Estimating the ground state energy of the Schrödinger equation for convex potentials

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Abstract

In 2011, the fundamental gap conjecture for Schrödinger operators was proven. This can be used to estimate the ground state energy of the time-independent Schrödinger equation with a convex potential and relative error $\varepsilon$. Classical deterministic algorithms solving this problem have cost exponential in the number of its degrees of freedom $d$. We show a quantum algorithm, that is based on a perturbation method, for estimating the ground state energy with relative error $\varepsilon$. The cost of the algorithm is polynomial in $d$ and $\varepsilon^{-1}$, while the number of qubits is polynomial in $d$ and $\log \varepsilon^{-1}$. In addition, we present an algorithm for preparing a quantum state that overlaps within $1-\delta$, $\delta \in (0,1)$, with the ground state eigenvector of the discretized Hamiltonian. This algorithm also approximates the ground state with relative error $\varepsilon$. The cost of the algorithm is polynomial in $d$, $\varepsilon^{-1}$ and $\delta^{-1}$, while the number of qubits is polynomial in $d$, $\log \varepsilon^{-1}$ and $\log \delta^{-1}$.

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1 Introduction

The power of quantum computers has been studied extensively. In some cases the results have been very exciting and encouraging while in others the results show limitations of quantum computation. Shor’s quantum algorithm for computing prime factors of a number [12] has provided an exponential speed-up compared to the fastest classical algorithm known, the number field sieve. Similarly, Grover’s algorithm for searching an unstructured database provides a quadratic speed-up compared to the best classical algorithm [4]. There are also results demonstrating that certain problems are very hard for quantum computers. For

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example, a decision problem about the ground state energy of a local Hamiltonian is QMA-complete [5].

One of the most important problems in computational sciences is to calculate the properties of physical and chemical systems. Such systems are described by the Schrödinger equation. Typically, this equation imposes significant computational demands in carrying out precise calculations [7].

Of particular interest is the estimation of the ground state energy of the time independent Schrödinger equation. In particular, consider the eigenvalue problem

\[
\begin{align*}
\left(-\frac{1}{2}\Delta + V\right)\Psi(x) &= E\Psi(x) \quad x \in I_d = (0,1)^d, \\
\Psi(x) &= 0 \quad x \in \partial I_d,
\end{align*}
\]

where \(\Psi\) is a normalized eigenfunction. Assume that all the masses and the normalized Planck constant are one, and that the potential \(V\) is a smooth function as we will explain below. Our problem is to estimate the ground state energy (i.e., the smallest eigenvalue), \(E_0\), with error \(\varepsilon\).

Such eigenvalue problems can be solved by discretizing the continuous Hamiltonian to obtain a symmetric matrix, and then by approximating the smallest matrix eigenvalue. Eigenvalue problems involving symmetric matrices are conceptually easy and methods such as the bisection method can be used to solve them with cost proportional to the matrix size, modulo polylog factors. The difficulty is that the discretization leads to a matrix of size that is exponential in \(d\). Hence, the cost for approximating the matrix eigenvalue is prohibitive when \(d\) is large. In fact, a stronger result is known, namely the cost of any deterministic classical algorithm must be at least exponential in \(d\), i.e., the problem suffers from the curse of dimensionality [9].

In certain cases, quantum algorithms may be able to break the curse of dimensionality by computing \(\varepsilon\)-accurate eigenvalue estimates with cost polynomial in \(\varepsilon^{-1}\) and in the degrees of freedom \(d\). This was shown in [10] where we see that if the potential is smooth, nonnegative and uniformly bounded by a relatively small constant there exists a quantum algorithm approximating the ground state energy with relative error \(\varepsilon\) and cost proportional to \(d\varepsilon^{-(3+\eta)}\), where \(\eta > 0\) is arbitrary.

It is interesting to investigate conditions for \(V\) beyond those of [9, 10] where quantum algorithms, possibly ones implementing perturbation methods, approximate the ground state energy without suffering from the curse of dimensionality. Indeed, in this paper we assume that \(V\) is convex and uniformly bounded by \(C > 1\), \(^1\) as opposed to \(C \leq 1\) in [9, 10]. In addition, just like in [10], the potential is non-negative and its partial derivatives are continuous and uniformly bounded by a constant \(C' > 0\). We derive a quantum algorithm estimating the ground state energy with relative error \(\varepsilon\) and cost polynomial in \(\varepsilon^{-1}\) and \(d\).

In particular our algorithm solves the eigenvalue problem for a sequence of Hamiltonians \(H_\ell = -\frac{1}{2}\Delta + V_\ell\), for \(\ell = 1, 2, \ldots, L\), where \(V_\ell = \ell \cdot V/L\). The algorithm proceeds in \(L\) stages; see Fig. 1.

\(^1\)We remark that \(C\) may depend on \(d\). The results of this paper hold for \(C = o\left(d^5\right)\), as we will see later in Section 3.2.
In each stage, the algorithm produces an approximate ground state eigenvector of $H_\ell$ which is passed on to the next stage. The fact that $V$ is convex allows us to use lower bounds on the fundamental gap [2] and to select $L$ accordingly so that the ground state eigenvectors of the successive Hamiltonians have a large enough “overlap” between them. This means that the (approximate) ground state eigenvector of $H_\ell$ is also an approximate ground state eigenvector of $H_{\ell+1}$. Our algorithm performs a measurement at every stage, which produces the desired outcome with a certain probability. We select the parameters of the algorithm so that the total success probability is at least $3/4$.

In terms of the number of quantum operations and queries, the resulting cost is

$$c(k) \cdot \varepsilon^{-(3+\frac{1}{2k})} \cdot C^{\frac{4-2\eta}{1-\eta} + \frac{5-2\eta}{2k(1-\eta)}} \cdot d^{1+\frac{4-2\eta}{1-\eta} + \frac{3}{2k(1-\eta)}}$$

and the number of qubits is

$$3 \log \varepsilon^{-1} + \frac{2-\eta}{1-\eta} \cdot \log(Cd) + \Theta(d \cdot \log \varepsilon^{-1}).$$

In the expressions above $k$ is a parameter such that the order of the splitting formula that we use for Hamiltonian simulation is $2k + 1$, $c(k)$ increases with $k$, and $\eta > 0$ is arbitrary. In fact, one can optimize the expressions above with respect to $k$, as in [11]. We do not pursue this direction, since it would overly complicate our analysis and the details of the quantum algorithm. In general, choosing $k = 2$ is sufficient.

