

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

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Abstract

Estimating the ground state energy of a multiparticle system with relative error ε using deterministic classical algorithms has cost that grows exponentially with the number of particles. The problem depends on a number of state variables d that is proportional to the number of particles and suffers from the curse of dimensionality. Quantum computers can vanquish this curse. In particular, we study a ground state eigenvalue problem and exhibit a quantum algorithm that achieves relative error ε using a number of qubits $C'd \log \varepsilon^{-1}$ with total cost (number of queries plus other quantum operations) $Cd\varepsilon^{-(3+\delta)}$, where $\delta > 0$ is arbitrarily small and C and C' are independent of d and ε .

Keywords: Eigenvalue problem, numerical approximation, quantum algorithms

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1 Introduction

A difficult and challenging problem in modern science is to accurately compute properties of physical and chemical systems. One of the difficulties in carrying out precise calculations arises from the computational demands the

Schrödinger equation presents. The computational resources needed to obtain accurate solutions appear to be exponential in the size of the physical system. As a result these problems are considered intractable on a classical computer for systems that are not trivial in size. For an overview of the numerical methods used for the solution of such problems see [5, 19] and the references therein.

So far there have been mixed results about the potential power of quantum computers relative to that of classical computers. For some problems, such as factoring large numbers, quantum computers offer exponential speedups relative to the best classical algorithms known. On the other hand, there are results about the limits of quantum computation [2], as well as results showing that certain problems are hard. For instance, estimating the ground state eigenvalue of arbitrary local Hamiltonians is a QMA complete problem [15].

Although there are fundamental problems in complexity theory that remain open, there is a distinct category of problems for which quantum computers can offer substantial speedups relative to classical computers. This includes problems, such as multivariate integration, path integration and multivariate approximation, that suffer from the *curse of dimensionality* in the classical deterministic worst case. Quantum computers can vanquish the curse; see e.g. [21, 22, 29]. R. E. Bellman introduced the term *curse of dimensionality* referring to multivariate problems whose complexity grows exponentially with the number of variables and so are impossible to solve when the number of variables is large.

An important problem in physics and chemistry that falls in this category is the estimation of the ground state eigenvalue of a time-independent Hamiltonian corresponding to a multiparticle system. Solving such problems on a classical computer in the worst case has cost exponential in the number of particles. In particular, the number of state variables d is proportional to the number of particles and the cost to solve the problem with relative accuracy ε may grow as ε^{-d} . For these reasons researchers have been experimenting with quantum computers to solve eigenvalue problems in quantum chemistry with very encouraging results [8, 17]. See also [13, 14] and the references therein.

We remark that recently there has been a fair amount of work dealing with eigenvalue problems see, e.g. [4, 11, 23, 28, 30, 31, 32]. However, our results are different. The other papers either address different eigenvalue problems, or use spin models, or study classical algorithms, or do not obtain

algorithm cost and error estimates.

In particular, we study a ground state eigenvalue problem and we exhibit a quantum algorithm that achieves relative error ε with cost $Cd\varepsilon^{-(3+\delta)}$, where $\delta > 0$ is an arbitrarily small positive number. The cost includes the number of queries plus all other quantum operations. The algorithm uses $C'd \log \varepsilon^{-1}$ qubits. The constants C and C' as well as all constants in our estimates throughout this paper are independent of d and ε .

We stress that we are not dealing with an arbitrary eigenvalue estimation problem. In our case we are able to obtain efficiently a rough but very useful approximation of the ground state eigenvector. Abrams and Lloyd [1] were the first to demonstrate the advantages of approximate eigenvectors in solving problems of physical interest. Consequently, the cost to implement and simulate the evolution of the Hamiltonian for the amount of time prescribed by the accuracy demand determines the cost to approximate the ground state eigenvalue.

