Near-optimal ground state preparation

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Joint work with Lin Lin (UC Berkeley, LBNL)

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The ground energy and the ground state

- Given a Hamiltonian $H = \sum_k \lambda_k |\psi_k\rangle\langle\psi_k| \in \mathbb{C}^{2^n \times 2^n}$, find its smallest eigenvalue λ_0 **(ground energy)**, and the corresponding eigenstate $|\psi_0\rangle$ **(ground state)**.

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- Without additional information, the task of finding the ground energy of a k-local Hamiltonian is QMA-complete.

The assumptions

(i) We assume we are given a circuit U_I to prepare an initial state $|\phi_0\rangle$ s.t. $|\langle\phi_0|\psi_0\rangle| \geq \gamma$.

(ii) **For ground state preparation only:** we assume there is a spectral gap at least Δ between λ_0 and λ_1.

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(2) U_I can also be constructed using variational algorithms (VQE, QAOA) and adiabatic evolution.

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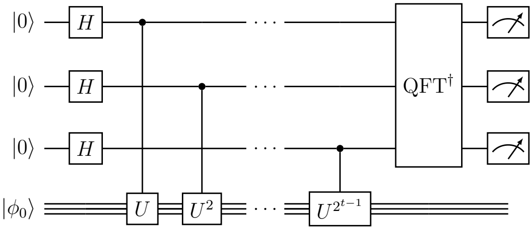

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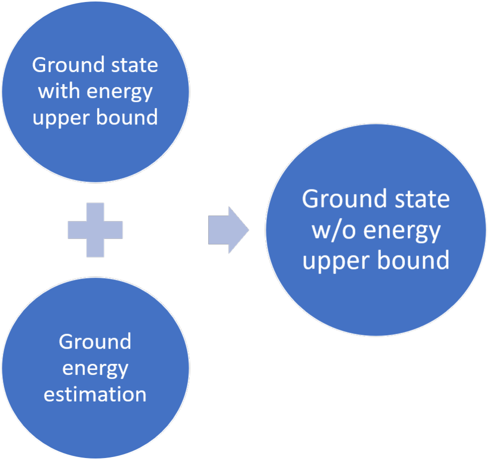
Outline of our results



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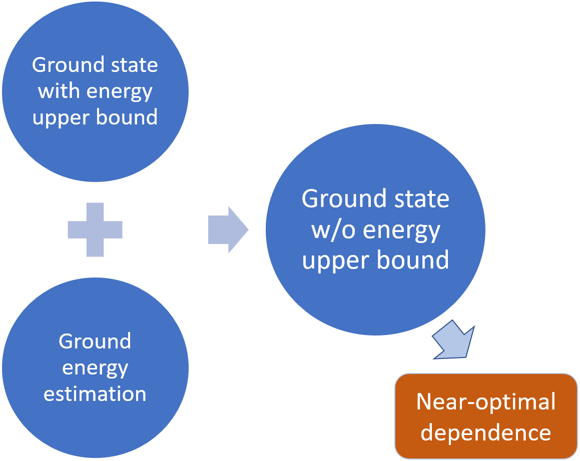

The main result

Ground energy (Theorem 8)

- **Oracles:** a unitary U_I such that $U_I |0^n\rangle = |\phi_0\rangle$, another unitary U_H that "block-encodes" H.
- **Assumption:** $|\langle\phi_0|\psi_0\rangle| \geq \gamma$ for some known $\gamma > 0$.
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- **Gate complexity:** roughly linear w.r.t. query complexity.

Compare with previous works

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- Get the best of both worlds!
- Near-optimal dependence on Δ and γ.

Block-encoding

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- Many matrices of practical interest can be effificently block-encoded (k-local, sparse, second-quantized fermionic Hamiltonians, etc.)
- First proposed in (Low and Chuang, 2019, "Hamiltonian simulation by qubitization") (standard form)

Quantum singular value transformation

- **Quantum signal processing (QSP)** (Low and Chuang, 2017), **quantum singular value transformation (QSVT)** (Gilyén, Su, Low, and Wiebe, 2019).
- For a Hermitian A,

$$U_A = \begin{pmatrix} A/\alpha & \cdot \\ \cdot & \cdot \end{pmatrix} \xrightarrow{\text{QSVT}} \begin{pmatrix} p(A/\alpha) & \cdot \\ \cdot & \cdot \end{pmatrix}.$$

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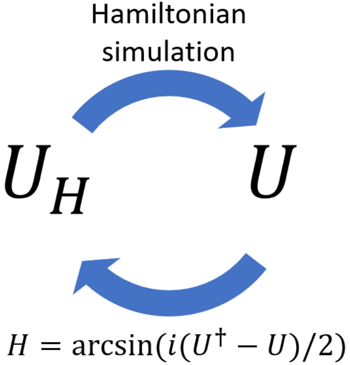
- Number of queries to U_A is d.
- Can prepare state $p(A/\alpha) |\phi\rangle$ (with amplitude amplification) and estimate $\| p(A/\alpha) |\phi\rangle \|$ (with amplitude estimation).