Furthermore, a direct consequence of our algorithm is that the state it produced at the end of the $L$th stage overlaps with the ground state of the discretized Hamiltonian within $1 - O((Cd)^{-\frac{2-\eta}{1-\eta}})$. We modify the algorithm to prepare approximations of the ground state of the discretized Hamiltonian that overlap within $1 - O(\delta)$, for $\delta = o((Cd)^{-\frac{2-\eta}{1-\eta}})$. The resulting cost is

$$c(k) \cdot C^{1+\frac{1}{2k}} \cdot d^{2-\frac{1}{2k}} \cdot \varepsilon^{-(3+\frac{1}{2k})} \cdot \delta^{-1-\frac{1}{2k} - \frac{1}{2-\eta} - \frac{1}{k(2-\eta)}}$$

and the number of qubits is

$$3 \log \varepsilon^{-1} + \log \delta^{-1} + \Theta(d \log \varepsilon^{-1}).$$

We use the expression “overlaps within $1 - \delta” to denote that the square of the magnitude of the projection of one state onto the other is bounded from below by $1 - \delta$, for $\delta \in (0, 1)$.


2 Discretization error

The finite difference method is frequently used to discretize partial differential equations, and approximate their solutions. The method with mesh size $h = \frac{1}{n+1}$ yields an $n^d \times n^d$ matrix $M_h = -\frac{1}{2} \Delta_h + V_h$, where $\Delta_h$ denotes the discretized Laplacian and $V_h$ the diagonal matrix whose entries are the evaluations of the potential on a regular grid with mesh size $h = \frac{1}{n+1}$.

$M_h$ is a symmetric positive definite and sparse matrix. For a potential function $V$ that has uniformly bounded first order partial derivatives, we have [16, 17]

$$|E_0 - E_{h,0}| \leq c_1 dh,$$

where $E_{h,0}$ is the smallest eigenvalue of $M_h$. Consider $\hat{E}_{h,0}$ such that

$$|E_{h,0} - \hat{E}_{h,0}| \leq c_2 dh.$$

Then we have $|1 - \frac{E_{h,0}}{E_0}| \leq c' h$, where $c'$ is a constant. The inequality follows by observing that $E_0 \geq d\pi^2/2$, for any $V \geq 0$. Hence we estimate $E_0$ with relative error $O(\varepsilon)$ by taking $h \leq \varepsilon$ and approximating the lowest eigenvalue of $M_h$ with absolute error $O(dh)$.

3 Quantum Algorithm

We consider the Hamiltonian $H_{\ell} = -\frac{1}{2} \Delta + \frac{\ell V}{L}$, and the respective discretized Hamiltonian $M_{h,\ell} = -\frac{1}{2} \Delta_h + \frac{\ell V_h}{L}$, where $\ell = 1, 2, \ldots, L$ and the value of $L$ will be chosen appropriately later. We proceed in $L$ stages. In the $\ell$th stage, we solve the eigenvalue problem for $H_{\ell}$ (and $M_{h,\ell}$) and pass the results to the next stage. In each stage the eigenvalue problem is solved using phase estimation.

In the following section we present some of the properties of phase estimation that we need for our algorithm. We present our algorithm in sections 3.2 and 3.3. The former section deals with the estimation of the ground state energy of $H$ and the latter section deals with the estimation of the ground state eigenvector of $M_h$.

3.1 Phase estimation improves approximate eigenvectors

Phase estimation [8, Fig. 5.2, 5.3] is used to approximate the eigenvalues of unitary matrices provided certain conditions hold. The input is the eigenvector that corresponds to the eigenvalue of interest and the eigenvalue estimate is computed using a measurement outcome at the end of the algorithm. Approximate eigenvectors can also be used input as long as the magnitude of their projection on the true eigenvector is not exponentially small [1]. In such a case, after the measurement, the quantum register that was holding the approximate eigenvector now holds a new state that is also an approximate eigenvector, often an improved one. This was observed in [15] without, however, showing rigorous error estimates and conditions. In this section we study the eigenvector approximation using phase estimation.

Let $A, \|A\| \leq R$, be an $n^d \times n^d$ Hermitian matrix. Then the eigenvalues of $U = e^{iA/R}$ have the form $e^{i\lambda/R}$, where $\lambda$ denotes an eigenvalue of $A$. Equivalently $e^{i\lambda/R} = e^{2\pi i \phi_\lambda}$, where $\phi_\lambda = \lambda/(2\pi R) \in [0, 1)$ is the phase corresponding to $\lambda$. 

4
Besides the (approximate) eigenvector, phase estimation uses matrix exponentials of the form $U^\tau = e^{i A \tau / R}$ to accomplish its task. Frequently, approximations $\tilde{U}_\tau$ are used instead. For instance, when $A$ is given as a sum of Hamiltonians each of which can be implemented efficiently one can use a splitting formula\cite{13, 14} to approximate $U_\tau$. Let the initial state and the matrix exponentials in phase estimation be as follows:

- **Initial state:** We have $|0\rangle^{\otimes b}$ in the top register, that deals with the accuracy, and $|\psi_{in}\rangle$ in the bottom register.

- **Matrix exponentials:** We have a unitary matrix $\tilde{U}_{2t}$ approximating $U_{2t} = e^{i A_{2t} / R}$, for $t = 0, 1, \ldots, b - 1$. Assume that the total error in the approximation of the exponentials is bounded by $\varepsilon_H$, i.e.

$$\sum_{j=0}^{b-1} \| U_{2j} - \tilde{U}_{2j} \| \leq \varepsilon_H,$$

which implies that

$$\| U_t - \tilde{U}_t \| \leq \varepsilon_H, \text{ for } t = 0, 1, \ldots, 2^b - 1$$

Denoting by $\{ \lambda_j, |u_j\rangle \}_{j=0,1,\ldots,n^d-1}$ the eigenpairs of $A$ we have

$$|\psi_{in}\rangle = \sum_j c_j |u_j\rangle.$$  \(\text{(6)}\)

Given a relatively rough approximation of the eigenvector of interest as input in the bottom register of phase estimation, we show conditions under which the bottom register at the end of the algorithm, and after the measurement, holds a state that is an improved approximation of the eigenvector of interest. To simplify matters we proceed in two steps. If the top register is $b$ qubits long as we discussed above, then the conditions for the improvement are shown in Proposition 1 in the Appendix, but the resulting success probability is not satisfactory. To increase the success probability we have extended the top register by $t_0$ qubits and modified part of the proof of Proposition 1 to obtain the theorem below.

(Proposition 1 is really a simplified version of this theorem.)