We now consider the problem in more detail. If the potential is a function of only state variables then the ground state energy is given by the smallest eigenvalue E_1 of the equation

$$\begin{aligned} (-\tfrac{1}{2}\Delta + V)\Psi_1(x) &= E_1\Psi_1(x) \quad \text{for all } x \in I_d := (0, 1)^d, \\ \Psi_1(x) &= 0 \quad \text{for all } x \in \partial I_d, \end{aligned}$$

where ∂I_d denotes the boundary of the unit cube, x is the position variable, and Ψ_1 is a normalized eigenfunction. For simplicity we assume that all masses and the normalized Planck constant are one. The boundary conditions are for particles in a box. Multiparticle systems on bounded domains with the wave function equal to zero on the boundary have been studied in the literature; see e.g. [5, p. 621].

This eigenvalue problem is called the time-independent Schrödinger equation in the physics literature and the Sturm-Liouville eigenvalue problem in the mathematics literature. We want to approximate E_1 with relative error ε .

Here, Δ is the d -dimensional Laplacian and $V \geq 0$ is a function of d variables. The dimension is proportional to the number of particles, e.g. $d = 3p$. For many applications the number of particles p and hence d is huge. We consider algorithms that approximate E_1 using finitely many function evaluations of V . Moreover, we assume that V and its first order partial derivatives $\partial V/\partial x_j$, $j = 1, \dots, d$, are continuous and uniformly bounded by 1.

2 Complexity of Classical algorithms and Discretization error

Decades of calculating ground state eigenvalues of systems with a large number of particles have suggested that such problems are hard. We sketch a proof that the cost of classical deterministic algorithms that approximate eigenvalues in the worst case grows exponentially with the number of variables.

Indeed, consider a potential function V and let \bar{V} be a perturbation of V . Then the eigenvalue $E_1(V)$ corresponding to V and the eigenvalue $E_1(\bar{V})$ corresponding to \bar{V} are related according to the formula

$$E_1(V) = E_1(\bar{V}) + \int_{I_d} (V(x) - \bar{V}(x)) \Psi_1^2(x; \bar{V}) dx + O(\|V - \bar{V}\|_\infty^2),$$

where $\Psi_1(\cdot; \bar{V})$ denotes the eigenfunction corresponding to $E_1(\bar{V})$. This implies that approximating E_1 is at least as hard as approximating a multivariate integral in the worst case. As a result, any classical deterministic algorithm for the eigenvalue problem with accuracy ε must use a number of function evaluations of V that grows as ε^{-d} ; see [24] for details.

Finite differences are often used for approximating E_1 . The discretization of the operator $-\frac{1}{2}\Delta + V$ with mesh size $h = (m+1)^{-1}$ yields an $m^d \times m^d$ matrix $M_h := M_h(V) = -\frac{1}{2}\Delta_h + V_h$. Then one solves the corresponding matrix eigenvalue problem $M_h z_{h,1} = E_{h,1} z_{h,1}$. Note that Δ_h denotes the discretization of the Laplacian and V_h is a diagonal matrix whose entries are evaluations of the potential V at the m^d grid points. The reader may assume that Δ_h is obtained using a $2d+1$ stencil for the Laplacian; see e.g. [18, p. 60].

For instance, if $d = 2$ we have

$$-\Delta_h = h^{-2} \begin{pmatrix} T_h & -I & & & & \\ -I & T_h & -I & & & \\ & \ddots & \ddots & \ddots & & \\ & & -I & T_h & -I & \\ & & & -I & T_h \end{pmatrix},$$

is an $m^2 \times m^2$ matrix, where I is the $m \times m$ identity matrix while

$$V_h = \begin{pmatrix} v_{11} & & & & \\ & \ddots & & & \\ & & v_{ij} & & \\ & & & \ddots & \\ & & & & v_{mm} \end{pmatrix},$$

where $v_{ij} = V(ih, jh)$, $i, j = 1, \dots, m$, and T_h is the $m \times m$ matrix given by

$$T_h = \begin{pmatrix} 4 & -1 & & & \\ -1 & 4 & -1 & & \\ & \ddots & \ddots & \ddots & \\ & & -1 & 4 & -1 \\ & & & -1 & 4 \end{pmatrix}.$$

M_h is symmetric positive definite and sparse and has been extensively studied in the literature [7, 9, 18]. For V that has bounded first order partial derivatives, using the results of [33, 34] we conclude

$$|E_1 - E_{h,1}| \leq c_1 dh \tag{1}$$

If $\hat{E}_{h,1}$ is such that $|E_{h,1} - \hat{E}_{h,1}| \leq c_2 dh$, we have relative error

$$|1 - \hat{E}_{h,1}/E_1| \leq c' h,$$

where c' is a constant. The inequality follows by observing that $2E_1$ is bounded from below by the smallest eigenvalue $4dh^{-2} \sin^2(\pi h/2)$ of the discretized Laplacian.

