On quantum to classical comparison for Davies generator

Thuy-Duong "June" Vuong

UC Berkeley/UC San Diego

Joint work with Joao Basso, Shirshendu Ganguly, Alistair Sinclair, Nikhil Srivastava, Zachary Stier

Quantum crash course

- Quantum operator on n qubits $\leftrightarrow f \in \mathbb{C}^{2^n \times 2^n}$
- Quantum state on n qubits $\leftrightarrow$ Hermitian $\sigma \in \mathbb{C}^{2^n \times 2^n}, tr(\sigma) = 1$
- Hamiltonian $H \in \mathbb{C}^{2^n \times 2^n}, H$ Hermitian
- Quantum Gibbs state of H at inverse temperature β: $\rho_\beta = \frac{\exp(-\beta H)}{\mathrm{tr}(\exp(-\beta H))}$

- Pure quantum states are sometimes represented by vectors $|\psi\rangle \in \mathbb{C}^{2^n}$
  $\leftrightarrow$ density matrix $|\psi\rangle\langle\psi| \in \mathbb{C}^{2^n \times 2^n}$
- General quantum states are statistical mixture of pure state

$$\sigma = \sum p_i |\psi_i\rangle\langle\psi_i|$$

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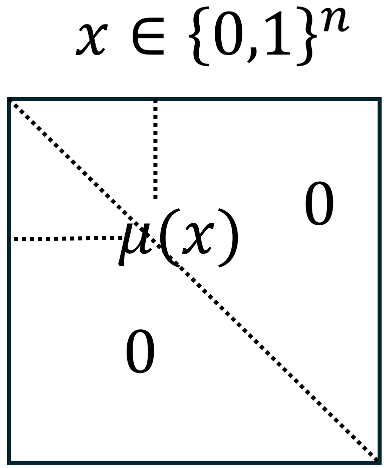
<u>Example</u>: classical distribution $\mu: \{0,1\}^n \to \mathbb{R}_{\geq 0} \to$ quantum state



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<u>Example</u>: classical distribution $\mu: \{0,1\}^n \to \mathbb{R}_{\geq 0} \leftarrow$ quantum state

$$\mu(i) = p_i \qquad \sigma = \sum p_i |\psi_i\rangle\langle\psi_i|$$

Quantum Markov processes (Davies generator)

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

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

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

Understand & predict how open quantum systems behave:

- Physics: models thermalization
- Quantum computing: prepare quantum Gibbs state → optimization, quantum ML, candidate quantum to classical speedup

Davies generator

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

$$[A,B] = AB - BA$$

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

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

- Linbladian dynamics $\sigma_t = e^{t\mathcal{L}^+}\sigma_0$
- 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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Π_λ : *projector to the eigenspace of* H *of eigenvalue* λ

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- Hamiltonian H: describes the internal quantum system
- Jump operators $\mathcal{S} = \{S\}$ s.t. $\mathcal{S}^\dagger = \{ S^\dagger : S \in \mathcal{S} \} = \mathcal{S}$
- Transition rate G s.t. $G(\omega) = G(-\omega)e^{-\beta\omega}$

$\Rightarrow$reversible

- (KMS) reversible: $\langle \mathcal{L}(f), g\rangle_\rho = \langle f, \mathcal{L}(g)\rangle_\rho$

$$\langle A, B\rangle_\rho := \mathrm{tr}(\rho^{1/2} A \rho^{1/2} B^\dagger)$$

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Central question: Rate of convergence