**Theorem 1.** Let $|\psi_{m'}\rangle$ be the final state in the bottom register after measuring $m'$ on the top register of the phase estimation with initial state $|0\rangle^{\otimes (b+t_0)}|\psi_{in}\rangle$ and unitaries $\tilde{U}_t$, $t = 0, 1, \ldots, 2^{b+t_0} - 1$ and $t_0 \geq 1$. Let $c_0 = \langle u_0 | \psi_{in} \rangle$ and $c'_0 = \langle u_0 | \psi_{m'} \rangle$, where $|u_0\rangle$ is the ground state eigenvector. If

- $b$ is such that the phases satisfy $|\phi_j - \phi_0| > \frac{5}{2} \frac{b}{\pi}$ for all $j = 1, 2, \ldots, n^d - 1$,

- $|c_0|^2 \geq \frac{4^2}{16}$,

then with probability $p \geq |c_0|^2 \left( 1 - \frac{1}{2 (2^b - 1)} \right) - \left( \frac{5 \pi^2}{2^b} + \frac{1 - \frac{\pi^2}{2^2}}{2^b} \right) \cdot \frac{1}{2^{t_0}} - 2 \sum_{j=0}^{b+t_0-1} \| U_{2j} - \tilde{U}_{2j} \|$ we obtain the measurement outcome $m'$ satisfying

- $m' \in G := \{ m \in \{0, 1, \ldots, 2^{b+t_0} - 1 \} : | \phi_0 - \frac{m'}{2^{b+t_0}} | \leq \frac{1}{2^b} \}$. 


and

- if \(1 - |c_0|^2 \leq \gamma \varepsilon_H\) then \(1 - |c'_0|^2 \leq (\gamma + 14) \varepsilon_H\)
- if \(1 - |c_0|^2 \geq \gamma \varepsilon_H^{1-\eta}\), for \(\eta \in (0, 1)\), then \(|c'_0| \geq |c_0|\)

where \(\gamma > 0\) is a constant.

Proof. Just like in Proposition 1 we derive an equation similar to (22), namely,

\[
|c'_0|^2 = |\langle m', \psi_{m'} | m', u_0 \rangle|^2 = \left| \frac{c_0 \alpha(m', \phi_0) + \frac{1}{2} \sum_{j=0}^{n^d-1} c_j \sum_{k=0}^{2^{b+t_0}-1} e^{-2\pi i m' k} 2^{b+t_0} \langle u_0 | x_{j,k} \rangle}{\| |\psi_{1,m'} \rangle + |\psi_{2,m'}\|} \right|^2,
\]

Without accounting for the error due to the approximations \(\tilde{U}_t\), \(t = 0, \ldots, 2^{b+t_0} - 1\), with probability at least \(|c_0|^2 \geq |c_0|^2 \cdot \left(1 - \frac{1}{2(2^0-1)}\right)\) we get a result \(m'\) such that \(m' \in \mathcal{G}\), with

\[
\mathcal{G} = \left\{ m \in \{0, 1, \ldots, 2^{b+t_0} - 1\} : |\phi_0 - \frac{m' c}{2^{b+t_0}}| \leq \frac{2^{t_0}}{2^{b+t_0}} = \frac{1}{2^{t_0}} \right\},
\]

see [3, Thm. 11]. Moreover, according to Lemma 4 the probability of getting a result \(m' \in \mathcal{G}\) with \(\frac{|\alpha(m', \phi_0)|^2}{|\alpha(m', \phi_0)|^2} \leq \frac{\pi^2}{32}\) for all \(j \geq 1\) is at least \(|c_0|^2 \left(1 - \frac{1}{2(2^0-1)}\right) - \left(\frac{5 \pi^2}{2^5} + \frac{1}{2^{t_0}}\right)\) \cdot \frac{1}{2^{t_0}}.

Accounting now for the error due to the approximation of the matrix exponentials, the probability of getting an outcome \(m'\) that belong to \(\mathcal{G}\) and also \(\frac{|\alpha(m', \phi_0)|^2}{|\alpha(m', \phi_0)|^2} \leq \frac{\pi^2}{32}\) for all \(j \geq 1\) is at least \(|c_0|^2 \left(1 - \frac{1}{2(2^0-1)}\right) - \left(\frac{5 \pi^2}{2^5} + \frac{1}{2^{t_0}}\right)\) \cdot \frac{1}{2^{t_0}} - 2 \sum_{j=0}^{b+t_0-1} \|U_j^2 - \tilde{U}_{2j}\|\), see [8, pg. 195].

From now on we consider only such outcomes.

As in Proposition 1, we have the equivalent of (23). Using \(\frac{|\alpha(m', \phi_0)|^2}{|\alpha(m', \phi_0)|^2} \leq \frac{\pi^2}{32}, j \geq 1,\) we obtain

\[
|c'_0| > |c_0| \left( \frac{1}{\sqrt{|c_0|^2 + \frac{\pi^2}{32} \cdot \sum_{j=1}^{n^d-1} |c_j|^2}} - \frac{7 \varepsilon_H}{|c_0|} \right)
\]

\[
= |c_0| \left( \frac{1}{\sqrt{|c_0|^2 + \frac{\pi^2}{32} \cdot (1 - |c_0|^2)}} - \frac{7 \varepsilon_H}{|c_0|} \right), \tag{7}
\]

since \(\sum_{j=0}^{n^d-1} |c_j|^2 = 1\).

Now we examine the different cases, depending on the magnitude of \(|c_0|\).

Case 1: \(1 - |c_0|^2 \leq \gamma \varepsilon_H\), for a constant \(\gamma\). Then (7) becomes

\[
|c'_0| > |c_0| \left( 1 - \frac{7 \varepsilon_H}{\sqrt{1 - \gamma \varepsilon_H}} \right),
\]
because \( f(x) = \frac{1}{\sqrt{x + \frac{\pi^2}{32}(1-x)}} \) is a monotonically decreasing function and \( |c_0|^2 \leq 1 \). Hence

\[
|c'_0|^2 > |c_0|^2 \left( 1 - \frac{14}{\sqrt{1 - \gamma \varepsilon_H}} + \frac{49}{1 - \gamma \varepsilon_H} \varepsilon_H^2 \right)
\]

\[
\geq (1 - \gamma \varepsilon_H) \cdot \left( 1 - \frac{14}{\sqrt{1 - \gamma \varepsilon_H}} + \frac{49}{1 - \gamma \varepsilon_H} \varepsilon_H^2 \right)
\]

\[
= 1 - \gamma \varepsilon_H - 14 \varepsilon_H \sqrt{1 - \gamma \varepsilon_H} + 49 \varepsilon_H^2
\]

\[
\geq 1 - \gamma \varepsilon_H - 14 \varepsilon_H + 49 \varepsilon_H^2 \geq 1 - (\gamma + 14) \varepsilon_H,
\]

since \( 1 - \gamma \varepsilon_H < 1 \). This concludes the first part of the theorem.