Such a discretization approach for a multiparticle system is not new; see e.g. [5, p. 621]. The problem is that the size of the resulting matrix is exponential in d and so is the cost of classical algorithms approximating its ground state eigenvalue.

3 Quantum algorithm

First we discuss our algorithm in general terms and then we provide a complete analysis. The key observation is that the discretization we outlined

above and the estimation of the smallest eigenvalue of the resulting matrix can be implemented on a quantum computer with cost that does not grow exponentially with d . This is accomplished by modifying quantum phase estimation, a well known quantum algorithm for approximating an eigenvalue of a unitary matrix W , see e.g., [20, p. 225]. First we provide a sketch of the algorithm and then give all its details and the resulting error and cost estimates.

Sketch of the algorithm

1. Consider the discretization $M_h = -\frac{1}{2}\Delta_h + V_h$ of $-\frac{1}{2}\Delta + V$ and let $h \leq \varepsilon$ leading to the desired accuracy. The matrix

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

is unitary since M_h is Hermitian.

2. For W use phase estimation to approximate the phase corresponding to $e^{iE_{h,1}/(2d)}$ with the following modifications:
 - (a) Use the approximate eigenvector

$$|0\rangle^{\otimes b} |\psi_1\rangle^{\otimes d}$$

as an initial state, where $|\psi_1\rangle^{\otimes d}$ is the ground state eigenvector of $-\Delta_h$ and can be implemented efficiently; see the discussion following (4) below for details.

- (b) Replace W^{2^t} , $t = 0, \dots, b-1$, that are required in phase estimation, using approximations given by high order splitting formulas that deal with the exponentials of $-\frac{1}{2}\Delta_h$ and V_h separately and can be implemented efficiently; see the discussion leading to (6) below for details.

The effect of the modifications is to somewhat decrease the success probability while increasing the cost of phase estimation. Nevertheless, the resulting success probability is at least $\frac{2}{3}$, and the cost for implementing the initial state and the approximate powers of W does not suffer from the curse of dimensionality. (The actual value of the success probability is not important since it exceeds $\frac{1}{2}$ and can be boosted to become arbitrarily close to one; see [20, p. 153] for details.)

Theorem 1. *Phase estimation with an approximate initial state and approximate powers of W with probability at least $\frac{2}{3}$ yields an estimate of E_1 with relative error ε and total cost*

$$Cd\varepsilon^{-(3+\delta)},$$

for any $\delta > 0$, using $C'd \log \varepsilon^{-1}$ qubits, where C and C' are constants.

Algorithm 1 GSE($n, M, |\psi_0\rangle, hC, hE, E_{\min}, E_{\max}$)

Require: n to be a positive integer representing the bits of accuracy

Require: M to be a positive integer representing the number of qubits in the bottom register and the number of basis functions

Require: τ to be a positive real number (scaling variable)

Require: $|\psi_0\rangle$ to be a prepared M -qubit quantum state (approximate ground state wave function)

Require: hC to be a list of M^2 complex numbers (Coulomb integrals)

Require: hE to be a list of M^4 complex numbers (exchange integrals)

Require: E_{\min} to be real number (lower bound for ground state energy)

Require: E_{\max} to be real number (upper bound for ground state energy)

Require: $E_{\min} < E_{\max}$

1: PauliH1(M, hC, L, \mathcal{H})

2: PauliH2(M, hE, L, \mathcal{H})