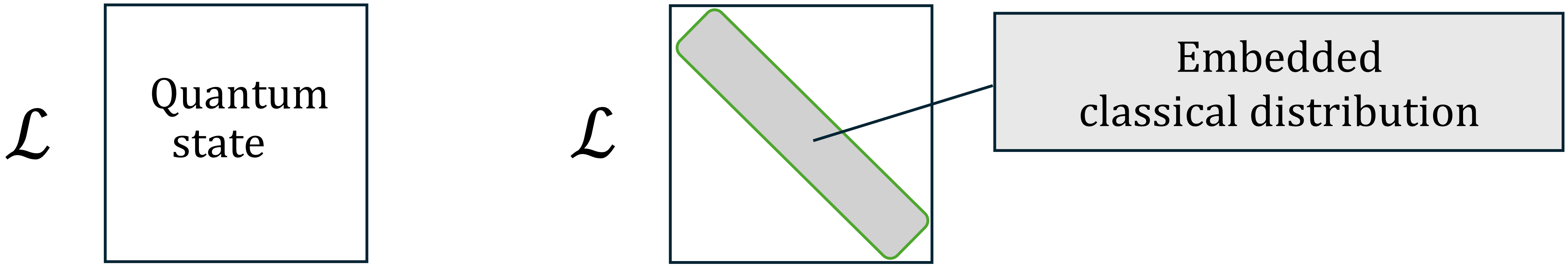
Rate of convergence is controlled by the generator's spectral gap

$$\lambda(\mathcal{L}) = \lambda_1 - \lambda_2 = |\lambda_2|$$

Eigenvalues of generator $\mathcal{L}$: $0 = \lambda_1 \geq \lambda_2 \geq \cdots$

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

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

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

Classical walks

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<u>Claim</u>: $f = \sum f_i |u_i\rangle\langle u_i|$. $\qquad$ Let $F : U \to \mathbb{R}$ where $F(u_i) = f_i$

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

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

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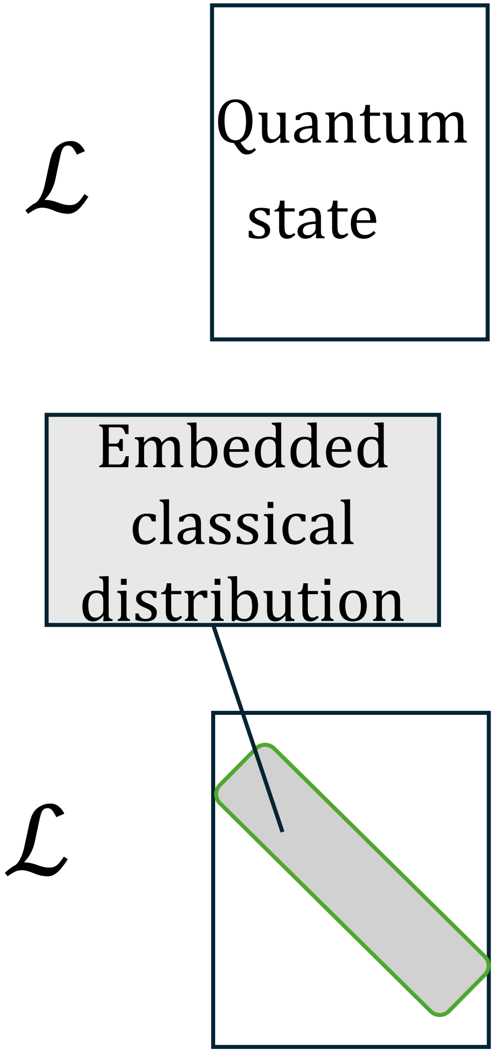
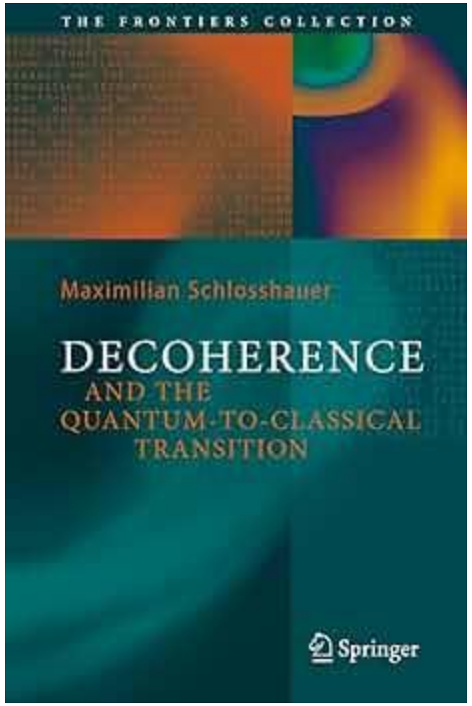
<u>Prop</u>: There exists $eigenbasis\ U^*\ of\ H$

