A fast algorithm for approximating the ground state energy on a quantum computer

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Overview

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Problem definition

Consider the eigenvalue problem

$$-\Delta u(x) + V(x)u(x) = E\,u(x) \qquad x \in I_d := (0,1)^d$$

$$u(x) = 0 \quad x \in \partial I_d$$

$$\Delta = \sum_{j=1}^{d} \frac{\partial^2}{\partial x_j^2}$$

for V in the class

$$F = \left\{ V : [0,1]^d \to [0,1] \;\middle|\; V,\ D_j V := \partial V / \partial x_j \text{ continuous},\ \text{and } \left\| D_j V \right\|_\infty \le 1,\ j = 1, \ldots, d, \text{ and } \left\| V \right\|_\infty \le 1 \right\}$$

Problem: Approximate the smallest eigenvalue

$$E_1 = E_1(V) \text{ with relative error } \varepsilon$$

Using function evaluations of V

For a p particle system $d = 3p$

and the smallest eigenvalue is the ground state energy

Since

$$E_1(0) \le E_1(V) \le E_1(0) + 1$$

and

$$E_1(0) = d\,\pi^2$$

So for relative error ε the interesting case is

$$d\,\pi^2\,\varepsilon < 1$$

Earlier work review

Classical worst case complexity

$$E_1(V) = E_1(\tilde{V}) + \int_{I_d} \left(V(x) - \tilde{V}(x)\right) u_1^2(x;\tilde{V})\, dx + O\left(\left\|V - \tilde{V}\right\|_\infty^2\right)$$

$u_1(\cdot;\tilde{V})$ eigenfunction corresponding to $\tilde{V}$

for $V, \tilde{V} \in F$

The problem is at least at hard as multivariate integration

Thm. [P07]

$$\varepsilon^{-d} \leq \ \mathrm{comp}(\varepsilon) \ \leq \varepsilon^{-d} + \varepsilon^{-d} \log \varepsilon^{-1}$$

info. cost comb. cost

Curse of dimensionality

Algorithm achieving the upper bound solves a matrix eigenvalue problem. The matrix size is exponential in the dimension

Quantum complexity

Thm. [P07]

$$\varepsilon^{-d/(d+1)} \leq \mathrm{comp}(\varepsilon) \leq \varepsilon^{-6} \log^4 \varepsilon^{-1}$$

- Upper bound by alg. derived from phase estimation
- The quantum complexity is not exponential in d
- Can we do better?