3: $\tau \leftarrow 2\pi / (E_{\max} - E_{\min})$

4: $b \leftarrow n + \lceil \log_2(2\pi/\tau) \rceil$

5: ApproxU($M, L, b, E_{\max}, \mathcal{H}, \tau, \hat{U}$)

6: Initial state : $|0\rangle^{\otimes b} |\psi_0\rangle$

7: Apply Hadamard: $\rightarrow \frac{1}{2^{b/2}} \sum_{j_0, j_1, \dots, j_{b-1}=0}^1 |j_{b-1} j_{b-2} \dots j_1 j_0\rangle |\psi_0\rangle$

8: Apply $\hat{U}_0^{j_0} \dots \hat{U}_{b-1}^{j_{b-1}}$: $\rightarrow \frac{1}{2^{b/2}} \sum_{j_0, j_1, \dots, j_{b-1}=0}^1 |j_{b-1} j_{b-2} \dots j_1 j_0\rangle |\psi_0\rangle \hat{U}_{b-1}^{j_{b-1}} \dots \hat{U}_1^{j_1} \hat{U}_0^{j_0} |\psi_0\rangle$

9: Apply FT^\dagger : $\rightarrow (FT^\dagger \otimes I) \left(\frac{1}{2^{b/2}} \sum_{j_0, j_1, \dots, j_{b-1}=0}^1 |j_{b-1} j_{b-2} \dots j_1 j_0\rangle \hat{U}_{b-1}^{j_{b-1}} \dots \hat{U}_1^{j_1} \hat{U}_0^{j_0} |\psi_0\rangle \right)$

10: Measure the first b qubits in the computational basis: outcome

$(m_{b-1}, \dots, m_1, m_0)$

11: $m \leftarrow \sum_{k=0}^{b-1} m_k 2^k$

12: $\hat{E}_0 \leftarrow E_{\max} - (E_{\max} - E_{\min})m/2^b$

13: **return** \hat{E}_0

Algorithm 2 ApproxU($M, L, b, \mathcal{H}, \tau, \hat{U}$)

Require: M to be a positive integer (number of basis functions)

Require: L to be a positive integer (number of groups of Hamiltonian terms)

Require: b to be a positive integer (number of qubits in top register of the PEA)

Require: \mathcal{H} to be a list of L Hamiltonian terms acting on M qubits (list of groups of Hamiltonian terms)

Require: τ to be a positive real number (scaling parameter)

Require: N to be a list of b positive integers (list of time intervals for Trotter approximations)

1: **for** $k = 0$ to $b - 1$ **do**

2: $N_k \leftarrow 100 \cdot 2^k$

3: $\hat{U}[k] \leftarrow e^{iE_{\max}\tau j_k 2^k} \left(\prod_{\ell=1}^L e^{-i\mathcal{H}_\ell \tau 2^{k-1}/N[k]} \right)$

4: **for** $j = 2$ to $N[k]$ **do**

5: $\hat{U}[k] \leftarrow \hat{U}[k] \left(\prod_{\ell=1}^L e^{-i\mathcal{H}_\ell \tau 2^{k-1}/N[k]} \right)$

6: **end for**

7: **end for**

8: **return**

Next we discuss the details of our algorithm and this will lead us to the proof of the theorem. Assume h is the largest mesh size satisfying $h \leq \min(\varepsilon, 1/4)$. This leads to the desired accuracy while ensuring the discretization is not trivial. The eigenvalue of W that corresponds to $E_{h,1}$ is $e^{iE_{h,1}/(2d)} = e^{2\pi i\varphi_1}$, where

$$\varphi_1 = E_{h,1}/(4\pi d)$$

is the phase and belongs to the interval $[0, 1)$ since $E_{h,1} \leq 2dh^{-2} \sin^2(\pi h/2) + 1 \leq d\pi^2/2 + 1$.