Case 2: \( 1 - |c_0|^2 \geq \gamma \varepsilon_H^{1-\eta} \), for some \( \eta \in (0, 1) \) and \( \gamma > 0 \). Then (7) becomes

\[
|c'_0| > |c_0| \left( \frac{1}{\sqrt{1 - (1 - \frac{\pi^2}{32}) \gamma \varepsilon_H^{1-\eta}}} - 7 \frac{\varepsilon_H}{\pi/4} \right),
\]

because \( f(x) = \frac{1}{\sqrt{x + \frac{\pi^2}{32}(1-x)}} \) is a monotonically decreasing function and \( |c_0|^2 \geq \frac{\pi^2}{16} \).

Note that \( \frac{1}{\sqrt{1-a}} \geq \sqrt{1+a} \), for \( |a| \leq 1 \). Hence

\[
|c'_0|^2 > |c_0|^2 \left( 1 + \left( 1 - \frac{\pi^2}{32} \right) \gamma \varepsilon_H^{1-\eta} - \frac{56}{\pi} \varepsilon_H \sqrt{1 + \left( 1 - \frac{\pi^2}{32} \right) \gamma \varepsilon_H^{1-\eta} + \frac{28^2}{\pi^2} \varepsilon_H^2} \right)
\]

\[
> |c_0|^2 \left( 1 + \left( 1 - \frac{\pi^2}{32} \right) \gamma \varepsilon_H^{1-\eta} - O(\varepsilon_H) \right) > |c_0|^2.
\]

This concludes the proof, since we can discard the \( O(\varepsilon_H) \) terms for \( \varepsilon_H \) sufficiently small. \( \square \)

### 3.2 Approximation of the ground state energy

As we already indicated our algorithm goes through \( L \) stages; recall Fig. 1. In the \( \ell \)th state the discretized potential is \( \ell \cdot V_h/L \) and we consider the Hamiltonian \( \tilde{M}_{h,\ell} = -\frac{1}{2} \Delta_h + \frac{1}{2} V_h \).

Let \( |u_{0,\ell} \rangle \) be its ground state eigenvector. We approximate the ground state energy (the minimum eigenvalue) of \( M_{h,\ell} \) within relative error \( \varepsilon \), \( \ell = 1, 2, \ldots, L \). We show how to set up the parameters of the algorithm so that the state produced after the measurement in the bottom register at the end of stage \( \ell - 1 \) is an approximation of both \( |u_{0,\ell-1} \rangle \) and \( |u_{0,\ell} \rangle \) and, therefore, can be used as input in the \( \ell \)th stage. We repeat this procedure until \( \ell = L \). The purpose of the stages \( \ell = 1, \ldots, L-1 \) is to gradually produce a relatively good approximation of the ground state eigenvector \( |u_{0,L} \rangle \) of the Hamiltonian \( M_h = M_{h,L} \), with high probability. The last stage computes the approximation of the ground state energy of \( M_h \).

We first introduce some useful notation. Phase estimation requires two quantum registers [8, Fig. 5.2, 5.3]. The top register determines the accuracy and the probability of success of the algorithm and the bottom register holds an approximation of the ground state of \( M_{h,\ell} \).

Let \( |\psi_{in,\ell} \rangle \) be the state on the bottom register at the beginning of the \( \ell \)th stage and let \( |\psi_{out,\ell} \rangle \) be the state on the same register at the end of the \( \ell \)th stage; see Fig. 2.
Phase Estimation on $W_{h,1}$

$|0\rangle \otimes (b + t_0)$

$|\psi_{in,1}\rangle \equiv |u_{0,0}\rangle$

$|\psi_{out,1}\rangle$

(a) First stage of the algorithm

$|0\rangle \otimes (b + t_0)$

$|\psi_{in,\ell-1}\rangle \equiv |\psi_{in,\ell}\rangle$

$|\psi_{out,\ell-1}\rangle \equiv |\psi_{in,\ell}\rangle$

Stage $\ell - 1$

Stage $\ell$

(b) Diagram of the algorithm for stages $\ell - 1$ and $\ell$, with $\ell = 2, 3, \ldots, L$. The phase estimation on stage $\ell$ runs for the unitary $W_{h,\ell} = e^{-iM_{h,\ell}/\Delta_h}$, with $M_{h,\ell} = -\frac{1}{2}\Delta_h + \ell \cdot \frac{V_h}{L}$

$|0\rangle \otimes (b + t_0)$

$|\psi_{in,L}\rangle \equiv |\psi_{in,L}\rangle$

$|\psi_{out,L}\rangle$

(c) Last stage of the algorithm. The result $j$ of the measurement of the top register provides the approximation to the ground state energy

Fig. 2 A detailed diagram describing the Repeated Phase Estimation algorithm
At the very beginning of the algorithm the bottom register is initialised to the state $|\psi_{n,1}\rangle = |u_{0,0}\rangle$, i.e. the ground state eigenvector of the discretized Laplacian. By choosing an appropriately large $L$, and using lower bounds for the gap between the first and the second eigenvalues of Hamiltonians involving convex potentials [2], we ensure that the initial state of the algorithm has a good overlap with the ground state of $M_{n,1}$. Theorem 1 shows that we can maintain this good overlap between approximate and actual ground state eigenvectors throughout all the stages with high probability. We use $b + t_0$ qubits on the top register. The $b$ qubits are used to control the accuracy in the eigenvalue estimates and the $t_0$ qubits are used to boost the probability of success of each stage.

We provide an overview of the algorithm.

1. **Number of qubits:** We have two resisters, the top and the bottom. The top register has $b + t_0$ qubits, while the bottom register has $d \log_2 h^{-1}$ qubits.

2. **Initial state:** The upper register is initialized to $|0\rangle^{b+t_0}$. The lower register is initialized to $|\psi_{n,1}\rangle = |u_{0,0}\rangle$.

3. **Phase estimation:** Run phase estimation for each of the unitary matrices $W_{h,\ell} = e^{-iM_{h,\ell}/R}$ in sequence, for $\ell = 1, 2, \ldots, L$. where $R$ a parameter to be defined later in this section. In each run the top register is set to $|0\rangle^{b+t_0}$, while the bottom register holds the approximate eigenstate produced in the previous stage, i.e., $|\psi_{n,\ell}\rangle := |\psi_{\text{out},\ell-1}\rangle$ for $\ell = 2, 3, \ldots, L$.

   - **Implementation of exponentials:** Implement each exponential $W_{h,\ell}^{2^j}$ with error $\varepsilon_{j,\ell} := ||W_{h,\ell}^{2^j} - \overline{W_{h,\ell}^{2^j}}||$, for $j = 0, 1, \ldots, t_0 + b - 1$ using Suzuki’s splitting formulas [13, 14].