Equivalence between query models

U_H block-encodes H, $U = e^{-i\tau H}$.



- Going from $U = e^{-i\tau H}$ to H: easy to construct a block-encoding of $i(U^\dagger - U)/2$;
- Apply QSVT to $i(U^\dagger - U)/2$ to get $\arcsin(i(U^\dagger - U)/2) = H$. (GSLW full version)

Ground state preparation through eigenstate filtering

- We have upper bound μ such that $\lambda_0 \leq \mu - \Delta/2 < \mu + \Delta/2 \leq \lambda_1$.
- Idea: use an **approximate projection operator** to filter out the unwanted eigenstates.
- **Filter polynomial** $p(x)$ satisfies

$$p(x) \begin{cases} \geq 1 - \epsilon' & -1 \leq x \leq -\delta \\ \leq \epsilon' & \delta \leq x \leq 1 \end{cases}$$

  and $0 \leq p(x) \leq 1$ for $x \in [-1, 1]$.
- Can find polynomial of degree $d = \mathcal{O}(\delta^{-1} \log(\epsilon'^{-1}))$ (Low and Chuang, 2017) (Eremenko-Yuditskii, 2007).

Eigenstate filtering

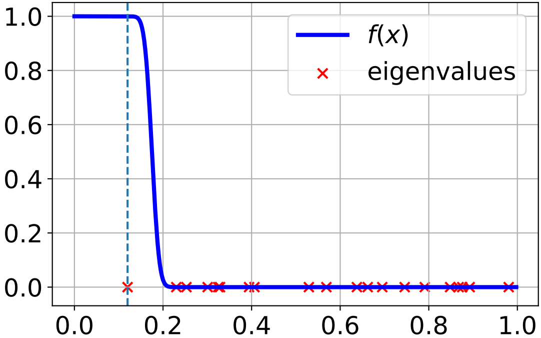


Figure: Applying QSVT with $f(x) = p((x - \mu)/2)$ to H.
$\lambda_0 \leq \mu - \delta < \mu + \delta \leq \lambda_1$, $\delta = \mathcal{O}(\Delta)$.

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- Requires knowledge of μ and Δ.

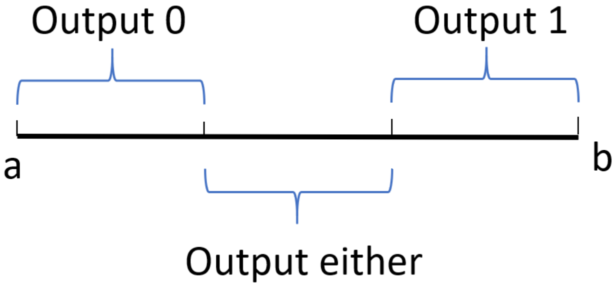
Ground energy estimation

The decision problem: $a \le \lambda_0 \le b$.

(i) When $a \le \lambda_0 \le \frac{2}{3}a + \frac{1}{3}b$, output 0;

(ii) When $\frac{2}{3}a + \frac{1}{3}b \le \lambda_0 \le \frac{1}{3}a + \frac{2}{3}b$, output 0 or 1;

(iii) When $\frac{1}{3}a + \frac{2}{3}b \le \lambda_0 \le b$, output 1.



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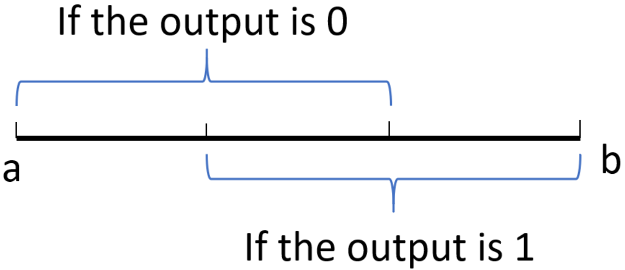

Ground energy estimation

- If the decision problem can be solved, then we can start with some $a \leq \lambda_0 \leq b$, and repeatedly solve the decision problem:
  (1) If the output is 0, it indicates $a \leq \lambda_0 \leq \frac{1}{3}a + \frac{2}{3}b$. We update $b \leftarrow \frac{1}{3}a + \frac{2}{3}b$;
  (2) If the output is 1, it indicates $\frac{2}{3}a + \frac{1}{3}b \leq \lambda_0 \leq b$. We update $a \leftarrow \frac{2}{3}a + \frac{1}{3}b$.