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





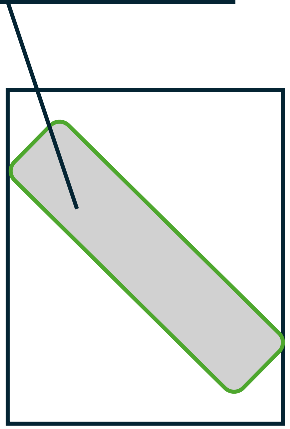
Q: quantum spectral gap comparable to classical spectral gap? $\lambda(\mathcal{L})$ vs. $\lambda(\mathcal{L}_{|V_0})$

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

$\mathcal{L}$

Quantum state

Embedded classical distribution



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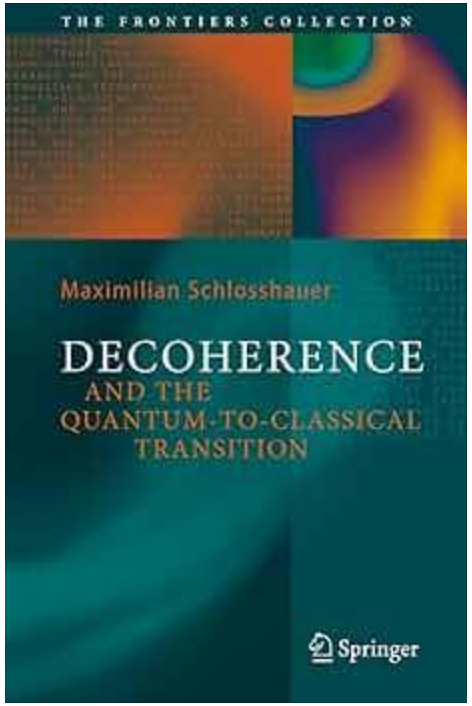

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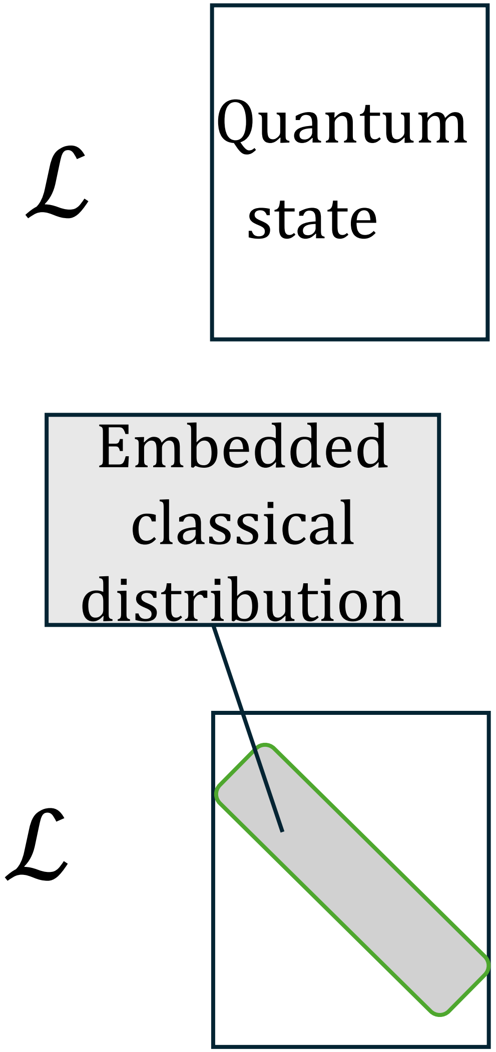
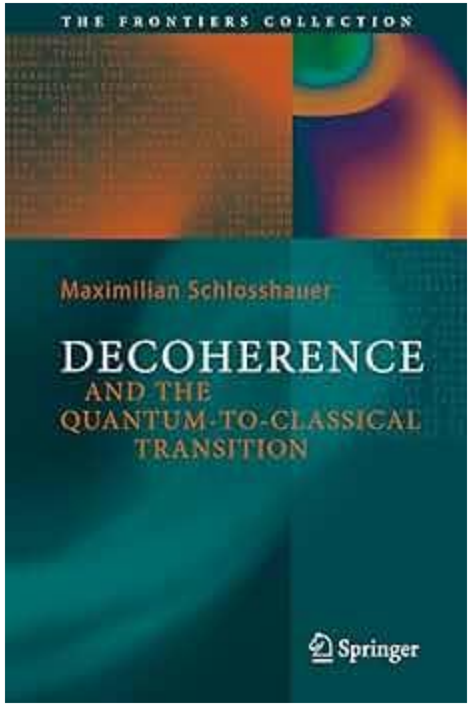
$\exists H, \mathcal{L}$:

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

n: #qubits





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

$\mathcal{L}$

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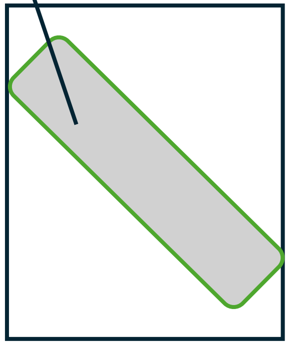

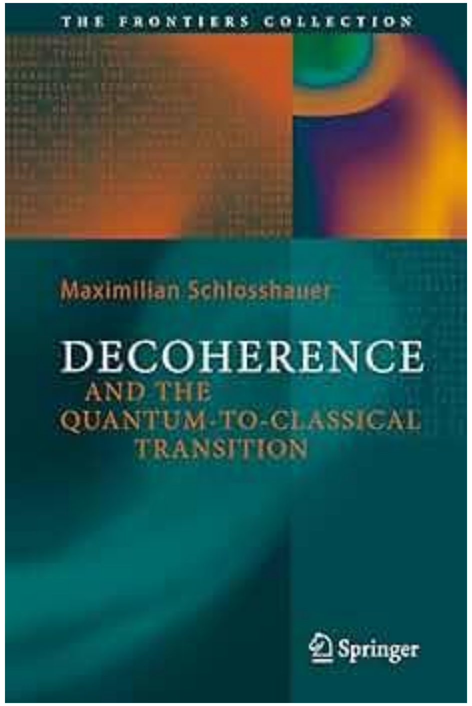

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- Our work: yes, for generic Hamiltonians, e.g. those obtained by perturbing a fixed Hamiltonian by a random external field.

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

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

$\mathcal{L}$

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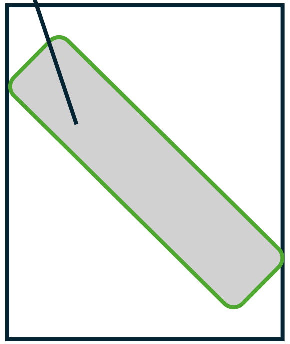