Fast quantum algorithm

Consider the matrix obtained from the discretization of the continuous problem

$$M_h = -\Delta_h + V_h, \quad h = (m+1)^{-1} \leq \varepsilon$$

symmetric, positive definite with size $m^d \times m^d$

Then for $$\left| E_{1,h} - \hat{E}_{1,h} \right| \leq c\ d\ h$$

smallest matrix eigenvalue and approximation

we have $$\left| \frac{E_1 - \hat{E}_{h,1}}{E_1} \right| \leq c'\,\varepsilon$$

For the unitary matrix

$$W = e^{iM_h/(2d)}$$

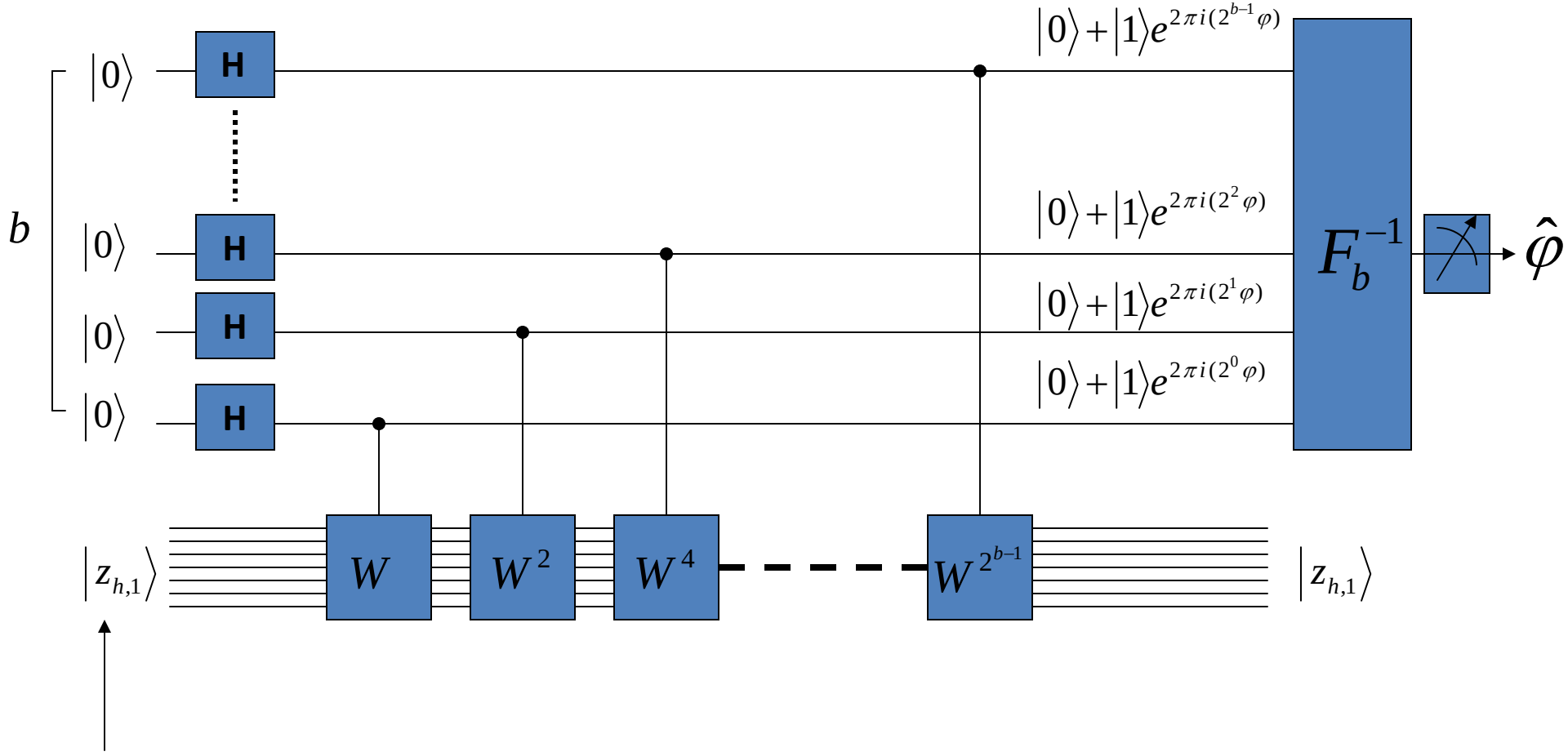
we have

$$e^{iE_{h,1}/(2d)} = e^{2\pi i\varphi}, \quad \varphi = E_{h,1}/(4\pi d) \in [0,1)$$

Suffices to approximate the phase φ

Use phase estimation with modifications

Phase estimation



corresponding eigenvector

$$|\varphi - \hat{\varphi}| \leq 2^{-b}, \quad b = \Theta\left(\log \varepsilon^{-1}\right)$$

$$\text{success prob.} \geq 8/\pi^2$$

Modification 1 – Initial state

Instead of $\left|z_{h,1}\right\rangle$

use $\left|\psi_1\right\rangle^{\otimes d}$, the

eigenvector of $-\Delta_h$ corresponding to min. eigenvalue

Implemented efficiently using Fourier transform with a number of quantum operations proportional to

$$d \cdot \log^2 \varepsilon^{-1}$$

Success probability is at least $\frac{8}{\pi^2}\left(1-\frac{1}{(3\pi^2-2)^2}\right) \geq \frac{4}{5}$