- Always guaranteed: $a \leq \lambda_0 \leq b$, $(b-a)_{\text{new}} = (2/3)(b-a)_{\text{old}}$.

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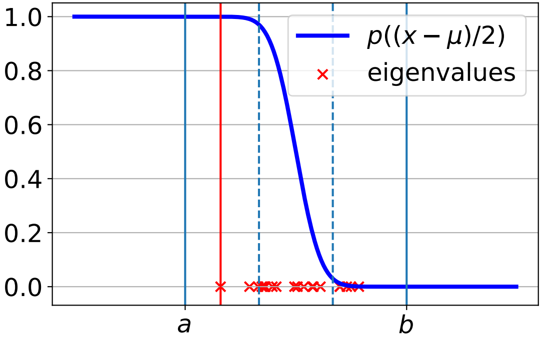
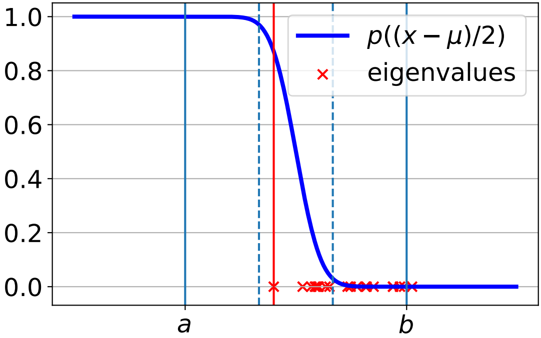
- Solve the decision problem through eigenstate filtering.

Solving the decision problem (i)



$$\lambda_0 \leq \frac{2}{3}a + \frac{1}{3}b \implies \|p((H-\mu)/2)\,|\phi_0\rangle\,\| \geq \gamma(1-\epsilon')$$

Solving the decision problem (ii)



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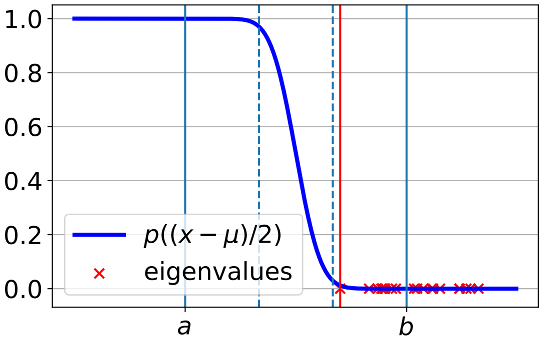

$$\lambda_0 \geq \frac{1}{3}a + \frac{2}{3}b \implies \| p((H-\mu)/2) \, |\phi_0\rangle \, \| \leq \epsilon'$$

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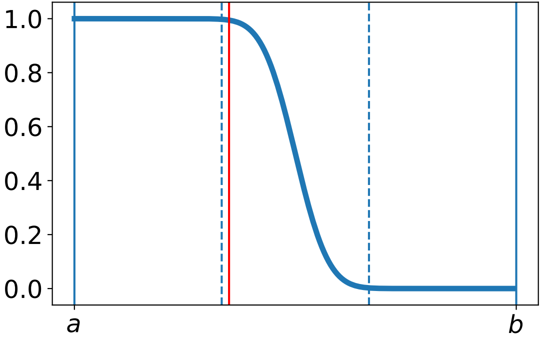
- Can use amplitude estimation to do so with overhead $\mathcal{O}(\gamma^{-1})$.
- Error probability can be exponentially suppressed using majority voting (Chernoff bound).