4. **Output:** Let $j \in \{0, 1, \ldots, 2^{t_0+b}-1\}$ the result of the measurement on the upper register after the last stage. Output $\hat{E}_{h,0} = 2\pi \cdot R \cdot j \cdot 2^{-(b+t_0)}$

Let $\lambda_{j,\ell}$ be the $j$th eigenvalue of $M_{n,\ell}$. The phase corresponding to this eigenvalue is

$$\phi_{j,\ell} = \frac{\lambda_{j,\ell}}{2\pi R}.$$  

Set $R = 3dh^{-2} \gg 2dh^{-2} + C \geq ||-\frac{i}{2}\Delta_h + V_h||$. 3 This choice of $R$ guarantees that $\phi_{j,\ell} \in [0, 1)$ for all $j = 0, 1, \ldots, n^d - 1$ and $\ell = 1, 2, \ldots, L$.

### 3.2.1 Error analysis

We know (eq. (3) and (4)) that we can achieve relative error $O(h)$ if we approximate the ground energy of $M_{h,L}$ with error at most $dh$. This implies that the algorithm has to approximate the eigenvalues $\lambda_{0,\ell}$ within error $dh$, for all $\ell = 0, 1, \ldots, L$, which in turn requires $\phi_{0,\ell}$ to be approximated with error $\frac{dh}{2\pi R}$. This translates to $2^{-b} \leq \frac{dh}{2\pi R}$, which in turn leads to

$$b = \left\lfloor \log \frac{2R\pi}{dh} \right\rfloor = \left\lfloor \log(6\pi h^{-3}) \right\rfloor = \log \Theta(h^{-3}). \tag{8}$$

3 Recall that $C = o(d^2)$ as stated in the Introduction and $h = o(d^{-2})$ as stated in the next section
3.2.2 Preliminary Analysis

In Theorem 1 we have shown conditions relating the state provided as input and the state produced after the measurement in the bottom register of phase estimation, without assuming a particular Hamiltonian form, as we do in this section. In the successive application of phase estimation we intend to use the results of one stage as input to the next. Thus we need to quantify how the results of one stage affect the success probability of the next stage in the case of the Schrödinger equation with a convex potential.

The fundamental gap for Hamiltonians of the form $-\frac{1}{2}\Delta + V$, where $V$ is a convex potential, is at least $\frac{3\pi^2}{2d}$ [2]. The gap between the first and second eigenvalues of $M_{h,\ell}$, for $\ell = 1, 2, \ldots, L$, is reduced by $O(dh)$ [16, 17]. Taking $h = o(d^{-2})$, the gap is at least $\frac{3\pi^2}{2d} - o(d^{-1}) \geq \frac{\pi^2}{d}$. \footnote{\[|\lambda_1(h) - \lambda_0(h)| \geq |\lambda_1(h) - \lambda_0| - |\lambda_1(h) - \lambda_1| \text{ since } \lambda_0(h) \leq \lambda_1, \ where \ the \ subscript \ zero \ denotes \ the \ smallest \ eigenvalue \ of \ a \ Hamiltonian \ and \ the \ subscript \ one \ denotes \ the \ second \ smallest \ eigenvalue.} As a result, the gap between the phases corresponding to the first two eigenvalues is at least $\frac{\pi^2}{d}$. Taking $h < \frac{2\pi^2}{5} \cdot \frac{1}{d^2}$, we have that $2^{-b} < \frac{1}{5} \cdot \frac{\pi^2}{d^2}$, according to (8). This leads to $|\phi_0 - \phi_j| \geq \frac{5}{2\pi}$, for all $j \geq 1$. Hence, for $h = o(d^{-2})$ the assumptions of Theorem 1 hold.

Let $L = \omega(d)$ that will be specified later. Consider the $(\ell - 1)$th stage, with initial state $|\psi_{in,\ell-1}\rangle$ and Hamiltonian $M_{h,\ell-1}$. Assume $|\langle \psi_{out,\ell-1}|u_{0,\ell-1}\rangle| = 1 - \kappa \delta$, where $\kappa > 0$ a constant and $\delta \in [0, 1)$ a quantity satisfying $\delta = \omega((Cd)^2/L^2)$. That is, $|\psi_{in,\ell-1}\rangle$ is not such a good approximation of the ground state eigenvector $|u_{0,\ell}\rangle$. Also assume that the error (5) due to the approximation of the matrix exponentials is $\varepsilon_H = o(\delta)$. Then the magnitude of the projection of the resulting state $|\psi_{out,\ell-1}\rangle$ of this stage onto the ground state eigenvector follows from Theorem 1 as we show in the corollary below.

**Corollary 1.** Let $|\langle \psi_{in,\ell-1}|u_{0,\ell-1}\rangle|^2 = 1 - \kappa \delta$, where $\kappa > 0$ is a constant, $\delta \in [0, 1)$ and $\delta = \omega(\varepsilon_H)$. Then

$$|\langle \psi_{out,\ell-1}|u_{0,\ell-1}\rangle|^2 \geq 1 - \frac{\pi^2 + 1}{32} \kappa \delta, \quad \ell \geq 2.$$  

**Proof.** We reconsider the case 2 of Theorem 1. Retracing the steps, we reach to

$$|\langle \psi_{out,\ell-1}|u_{0,\ell-1}\rangle|^2 > |\langle \psi_{in,\ell-1}|u_{0,\ell-1}\rangle|^2 \left(1 + \left(1 - \frac{\pi^2}{32}\right) \kappa \delta - O(\varepsilon_H)\right)$$

$$= (1 - \kappa \delta) \left(1 + \left(1 - \frac{\pi^2}{32}\right) \kappa \delta - O(\varepsilon_H)\right)$$

$$= 1 - \frac{\pi^2}{32} \kappa \delta - O(\varepsilon_H) + \kappa \delta \cdot O(\varepsilon_H)$$

$$\geq 1 - \frac{\pi^2 + 1}{32} \kappa \delta,$$

where the last inequality is due to $\delta = \omega(\varepsilon_H)$. \hfill \square

Observe after stage $\ell - 1$ is complete, that phase estimation has improved the approximation of $|u_{0,\ell-1}\rangle$. Note that $|\psi_{out,\ell-1}\rangle = |\psi_{in,\ell}\rangle$ and $|\langle u_{0,\ell}|\psi_{in,\ell}\rangle|$ determines the success probability of the $\ell$th stage. To calculate this, we need to take into account the projection of the ground state eigenvector $|u_{0,\ell-1}\rangle$ onto $|u_{0,\ell}\rangle$.\footnote{\[|\lambda_1(h) - \lambda_0(h)| \geq |\lambda_1(h) - \lambda_0| \geq |\lambda_1(h) - \lambda_1| \text{ since } \lambda_0(h) \leq \lambda_1, \ where \ the \ subscript \ zero \ denotes \ the \ smallest \ eigenvalue \ of \ a \ Hamiltonian \ and \ the \ subscript \ one \ denotes \ the \ second \ smallest \ eigenvalue.}
Taking into account the lower bound on the gap between the first two eigenvalues of $M_{h, \ell}$, we express $|u_{0, \ell-1}\rangle$ in terms of the eigenstates of $M_{h, \ell}$ to get

$$\|V/L\|_\infty^2 \geq (1 - |\langle u_{0, \ell-1} | u_{0, \ell} \rangle|^2) \left( \frac{\pi^2}{d} \right)^2 \Rightarrow |\langle u_{0, \ell-1} | u_{0, \ell} \rangle|^2 \geq 1 - \left( \frac{Cd}{\pi^2 L} \right)^2,$$

(9) for $\ell = 2, \ldots, L$, see [9].