Quantum phase estimation approximates the phase φ_1 with b -bit accuracy, where $b = \lceil \log_2 h^{-1} \rceil$. The output of the algorithm is an index $j \in [0, 2^b - 1]$ such that $|\varphi_1 - j 2^{-b}| \leq 2^{-b}$. Hence,

$$|E_{h,1} - 4\pi dj 2^{-b}| \leq c_2 dh. \quad (2)$$

Combining (1) and (2) we conclude

$$|E_1 - 4\pi dj 2^{-b}| \leq c_1 d\varepsilon + c_2 d\varepsilon = cd\varepsilon. \quad (3)$$

Hence the algorithm approximates the ground state eigenvalue E_1 by

$$\hat{E}_{h,1} := 4\pi dj 2^{-b}.$$

This estimate holds with probability at least $\frac{8}{\pi^2}$ (see, e.g., [3]) assuming:

- The initial state of the algorithm is $|0\rangle^{\otimes b} |z_{h,1}\rangle$, where $|z_{h,1}\rangle$ is the eigenvector of M_h that corresponds to $E_{h,1}$.
- We are given the matrix exponentials W^{2^t} , $t = 0, \dots, b - 1$.

In our case, however, we do not know $|z_{h,1}\rangle$ and we use an approximation. Similarly, we use approximations of the W^{2^t} , $t = 0, \dots, b - 1$, to simulate the evolution of the quantum system that evolves with Hamiltonian $H = M_h/(2d)$. We will compute the cost to implement these approximations so that (3) holds. All these approximations affect the estimate $\frac{8}{\pi^2}$ of the success probability of phase estimation, but only by a small amount.

The initial state of our algorithm is

$$|0\rangle^{\otimes b} |\psi_1\rangle^{\otimes d}, \quad (4)$$

where $|\psi_1\rangle^{\otimes d}$ is the ground state eigenvector of the discretized Laplacian. We know [7] that the coordinates of $|\psi_1\rangle$ are

$$\psi_{1j} = \sqrt{2h} \sin(j\pi h), \quad j = 1, \dots, m,$$

and $|\psi_1\rangle^{\otimes d}$ has unit length. Since h is proportional to ε , the matrix M_h has size $m^d \times m^d$, with $m = \Theta(\varepsilon^{-1})$. Therefore, $|\psi_1\rangle^{\otimes d} \in \mathbb{C}^{m^d}$ and can be represented using $\log_2 m^d = O(d \log_2 \varepsilon^{-1})$ qubits and can be implemented with $d \cdot O(\log^2 \varepsilon^{-1})$ quantum operations using the Fourier transform; see e.g., [16, 35]. We point out that here and elsewhere the implied constants in the big- O and Θ notation are independent of d and ε . (From a practical standpoint, it is possible to further reduce the cost of the initial state using the algorithm in [12] but we do not pursue this alternative since the analysis of the algorithm becomes more involved.)

Expanding $|\psi_1\rangle^{\otimes d}$ using the eigenvectors of M_h we have

$$|\psi_1\rangle^{\otimes d} = \sum_{k=1}^{m^d} d_k |z_{h,k}\rangle.$$

The approximate initial state reduces the success probability of phase estimation by a factor equal to the square of the magnitude of the projection of $|\psi_1\rangle^{\otimes d}$ onto $|z_{h,1}\rangle$, to become $\frac{8}{\pi^2}|d_1|^2$; see, e.g., [1, 12].

We will see that $|d_1|^2 > \pi^2/10$. Indeed, we estimate $|d_1|$ using the approach in [36, p. 172] which is based on the separation of the eigenvalues of M_h . In particular, we have

$$1 \geq (E_{h,2} - E_{h,1})^2(1 - |d_1|^2),$$

where $E_{h,1}$ and $E_{h,2}$ are the smallest and second smallest eigenvalues of M_h . We estimate $E_{h,2} - E_{h,1}$ from below using the two smallest eigenvalues of $-\Delta_h$ to obtain $E_{h,2} - E_{h,1} \geq 2h^{-2}(\sin^2(\pi h) - \sin^2(\pi h/2)) - 1$.

This yields that the success probability of phase estimation with the approximate ground state eigenvector is at least

$$\frac{8}{\pi^2} \left(1 - \frac{1}{(2h^{-2}(\sin^2(\pi h) - \sin^2(\pi h/2)) - 1)^2} \right) > \frac{4}{5}, \quad (5)$$

$h \leq 1/4$. (The overall success probability of the algorithm is affected by an additional factor and once we address that we will provide a final estimate.)

