Exact and efficient Lanczos method on an quantum computer

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1. Lanczos method

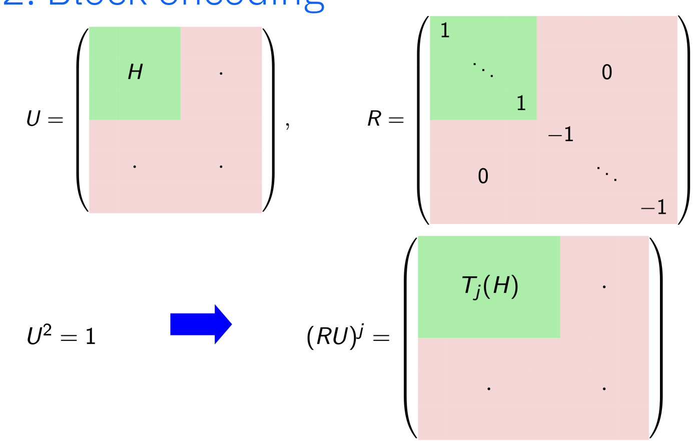
Krylov space

1. Initial guess $|\psi_0\rangle \Rightarrow H|\psi_0\rangle \Rightarrow \cdots \Rightarrow H^{D-1}|\psi_0\rangle$
2. $(\mathbf{H}, \mathbf{S})$ = project H onto span$\underbrace{[|\psi_0\rangle, H|\psi_0\rangle, H^2|\psi_0\rangle, \ldots, H^{D-1}|\psi_0\rangle]}_{V}$

$$V^\dagger \; H \; V = \mathbf{H}, \qquad V^\dagger \; V = \mathbf{S}$$

3. Lowest eigenvalue of $\mathbf{Hv} = \lambda \mathbf{Sv}$ approximates lowest eigenvalue of H

2. Block encoding



e.g., $H = \sum_i \alpha_i P_i$

$$\Rightarrow U = \sum_i |i\rangle\langle i| \otimes P_i$$

$$|G\rangle = \sum_i \sqrt{\alpha_i}|i\rangle$$

$$\Rightarrow R = 2|G\rangle\langle G| - 1$$

$T_j(H) = j$th Chebyshev polynomial

3. Quantum Lanczos method

Idea: replace V by $[|\psi_0\rangle, T_1(H)|\psi_0\rangle, T_2(H)|\psi_0\rangle, \ldots, T_{D-1}(H)|\psi_0\rangle]$

Same span $\Rightarrow$ same Krylov space!

Advantages:

- Krylov basis constructed exactly (no error from simulating time evolution)
- Energy error converges exponentially quickly with D

4. Required matrix elements

$$\mathbf{S_{ij}} = \langle T_i(H) T_j(H) \rangle = \left(\langle T_{i+j}(H) \rangle + \langle T_{|i-j|}(H) \rangle \right)/2$$

$$\mathbf{H_{ij}} \propto \langle T_{i+j+1}(H) \rangle + \langle T_{|i+j-1|}(H) \rangle + \langle T_{|i-j+1|}(H) \rangle + \langle T_{|i-j-1|}(H) \rangle$$

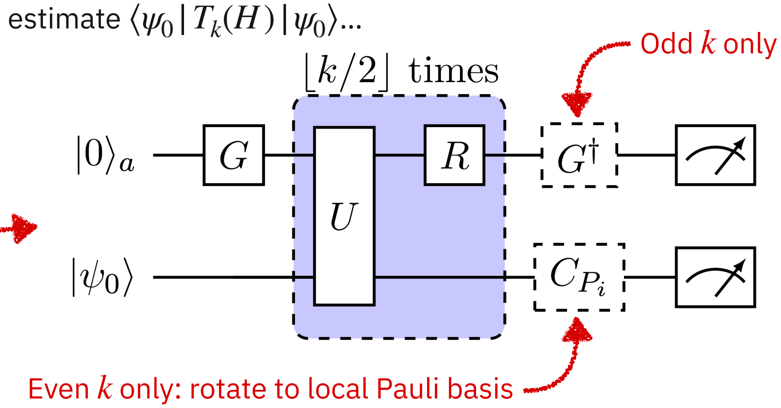
for $i, j = 0,1,2,\ldots,D-1$. $\Rightarrow$ only need to estimate

$$\langle T_k(H) \rangle = \langle \psi_0 | T_k(H) | \psi_0 \rangle$$

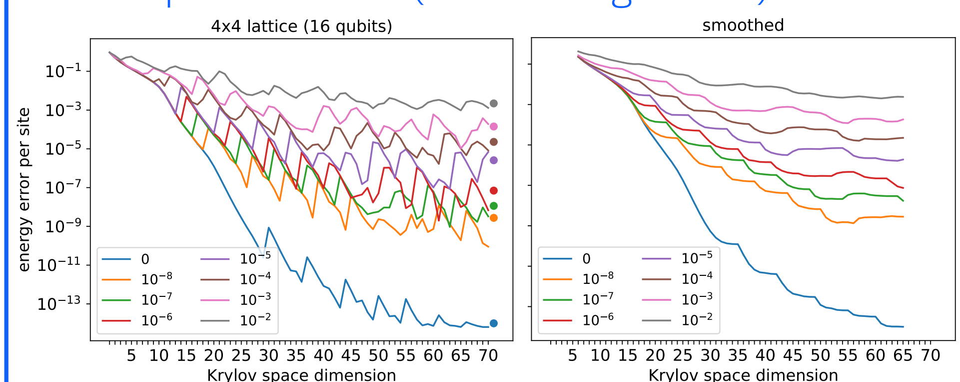
for $k = 0,1,2,\ldots,2D-1$.

5. Resulting circuits

To estimate $\langle \psi_0 | T_k(H) | \psi_0 \rangle$...



6. Example numerics (Heisenberg model)



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