**Lemma 1.** Let

$$|\langle \psi_{\text{out}, \ell-1} | u_{0, \ell-1} \rangle|^2 \geq 1 - \kappa' \delta$$

$$|\langle u_{0, \ell-1} | u_{0, \ell} \rangle|^2 \geq 1 - \left( \frac{Cd}{\pi^2 L} \right)^2,$$

with $\delta = \omega \left( \left( \frac{Cd}{\pi^2 L} \right)^2 \right)$. Then

$$|\langle \psi_{\text{out}, \ell-1} | u_{0, \ell} \rangle|^2 \geq 1 - \kappa' \delta - o(\delta), \quad \ell \geq 2,$$

where $\kappa' > 0$ is a constant.

**Proof.** Let $\theta_1 := \arccos |\langle \psi_{\text{out}, \ell-1} | u_{0, \ell-1} \rangle|$ and $\theta_2 = \arccos |\langle u_{0, \ell-1} | u_{0, \ell} \rangle|$.

![Fig. 3](image)

**Fig. 3** The magnitude of the projection of $|\psi_{\text{out}, \ell-1}\rangle$ onto $|u_{0, \ell}\rangle$ in the worst case

Then $|\langle \psi_{\text{out}, \ell-1} | u_{0, \ell} \rangle|^2 \geq \cos^2(\theta_1 + \theta_2)$ (see Fig. 3). Note that

$$\cos^2(\theta_1 + \theta_2) = \frac{1}{2} [1 + \cos(2(\theta_1 + \theta_2))] = \frac{1}{2} [1 + \cos(2\theta_1) \cos(2\theta_2) - \sin(2\theta_1) \sin(2\theta_2)].$$

Now $\cos^2(\theta_1) = \frac{1}{2} \left[ 1 + \cos(2\theta_1) \right] \geq 1 - \kappa' \delta$, which leads to

$$\cos(2\theta_1) \geq 1 - 2\kappa' \delta.$$
Similarly
\[ \cos(2\theta_2) \geq 1 - 2 \left( \frac{Cd}{\pi^2 L} \right)^2. \]

Furthermore
\[ \sin^2(2\theta_1) = 1 - \cos^2(2\theta_1) \leq 1 - \left[ 1 - 2\kappa' \delta \right]^2 \leq 4\kappa' \delta, \]
and similarly \( \sin^2(2\theta_2) \leq 4 \left( \frac{Cd}{\pi^2 L} \right)^2. \) According to the above
\[
\cos^2(\theta_1 + \theta_2) \geq \frac{1}{2} \left[ 1 + (1 - 2\kappa' \delta) \cdot \left( 1 - 2 \left( \frac{Cd}{\pi^2 L} \right)^2 \right) - \sqrt{4\kappa' \delta} \cdot \sqrt{4 \left( \frac{Cd}{\pi^2 L} \right)^2} \right] \\
\geq 1 - \kappa' \delta + 2\kappa' \delta \left( \frac{Cd}{\pi^2 L} \right)^2 - \left( \frac{Cd}{\pi^2 L} \right)^2 - 2\sqrt{\kappa' \delta} \cdot \sqrt{\delta} \cdot \left( \frac{Cd}{\pi^2 L} \right)^2 \\
\geq 1 - \kappa' \delta - o(\delta)
\]
since \( \left( \frac{Cd}{\pi^2 L} \right)^2 = o(\delta) \) and \( \sqrt{\delta} \left( \frac{Cd}{\pi^2 L} \right)^2 = \sqrt{\delta} \cdot o(\delta) = o(\delta). \)

Consider errors \( \varepsilon_{j,\ell}^S \) for the exponentials \( W_{\pi h,\ell}^{2j} \) such that the total error for each stage is
\[
\sum_{j=0}^{b-1} \varepsilon_{j,\ell}^S \leq \varepsilon_H = O \left( \left( \frac{Cd}{\pi^2 L} \right)^2 \right). \]
We use Corollary 1, and Lemma 1 to get
\[
|\langle \psi_{\text{out},\ell-1} | u_{0,\ell} \rangle|^2 = 1 - \frac{\pi^2}{32} + \frac{1}{\kappa \delta} - o(\delta) \geq 1 - \left( \frac{\pi^2}{32} + 10^{-3} \right) \kappa \delta, \quad (10)
\]
where \( \kappa > 0 \) is a constant, \( \delta = \omega \left( \left( \frac{Cd}{\pi^2 L} \right)^2 \right) \) and \( \ell \geq 2. \)

3.2.3 Initial state
The initial state of our algorithm is the ground state eigenvector \( |u_{0,0}\rangle \) of the discretized Laplacian. Hence, \( |\psi_{\text{in},1}\rangle := |u_{0,0}\rangle = |z\rangle^\otimes d \), where \( |z\rangle \) is the ground state eigenvector of the \( n \times n \) matrix corresponding to the (one dimensional) discretization of the second derivative. The coordinates of \( |z\rangle \) are
\[
z_j = \sqrt{2} h \sin(j \pi h), \quad \text{for } j = 1, 2, \ldots, n.
\]
and it can be implemented using the quantum Fourier transform with a number quantum operations proportional to \( \log^2 h^{-1} \) [6]. Thus, the implementation of the initial state of the algorithm \( |u_{0,0}\rangle \) requires a number of quantum operations proportional to \( d \log^2 h^{-1} \).
According to (9) we have
\[
|\langle \psi_{\text{in},1} | u_{0,1} \rangle|^2 \geq 1 - \left( \frac{Cd}{\pi^2 L} \right)^2. \quad (11)
\]
3.2.4 Success probability

According to the analysis in Sections 3.2.2, 3.2.3, and, particularly, observing that the output of one stage is the input to the next from (10,11) we have

$$|\langle \psi_{in,\ell}|u_{0,\ell}\rangle|^2 \geq 1 - \delta,$$

for any $\delta = \omega \left( \left( \frac{Cd}{L} \right)^2 \right)$ and $\ell = 1, 2, \ldots, L$, as long as the total error due to the approximation of the exponentials at each stage is $O \left( \left( \frac{Cd}{L} \right)^2 \right)$, i.e. $\varepsilon_H = O \left( \left( \frac{Cd}{L} \right)^2 \right)$. As a result,

$$|\langle \psi_{in,\ell}|u_{0,\ell}\rangle|^2 \geq 1 - \kappa_1 \left( \frac{Cd}{L} \right)^{2-\eta},$$

(12)

for $\kappa_1$ a constant and any $\eta > 0$.