Now let us turn to the approximation of the matrix exponentials. We simulate the evolution of a quantum system with Hamiltonian $H = M_h/(2d)$ for time 2^t , $t = 0, 1, \dots, b-1$. Let $H = H_1 + H_2$ where $H_1 = -\Delta_h/(4d)$ and $H_2 = V_h/(2d)$. Recall that h is the largest mesh size satisfying $h \leq \min(\varepsilon, 1/4)$. The eigenvalues and eigenvectors of the discretized Laplacian

are known and the evolution of a system with Hamiltonian H_1 can be implemented with $d \cdot O(\log^2 \varepsilon^{-1})$ quantum operations using the Fourier transform in each dimension; see e.g., [20, p. 209]. The evolution of a system with Hamiltonian H_2 can be implemented using two quantum queries and phase kickback. The queries are similar to those in Grover's algorithm [20] and return function evaluations of V truncated to $O(\log \varepsilon^{-1})$ bits.

In particular, we use a splitting formula of order $2k + 1$, $k \geq 1$, to approximate $W^{2^t} = e^{i(H_1+H_2)2^t}$ by

$$\prod_{\ell=1}^{N_t} e^{iA_\ell z_\ell}, \quad (6)$$

where $A_\ell \in \{H_1, H_2\}$ and suitable z_ℓ that depend on t and k as described in [26, 27].

From [25] (see p. 2 using $m = 2$), the number N_t of exponentials needed to approximate W^{2^t} by a splitting formula of order $2k + 1$ with error ε_t , $t = 0, \dots, b - 1$, is

$$N_t \leq 16e\|H_1\|2^t \left(\frac{25}{3}\right)^{k-1} \left(\frac{8e2^t\|H_2\|}{\varepsilon_t}\right)^{1/(2k)},$$

for any $k \geq 1$. The total number of exponentials required for the approximation of all the W^{2^t} is bounded from above as follows

$$\begin{aligned} N &= \sum_{t=0}^{b-1} N_t \leq 16e\|H_1\| \left(\frac{25}{3}\right)^{k-1} (8e\|H_2\|)^{1/(2k)} \\ &\quad \times \sum_{t=0}^{b-1} 2^t \left(\frac{2^t}{\varepsilon_t}\right)^{1/(2k)} \\ &\leq 16e\|H_1\|2^b \left(\frac{25}{3}\right)^{k-1} (160e2^b\|H_2\|)^{1/(2k)}, \end{aligned} \quad (7)$$

where we obtained the last inequality by setting $\varepsilon_t = \frac{2^{t+1-b}}{40}$, $t = 0, \dots, b - 1$. It is easy to check that $\sum_{t=0}^{b-1} \varepsilon_t \leq \frac{1}{20}$. Thus the success probability of phase estimation can be reduced by twice this amount [20, p. 195]. Using (5) we conclude our algorithm succeeds with probability at least

$$\frac{4}{5} - \frac{1}{10} > \frac{2}{3}.$$

Since $\|H_1\| \leq \frac{4dk^{-2}}{4d} \leq \varepsilon^{-2}$ and $\|H_2\| \leq 1/(2d)$, the algorithm uses a number of exponentials of H_1 and H_2 that satisfies

$$N \leq 16e \left(\frac{80e}{d}\right)^{1/(2k)} \left(\frac{25}{3}\right)^{k-1} \varepsilon^{-2} 2^{b(1+1/(2k))}.$$

Since we have chosen $2^b = \Theta(1/\varepsilon)$ we obtain

$$N \leq \tilde{C} \left(\frac{80e}{d}\right)^{1/(2k)} \left(\frac{25}{3}\right)^{k-1} \varepsilon^{-(3+\frac{1}{2k})},$$

for any $k > 0$, where \tilde{C} is a constant.

