H(u_{i_{j+1}}) = H(u_{i_j}) - \omega \forall j$

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$\boxed{\text{but } v_{i_k} \text{ not in spectral decomposition of } g}$

$H(u_{i_1}), \cdots, H(u_{i_k}), H(v_{i_k}) : (k+1)\text{-AP} \Rightarrow k+1 \leq D$

$$\mathrm{Var}(g) + \mathrm{Var}(h) \geq \frac{1}{D} \mathrm{Var}(f)$$

$\{u_i\}_i$ and $\{v_i\}_i$ are orthonormal eigenbasis of H, eigenvalue $H(u_i), H(v_i)$

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Assume $\beta\omega \geq 0$: show $\boxed{1 - \sum \rho(u_i) \geq 1/D} \quad \Rightarrow \quad \mathrm{Var}(g) \geq \frac{1}{D} \mathrm{Var}(f)$

Take maximal sequence $u_{i_1}, \ldots, u_{i_k}$, where $H(u_{i_{j+1}}) = H(u_{i_j}) - \omega \forall j$

$H(v_{i_k}) = H(u_{i_k}) - \omega$ is also in $\mathrm{spec}(H)$ but $v_{i_k} \notin SVD(g)$

$H(u_{i_1}), \cdots, H(u_{i_k}), H(v_{i_k})$: $(k+1)$-AP $\Rightarrow$ $k + 1 \leq D$

$$\boxed{\sum_{v \notin SVD(g)} \rho(v) \geq \frac{1}{D-1} \sum_{u \in SVD(g)} \rho(u) \Rightarrow 1 - \sum_{u \in SVD(g)} \rho(u) = \sum_{v \notin SVD(g)} \rho(v) \geq \frac{1}{D}}$$

Open question

- Applications
- Modified Log-Sobolev inequality (MLSI) instead of spectral gap?