From Theorem 1, the total probability of success of the algorithm after $L$ steps is

$$P_{total} \geq \left( \min_{\ell=1,2,\ldots,L} |\langle \psi_{in,\ell}|u_{0,\ell}\rangle|^2 \cdot \left( 1 - \frac{1}{2^{(2t_0-1)}} \right) \right) - \left( \frac{5\pi^2}{2^5} + \frac{1 - \pi^2/16}{2^5} \right) \frac{1}{2^{t_0}} - 2 \sum_{j=0}^{b+t_0-1} \|W_{h,\ell}^{2^j} - \tilde{W}_{h,\ell}^{2^j}\| \right)^L. \tag{13}$$

We use Suzuki’s decomposition formulas to approximate the exponentials $W_{h,\ell}^{2^j}$, for $j = 0, 1, \ldots, t_0 + b - 1$; see [13, 14]. We select

$$\varepsilon_{j,\ell}^S := 2^{j-(b+t_0)} \cdot \left( \frac{Cd}{L} \right)^2.$$

The total error at each stage is

$$\sum_{j=0}^{b+t_0-1} \varepsilon_{j,\ell}^S \leq \left( \frac{Cd}{L} \right)^2.$$

As in (5), the choice of $\varepsilon_{j,\ell}^S$ also implies that

$$\|W_{h,\ell}^k - \tilde{W}_{h,\ell}^k\| \leq \left( \frac{Cd}{L} \right)^2,$$

for $k = 0, 1, \ldots, 2^{t_0+b} - 1$. Using (12) and the inequality above, (13) becomes

$$P_{total} \geq \left( \left( 1 - \kappa_1 \left( \frac{Cd}{L} \right)^{2-\eta} \right) \cdot \left( 1 - \frac{1}{2^{(2t_0-1)}} \right) \right) - \left( \frac{5\pi^2}{2^5} + \frac{1 - \pi^2/16}{2^5} \right) \frac{1}{2^{t_0}} - 2 \left( \frac{Cd}{L} \right)^2 \right)^L. \tag{14}$$
Select $t_0$ to satisfy $\frac{1}{2(2^{t_0-1})} \leq \left(\frac{Cd}{L}\right)^{2-\eta}$, by setting
\[
t_0 = \left\lceil \log \left(\frac{L}{Cd}\right)^{2-\eta} \right\rceil.
\] (15)

Then (14) becomes
\[
\begin{align*}
P_{\text{total}} & \geq \left[\left(1 - \kappa_1 \left(\frac{Cd}{L}\right)^{2-\eta}\right) \cdot \left(1 - \left(\frac{Cd}{L}\right)^{2-\eta}\right) - \frac{6\pi^2}{2^5} \left(\frac{Cd}{L}\right)^{2-\eta} - 2 \left(\frac{Cd}{L}\right)^2 \right]^L \\
& \geq \left[1 - \left(\kappa_1 + 3 + \frac{6\pi^2}{2^5}\right) \left(\frac{Cd}{L}\right)^{2-\eta}\right]^L
\end{align*}
\]

Let $\kappa_2 := \kappa_1 + 3 + \frac{6\pi^2}{2^5}$ for brevity. Then
\[
P_{\text{total}} \geq \left[1 - \kappa_2 \left(\frac{Cd}{L}\right)^{2-\eta}\right]^L \geq \left(1 - \frac{\kappa_2 \cdot (Cd)^{2-\eta} / L^{1-\eta}}{L}\right) \cdot e^{-\kappa_2 \cdot (Cd)^{2-\eta} / L^{1-\eta}},
\]

since $(1 - \frac{2}{n})^n \geq (1 - \frac{2}{n}) \cdot e^{-x}$ for $|x| \leq n$ and $n > 1$. In our case $x = \frac{\kappa_2 \cdot (Cd)^{2-\eta}}{L^{1-\eta}}$, $n = L$ and the inequality is satisfied when $L$ is sufficiently large, which we choose by
\[
L = (Cd)^{(2-\eta)/(1-\eta)}.
\] (16)

Then the probability of success becomes
\[
P_{\text{total}} \geq \left(1 - \frac{\kappa_2^2}{L}\right) \cdot e^{-\kappa_2} = \left(1 - \frac{\kappa_2^2}{(Cd)^{(2-\eta)/(1-\eta)}}\right) \cdot e^{-\kappa_2} \geq \frac{1}{2} \cdot e^{-\kappa_2} = \Omega(1),
\]
for $d$ sufficiently large. Hence, the choice of $L$ in (16) guarantees that the algorithm has constant probability of success. Moreover, we can get $P_{\text{total}} \geq 3/4$ if we repeat the algorithm and choose the median as the final result.

### 3.2.5 Cost

We use Suzuki splitting formulas [13, 14] in order to express the exponentials $W_{h,t}^{2j} = e^{-iM_h,t/R}$, with respect to exponentials involving either $-\Delta_h$ or $V_h$.

The Suzuki splitting formula $S_{2k}$ of order $2k+1$ for $k = 1, 2, 3, \ldots$ approximates exponentials of the form $e^{-i(A+B)\Delta t}$, where $A$, $B$ are Hermitian matrices. The formula is constructed recursively by
\[
S_2(A, B, \Delta t) = e^{-iA\Delta t/2}e^{-iB\Delta t}e^{-iA\Delta t/2}
\]
\[
S_{2k}(A, B, \Delta t) = [S_{2k-2}(A, B, p_k \Delta t)]^2 \cdot S_{2k-2}(A, B, (1 - 4p_k)\Delta t) \\
\cdot [S_{2k-2}(A, B, p_k \Delta t)]^2,
\]
where \( k = 2, 3, \ldots \). Unfolding the recurrence and according to \([11, \text{Thm. 1}]\) we obtain the approximation of \( W_{h, \ell}^{2j} \) by
\[
\widetilde{W}_{h, \ell}^{2j} = e^{-iH_{1, \ell}s_{j, 0}} \cdot e^{-iH_{2, \ell}s_{j, 1}} \cdots e^{-iH_{1, \ell}s_{j, 1}} \cdot e^{-iH_{2, \ell}s_{j, K_j, \ell}} \cdot e^{-iH_{1, \ell}s_{j, K_j, \ell}},
\]
where \( s_{j, 0}, \ldots, s_{j, K_j, \ell}, z_{j, 1}, \ldots, z_{j, K_j, \ell} \) and \( K_j, \ell \) are parameters with \( j = 0, 1, \ldots, t_0 + b - 1 \) and \( \ell = 1, 2, \ldots, L \). The Hermitian matrices \( H_{1, \ell} \) and \( H_{2, \ell} \) are defined for each stage \( \ell \) as \( H_{1, \ell} = -\Delta_h/(2R) \) and \( H_{2, \ell} = \ell \cdot V_h/(LR) \).