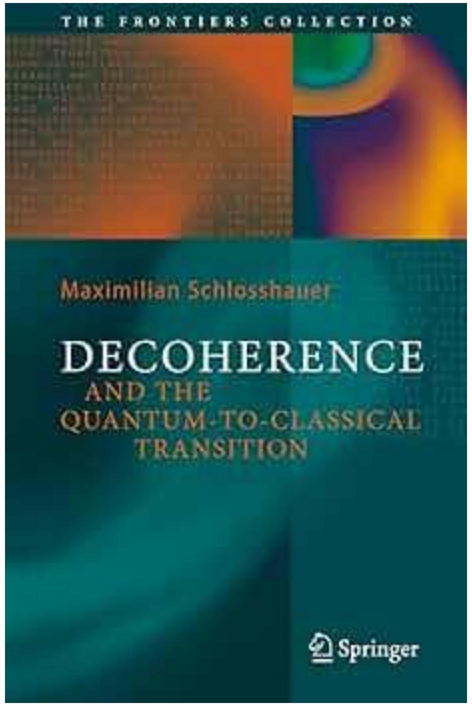

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- Mathematicians' findings: no, for some Hamiltonian [Tem'13]
- Our work: yes, for generic Hamiltonians, e.g. those obtained by perturbing a fixed Hamiltonian by a random external field.
- Implication:
  - Open the way to use classical techniques to analyze quantum walk
  - Match physicists' prediction

Proof

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

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

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

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

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

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

Proof (insipired by [Huang-Harrow'23]):

Create polynomial F, G s.t $H_{\boldsymbol{h}}$ doesn't have 3-APs $\Leftrightarrow F(\boldsymbol{h}) \neq 0$

$H_{\boldsymbol{h}}$ doesn't have repeated eigenvalues $\Leftrightarrow G(\boldsymbol{h}) \neq 0$

$$F := \prod_{i,j,k \text{ distinct}} (\lambda_i + \lambda_j - 2\lambda_k) \qquad G(h_1, \ldots, h_n) := \prod_{i,j:i \neq j} (\lambda_i - \lambda_j)$$

$\boldsymbol{h} = R\,\widetilde{\boldsymbol{h}}$, $\mathrm{R} \to +\infty$, $H_{\boldsymbol{h}} \to \mathrm{R}\sum \widetilde{h}_i Z_i$

Reducing to prove that $\sum h_i Z_i$ doesn't have 3-AP or repeated eigenvalues for generic (e.g. linearly independent) $h_1, \cdots, h_n$

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

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

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

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

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

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

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

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

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

$$\mathcal{E}(f) = \frac{1}{2} \sum_{S \in \mathcal{S}, \omega} \tilde{G}(\omega) \| [S(\omega), f] \|_{\rho}^{2} \quad where\ \tilde{G}(\omega) = G(\omega) e^{\frac{\beta\omega}{2}}$$

$$\tilde{G}(\omega) = G(\omega) e^{\frac{\beta\omega}{2}} = \tilde{G}(-\omega),$$

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

$$T(\tilde{\omega}) := \|[S(\tilde{\omega}), f]\|_\rho^2 + \|[S^\dagger(-\tilde{\omega}), f]\|_\rho^2 - \frac{1}{2}(\|[S(\tilde{\omega}), g]\|_\rho^2 + \|[S^\dagger(-\tilde{\omega}), g]\|_\rho^2 + \|[S(\tilde{\omega}), h]\|_\rho^2 + \|[S^\dagger(-\tilde{\omega}), h]\|_\rho^2)$$

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

$$\tilde{f} = \rho^{1/4}f\rho^{1/4}, \tilde{g} = \rho^{1/4}g\rho^{1/4}, \tilde{h} = \rho^{1/4}h\rho^{1/4} \qquad \tilde{g} = (\tilde{f}\tilde{f}^\dagger)^{1/2} \quad \tilde{h} = (\tilde{f}^\dagger\tilde{f})^{1/2}$$

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

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

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

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

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

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

Orthonormal eigenbasis $\{u_i\}_i, \{v_i\}_i$ of H $\quad H(v_i) = H(u_i) - \omega$

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

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 spec(H)

but v_{i_k} not in spectral decomposition of g

WLOG assume $\beta\omega \geq 0 \Rightarrow \rho(v_{i_k}) \geq \frac{1}{k}\sum_{i=1} \rho(u_{i_j})$

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

$$1 - \sum \rho(u_i) \geq 1/D$$

$$\mathrm{Var}(g) \geq \tfrac{1}{D}\mathrm{Var}(f)$$