Exact and efficient Lanczos* method on a quantum computer

Will Kirby[1,2], Mario Motta[3], and Antonio Mezzacapo[2]
[1]Department of Physics and Astronomy, Tufts University, Medford, MA
[2]IBM Quantum, T. J. Watson Research Center, Yorktown Heights, NY
[3]IBM Quantum, IBM Research Almaden, San Jose, CA 95120, USA

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Motivation

Goal: estimate ground state energy of quantum Hamiltonian.

Abstract perspective: approximate lowest eigenvalue of Hermitian matrix.

Example applications:

- Quantum chemistry.
- Condensed matter physics.
- High-energy physics.
- Nuclear physics.

Goal is classically challenging due to exponential Hilbert space dimension.

Lanczos* method

Lanczos method = classical method for approximating lowest eigenvalues:

1. Initial guess $|\psi_0\rangle \quad \Rightarrow \quad H|\psi_0\rangle \quad \Rightarrow \quad H^2|\psi_0\rangle \quad \cdots \Rightarrow \quad H^{D-1}|\psi_0\rangle$.
2. $(\mathbf{H}, \mathbf{S})$ = project H onto span$\{|\psi_0\rangle,\ H|\psi_0\rangle,\ H^2|\psi_0\rangle,\ \ldots,\ H^{D-1}|\psi_0\rangle\}$.
3. lowest eigenvalue of $(\mathbf{H}, \mathbf{S}) \sim$ lowest eigenvalue of H.

Advantage: converges exponentially with D (in ∞ precision arithmetic).

Disadvantage: classically, requires storing entire statevectors $H^i|\psi_0\rangle$ $\Rightarrow$ exponential overhead.

Can we construct a quantum version that mitigates the overhead to represent statevectors while keeping fast convergence?[1]

[1] Klymko *et al.* (2022), Epperly *et al.* (2022), and many more.

Block encoding

Idea: for H on n qubits (s.t. $\|H\| \leq 1$), find U on $m+n$ qubits s.t.[2]

$$U = \begin{pmatrix} H & \cdot \\ \cdot & \cdot \end{pmatrix}, \qquad R = \begin{pmatrix} 1 & & & & & \\ & \ddots & & & 0 & \\ & & 1 & & & \\ & & & -1 & & \\ & 0 & & & \ddots & \\ & & & & & -1 \end{pmatrix}$$

$$U^2 = 1 \quad \Rightarrow \quad (RU)^j = \begin{pmatrix} T_j(H) & \cdot \\ \cdot & \cdot \end{pmatrix}$$

[2]Low and Chuang, Quantum 3 (2019).

Quantum Lanczos method

$$\Rightarrow \quad (RU)^j = \begin{pmatrix} T_j(H) & \cdot \\ \cdot & \cdot \end{pmatrix}$$

$\Rightarrow$ can use block encoding to exactly construct $T_j(H)|\psi_0\rangle$.

Recall: Lanczos method $\sim$ project H onto

$$\begin{aligned} &\text{span}\{|\psi_0\rangle,\ H|\psi_0\rangle,\ H^2|\psi_0\rangle,\ \dots,\ H^{D-1}|\psi_0\rangle\} \\ &= \text{span}\{|\psi_0\rangle,\ T_1(H)|\psi_0\rangle,\ T_2(H)|\psi_0\rangle,\ \dots,\ T_{D-1}(H)|\psi_0\rangle\}. \end{aligned}$$

Quantum Lanczos method

To diagonalize H projected onto subspace, estimate

$$\mathbf{H}_{ij} := \langle\psi_0|T_i(H)HT_j(H)|\psi_0\rangle, \quad \mathbf{S}_{ij} := \langle\psi_0|T_i(H)T_j(H)|\psi_0\rangle$$

on quantum computer for $i, j = 0, 1, 2, ..., D-1$, then solve

$$\mathbf{H}\vec{v} = \lambda\mathbf{S}\vec{v}.$$

Required quantities

So the quantities we need are

$$\langle\psi_0|T_i(H)HT_j(H)|\psi_0\rangle = \frac{1}{4}\Big(\big\langle T_{i+j+1}(H)\big\rangle_0 + \big\langle T_{|i+j-1|}(H)\big\rangle_0 + \big\langle T_{|i-j+1|}(H)\big\rangle_0 + \big\langle T_{|i-j-1|}(H)\big\rangle_0 \Big),$$

$$\langle\psi_0|T_i(H)T_j(H)|\psi_0\rangle = \frac{1}{2}\Big(\big\langle T_{i+j}(H)\big\rangle_0 + \big\langle T_{|i-j|}(H)\big\rangle_0 \Big)$$