The *optimal* k^* , i.e., the one minimizing the upper bound for N in (7), is obtained in [25, Sec. IV] and is given by

$$k^* = \sqrt{\frac{1}{2} \log_{25/3} \frac{80e 2^b}{d}} = O\left(\sqrt{\ln \frac{1}{d\varepsilon}}\right) \quad \text{as } d\varepsilon \rightarrow 0,$$

The number of exponentials corresponding to k^* satisfies

$$N^* = O\left(\varepsilon^{-3} e^{\sqrt{\ln \frac{1}{d\varepsilon}}}\right) \quad \text{as } d\varepsilon \rightarrow 0. \quad (8)$$

We remark that of the N^* matrix exponentials half involve H_1 and the other half involve H_2 ; see the detailed definition of the high order splitting formula [26, 27]. Since each exponential involving H_2 requires two queries the total number of queries is also N^* .

Hence, the number of quantum operations, excluding queries, to implement the initial state, the matrix exponentials involving H_1 and the inverse Fourier transform yielding the final state of phase estimation is

$$N^* \cdot O(d \log^2 \varepsilon^{-1}). \quad (9)$$

Equations (7), (8) and (9) yield that the total cost of the algorithm, including the number of queries and the number of all other quantum operations, is

$$Cd\varepsilon^{-(3+\delta)},$$

where $\delta > 0$ is arbitrarily small and C is a constant.

Summarizing our results we see that the dependence on d of the number of qubits and the cost is linear. As far as the number of qubits is concerned

this is not really surprising. The algorithm uses phase estimation to approximate an eigenvalue of a matrix whose size is proportional to $\varepsilon^{-d} \times \varepsilon^{-d}$. The corresponding eigenvector has a number of coordinates proportional to ε^{-d} and, therefore, is represented using a number of qubits proportional to $d \log_2 \varepsilon^{-1}$.

We now turn to the cost. The depth of the quantum circuit realizing the algorithm grows as N^* which is given in (8). Clearly, $\varepsilon^{-3} e^{\sqrt{\ln \frac{1}{d\varepsilon}}} \leq \varepsilon^{-3} e^{\sqrt{\ln \frac{1}{\varepsilon}}}$, for any d . Thus N^* is bounded from above by a quantity independent of d . Recall that N^* is the total number of matrix exponentials the algorithm uses. Half of these exponentials involve the discretized Laplacian Δ_h and the other half involve the discretized potential V_h .

Each of the matrix exponentials involving the d dimensional Δ_h is implemented efficiently with cost proportional to $d \log^2 \varepsilon^{-1}$ using the quantum Fourier transform. Hence the cost of all matrix exponentials involving Δ_h depends linearly on d .

We consider the cost of the matrix exponentials involving V_h . Each exponential can be implemented with two quantum queries. We assume the cost of each query is constant. Hence the cost of all matrix exponentials involving V_h is $2N^*$ times the cost of a quantum query.

Thus the sum of the cost of all matrix exponentials and, therefore, the cost of the algorithm depends linearly on d .

This cost analysis has the advantage that it reveals the computational effort spent on solving the ground state eigenvalue problem unobscured by the actual cost of evaluating V (i.e., the the cost of a quantum query). It is not limited in any way, since for any particular choice of V when the actual cost of a query is known, it suffices to multiply it by the number of queries and add the product to (9) to obtain an aggregate cost estimate.

For multiparticle systems studied in physics and chemistry the number of dimensions d is directly proportional to the number of particles p . For instance, p particles in three dimensions yield $d = 3p$. Thus the dependence on p of the number of qubits and the cost of the algorithm is linear.

Finally, our analysis assumes a perfect physical realization of a quantum computer. However, for the implementation of the algorithm, one needs to address decoherence and other sources of error for a specific underlying architecture. This may significantly increase the required computational resources. Such a study exists for phase estimation and the Abrams and Lloyd algorithm [1] applied to the ground state eigenvalue of the transverse Ising

model [6]; see also the references therein and [10]. This study is broad enough to cover Shor's algorithm and conveys the general idea in our case as well. It concludes that for the current state of the art in quantum logic array architectures the existing fault tolerance and error correction techniques impose significant resource requirements in the implementation of these algorithms.

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