The search process



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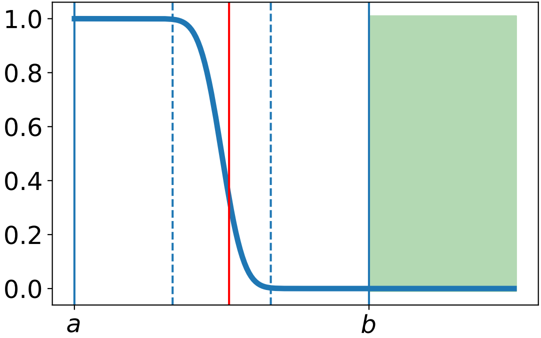

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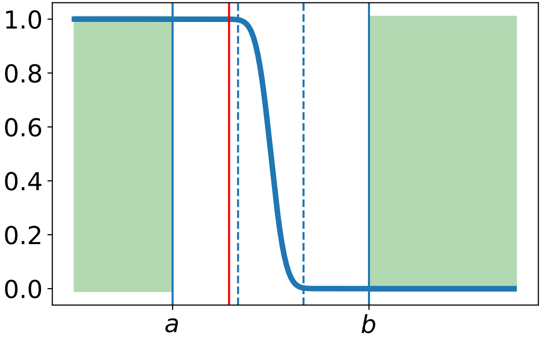

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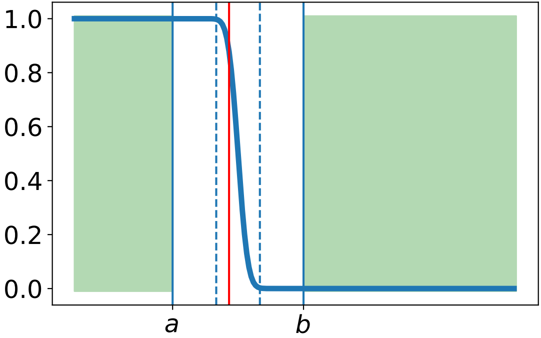

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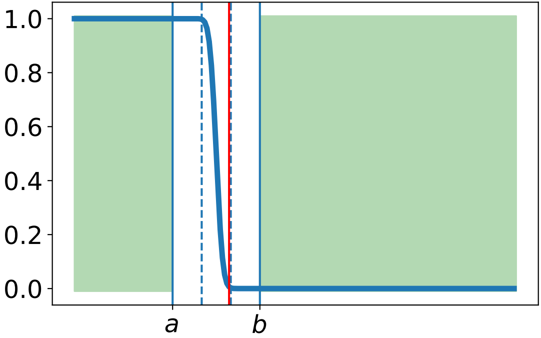

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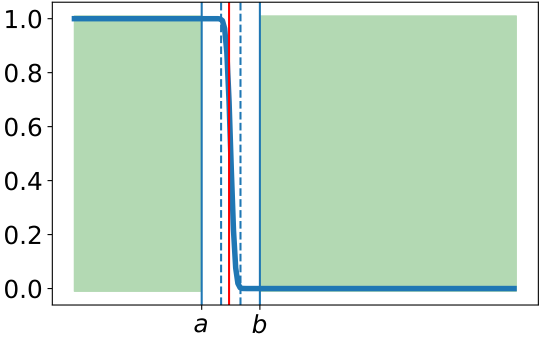

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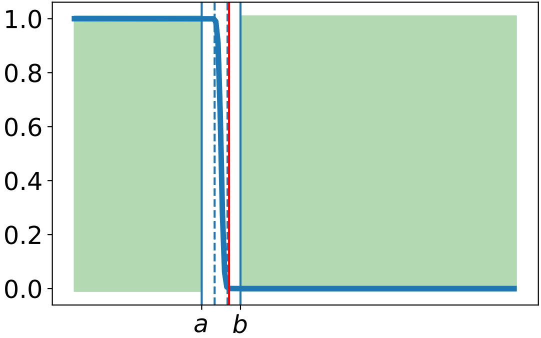

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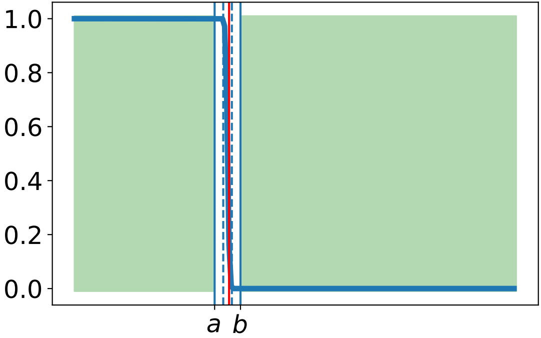

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- There are $\mathcal{O}(\log(\epsilon^{-1}))$ steps, and $\delta = \frac{1}{3}, \frac{1}{3^2}, \frac{1}{3^3}, \ldots, \epsilon$;
- Total number of queries to U_I is $\mathcal{O}(\gamma^{-1})$ and number of queries to U_H is $\mathcal{O}(\epsilon^{-1}\gamma^{-1})$.