Modification 2 – Matrix exponentials

Idea: Approximate

$$W^{2^t} = e^{i(-\Delta_h + V_h)2^t/(2d)}, \quad t = 0, \ldots, b-1$$

using Suzuki's high order splitting formulas of the form

$$\prod_{l=1}^{N_t} e^{iA_l z_l}$$

$A_l \in \{-\Delta_h, V_h\}$ and suitably chosen numbers z_l and with sufficient accuracy such that the success probability of the alg. is at least 2/3

Total number of matrix exponentials is $N = \sum_{t=0}^{b-1} N_t$

Let $H_1 = -\Delta_h/(2d), \quad H_2 = V_h/(2d)$

Thm. [S90, S91] The splitting formula

$$S_2(\tau) = e^{iH_1\tau/2} e^{iH_2\tau} e^{iH_1\tau/2}$$ Strang splitting

$$S_{2k}(\tau) = S_{2k-2}^2(p_k\tau) S_{2k-2}((1-4p_k)\tau) S_{2k-2}^2(p_k\tau), \quad k \geq 2$$

$$p_k = 1/(4 - 4^{1/(2k-1)})$$

approximates $W^\tau = e^{i(H_1+H_2)\tau}$

(approximates the evolution of a system evolving with Hamiltonian $H_1 + H_2$ for an amount of time τ)

with error $O(|\tau|^{2k+1})$

i.e., the order is $2k+1, \quad k \geq 1$

Using ideas from [PZ10] we approximate

$$W^{2^t} \approx \left(S_{2k}(\tau)\right)^{2^t/\tau}$$

Length of interval Number of intervals

with error $2^{t+1-b}/40, \quad t = 0, \ldots, b-1$

This yields an upper bound for the number of matrix exponentials N_t required for the approximation of W^{2^t} with the required accuracy

The sum errors for the approximation of all the

$$W^{2^t}, \quad t = 0, \ldots, b-1$$

is at most 1/20 and therefore the success probability is at least

$$\frac{8}{\pi^2}\left(1-\frac{1}{(3\pi^2-2)^2}\right)-\frac{1}{10} \geq \frac{2}{3}$$

The total number of matrix exponentials satisfies

$$N = \sum_{t=0}^{b-1} N_t \leq \tilde{C}\,\frac{1}{2k+1}\left(\frac{40}{d}\right)^{1/(2k)} 10^k\, \varepsilon^{-(3+1/(2k))}$$

We find the optimal k^* that minimizes the upper bound and this yields a total number of matrix exponentials

$$N^* = O\left(\varepsilon^{-3} e^{\sqrt{\ln \frac{1}{d\varepsilon}}} \right)$$

Half of them involve $-\Delta_h$

The other half V_h

Each matrix exponential involving $-\Delta_h$

is implemented using Fourier transform with a number of quantum operations proportional to

$$d \cdot \log^2 \varepsilon^{-1}$$

Each matrix exponential involving V_h

is implemented using a quantum query that returns a

$$\Theta\left(\log \varepsilon^{-1}\right)$$

bit truncation of the potential evaluation

Thm. For relative error ε

Total cost - number of queries and other quantum operations

$$N^* \; d \; O(\log^2 \varepsilon^{-1})$$

or equivalently

$$C \; d \; \varepsilon^{-(3+\delta)}$$

for $\delta > 0$ arbitrarily small

Total number of qubits

$$C' \; d \; \log \varepsilon^{-1}$$

Summary

- Fast quantum algorithm

$$C\, d\, \varepsilon^{-(3+\delta)} \qquad \delta > 0$$

  - Best known algorithm
  - Cost of known classical algorithms is exponential in the dimension

- Open problems
  - How to improve the cost?
  - What happens if we consider other classes of potential functions?