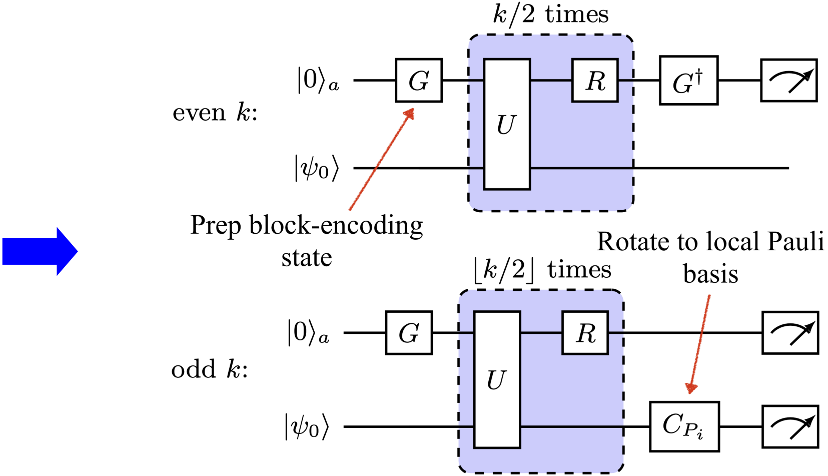
for $i, j = 0, 1, 2, ..., D-1$. In other words, need to estimate

$$\langle T_k(H)\rangle_0 := \langle\psi_0|T_k(H)|\psi_0\rangle$$

for each $k = 0, 1, 2, ..., 2D-1$.

Required circuits

Hence, required circuits are: for each $k = 0, 1, 2, ..., 2D - 1$,



where $G|0\rangle_a$ identifies the block in the block encoding.

"In practice" error analysis[4]

Can bound energy error $\mathcal{E}$ as function of noise rate, Krylov space dimension, problem parameters.

Assuming noise only from finite shots, to reach energy error $\mathcal{E}$ we require

$$D = \Theta\left[\left(\log\frac{1}{|\gamma_0|} + \log\frac{1}{\mathcal{E}}\right)\min\left(\frac{1}{\mathcal{E}}, \frac{1}{\Delta}\right)\right]$$

and

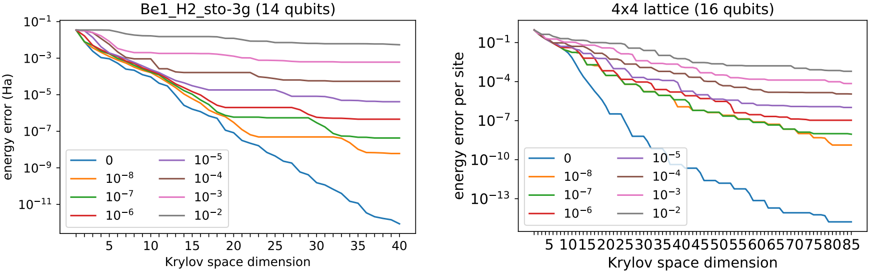
$$M = \Theta\left[D\left(\frac{1}{\mathcal{E}^2} + \frac{1}{\mathcal{E}|\gamma_0|^4}\right)\right].$$

measurements in total, for initial state overlap γ_0 and spectral gap Δ.[3]

[3] Uses analysis based on Epperly *et al.*, 2022.

[4] "In practice" because theoretical bound only guarantees first term in M is $\mathcal{E}^{-p}$ for $p \in [2, 3]$; $p = 2$ is based on numerics.

Numerical examples



Left plot shows energy error versus Krylov space dimension for BeH_2 in STO-3G, equilibrium configuration (bondlength 1.3264 Å), with different noise rates per matrix element. Right plot shows energy error per site versus Krylov space dimension for J1-J2 model on 4×4 square lattice with couplings $J_1 = 1$ and $J_2 = 0.5$.

Thank you!

Preprint: https://arxiv.org/abs/2208.00567