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- Only need a weaker assumption $\lambda_1 - \lambda_0 \geq \Delta$;
- Also $|\langle \phi_0 | \psi_0 \rangle| \geq \gamma$;
- First estimate the ground energy to precision $\Delta/4$ to get a λ_0', let $\mu = \lambda_0' + \Delta/2$, this μ satisfies

$$\lambda_0 \leq \mu - \Delta/4 < \mu + \Delta/4 \leq \lambda_1.$$

  Then we apply eigenstate filtering.

Ground state preparation

- We want to prepare the ground state without knowing μ such that $\lambda_0 \leq \mu - \Delta/2 \leq \mu + \Delta/2 \leq \lambda_1$.
- Only need a weaker assumption $\lambda_1 - \lambda_0 \geq \Delta$;
- Also $|\langle \phi_0 | \psi_0 \rangle| \geq \gamma$;
- First estimate the ground energy to precision $\Delta/4$ to get a λ_0', let $\mu = \lambda_0' + \Delta/2$, this μ satisfies

$$\lambda_0 \leq \mu - \Delta/4 < \mu + \Delta/4 \leq \lambda_1.$$

  Then we apply eigenstate filtering.
- $\mathcal{O}(\gamma^{-1}\Delta^{-1}\log(\epsilon^{-1}))$ queries to U_H and $\mathcal{O}(\gamma^{-1})$ queries to U_I.

The unstructured search problem

- The unstructure search problem: among n-bit strings, given oracle U_w such that

$$U_w |x\rangle = \begin{cases} |x\rangle, & x \neq w \\ -|x\rangle, & x = w, \end{cases}$$

  find w.
- Cannot be solved with $o(\sqrt{N})$ queries to U_w (BBBV Theorem).
- This is a ground state preparation problem with Hamiltonian U_w.

Lower bound on the overlap dependence

- We let $U_H = H = U_w$;
- $|\phi_0\rangle = |u\rangle = U_I |0^n\rangle$, $U_I = \mathrm{H}^{\otimes n}$;
- $\gamma = 1/\sqrt{N}$, $\Delta = 2$.

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- Then this algorithm solves the unstructured search problem with $o(\sqrt{N})$ queries to $U_H = U_w$.
- Contradiction!

Overlap-gap trade-off

- Childs, Deotto, Farhi, and Goldstone, 2002, "Quantum search by measurement".
- $D = I - 2|u\rangle\langle u|$, $|u\rangle = |+\rangle^{\otimes n}$,
  $H(t) = (1-t)D + tU_w$.

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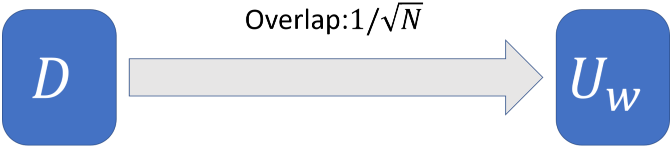

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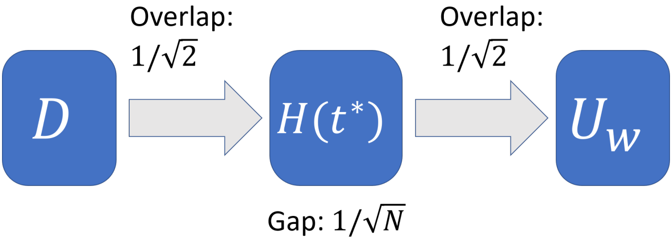

$$t^* = 1/2$$

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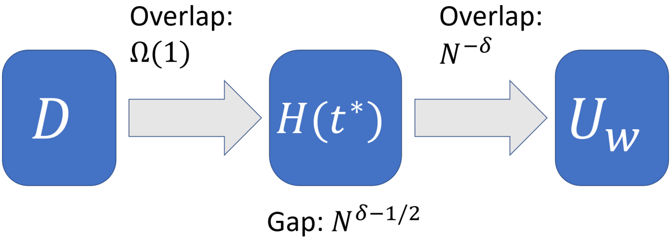

$$t^* = 1/2 - N^{-1/2+\delta}$$

Summary of results

- Preparation of the ground state with knowledge of μ through eigenstate filtering;
- Ground energy estimation through repeated solving a decision problem;
- Ground state preparation with near-optimal dependence on the overlap and the spectral gap.