The exponentials involving \( -\Delta_h \) can be implemented in \( O(d \log^2 h^{-1}) \) quantum operations using the quantum Fourier transform \([6, 18]\). The exponentials involving \( V_h \) can be implemented with two bit queries. Approximately half of the exponentials involve \( -\Delta_h \) and the other half involve \( V_h \). Consequently the number of exponentials provides a good estimate on the cost of the algorithm. The application of Suzuki’s splitting formulas in the case of the time independent Schrödinger equation is discussed in detail in \([10]\).

Let \( N_{j, \ell} \) be the total number of exponentials required for the simulation of \( W_{h, \ell}^{2j} \), \( N_{\ell} \) be the total number of the exponentials required for the \( \ell \)th stage and \( N \) be the total number of exponentials required for all the stages of the algorithm. Using the results of \([11]\) we have
\[
N_{\ell} = \sum_{j=0}^{t_0+b-1} N_{j, \ell} \lesssim \sum_{j=0}^{t_0+b-1} 2 \cdot 5^{k-1} \cdot \| -\Delta_h/R \|_2 \cdot 2^j \left( \frac{4e \cdot 2 \cdot 2^j}{\varepsilon R} \right)^{1/(2k)} \cdot \frac{4e \cdot 2}{3} \left( \frac{5}{3} \right)^{k-1},
\]
where \( k \) is chosen so that the order of the Suzuki splitting formula is \( 2k + 1, k \geq 1 \). However \( \| -\Delta_h/R \|_2 \leq 1 \) and \( \| \frac{\ell}{L} \cdot \frac{V_h}{R} \| \leq \frac{\ell}{L} \cdot \frac{C}{3dh^{-2}} \), which leads to
\[
N_{\ell} \lesssim \sum_{j=0}^{t_0+b-1} \frac{80e}{3} \cdot 5^{k-1} \cdot \left( \frac{5}{3} \right)^{k-1} \cdot 1 \cdot 2^j \cdot \left( \frac{4e \cdot 2 \cdot 2^j}{\varepsilon R} \right)^{1/(2k)} \cdot \frac{4e \cdot 2}{3} \left( \frac{5}{3} \right)^{k-1} \cdot \left( \frac{2^j}{2^j+b+1} \right)^{1/(2k)} \cdot C \cdot d \left( \frac{2^j+b+1}{2^j+b+1} \right)^{1/(2k)}.
\]

Since \( \sum_{j=0}^{t_0+b-1} 2^j \leq 2^{t_0+b} \leq 24\pi \cdot (C \ell)^{\frac{2}{2}} \cdot h^{-3} \). Denote by \( c(k) \) the constant on the expression above that depends on \( k \), namely, \( c(k) := \frac{80e}{3} \cdot \left( \frac{25}{3} \right)^{k-1} \cdot \left( \frac{8e}{3} \right)^{1/(2k)} \cdot (40\pi)^{1+\frac{1}{2k}} \cdot C \cdot d \left( \frac{2^j+b+1}{2^j+b+1} \right)^{1/(2k)} \). We have
\[
N = \sum_{\ell=1}^{L} N_{\ell} \leq c(k) \cdot \sum_{\ell=1}^{L} \left( \frac{\ell}{L} \right)^{1/(2k)} \cdot \left( \frac{2^j+b+1}{2^j+b+1} \right)^{1/(2k)} \cdot \left( \frac{2^j+b+1}{2^j+b+1} \right)^{1/(2k)} \cdot \left( \frac{2^j+b+1}{2^j+b+1} \right)^{1/(2k)} \cdot \left( \frac{2^j+b+1}{2^j+b+1} \right)^{1/(2k)}.
\]
For relative error $O(\varepsilon)$, it suffices to set $h \leq \varepsilon$. In that case

$$N \leq c(k) \cdot \varepsilon^{-(3 + \frac{1}{2k})} \cdot C \left( \frac{4 - 2\eta}{1 - \eta} + \frac{5 - 2\eta}{2k(1 - \eta)} \right) \cdot d^{1 + \frac{4 - 2\eta}{1 - \eta} + \frac{3}{2k(1 - \eta)}}. \quad (17)$$

Recall that the eigenvalues and eigenvectors of the discretized Laplacian are known and the evolution of a system with a Hamiltonian involving $-\Delta_h$ can be implemented with $d \cdot O(\log^2 \varepsilon^{-1})$ quantum operations using the Fourier transform in each dimension; see e.g., [8, p. 209]. The evolution of a system with a Hamiltonian involving $V_h$ can be implemented using two quantum queries and phase kickback. Hence the number of quantum operations required to implement the algorithm is proportional to

$$c(k) \cdot \varepsilon^{-(3 + \frac{1}{2k})} \cdot C \left( \frac{4 - 2\eta}{1 - \eta} + \frac{5 - 2\eta}{2k(1 - \eta)} \right) \cdot d^{1 + \frac{4 - 2\eta}{1 - \eta} + \frac{3}{2k(1 - \eta)}}. $$

The analysis leads to the following theorem.

**Theorem 2.** Consider the ground state energy estimation problem for the time-independent Schrödinger equation (1),(2). The quantum algorithm that applies $L = (Cd)^{(2-\eta)/(1-\eta)}$ stages of repeated phase estimation with:

- **Number of qubits**: The top register has $q := b + t_0 = 3\log \varepsilon^{-1} + \frac{2 - \eta}{1 - \eta} \cdot \log(Cd) + O(1)$ qubits, while the bottom register has $\Theta(d \log \varepsilon^{-1})$ qubits.

- **Input state**: The top register is initialized to $|0\rangle^\otimes q$. The bottom register of the first stage is initialized to $|u_{0,0}\rangle$. Furthermore we set $|\psi_{in,\ell}\rangle := |\psi_{out,\ell-1}\rangle$ for $\ell = 2, 3, \ldots, L$.

- **Implementation of exponentials**: Implement each exponential $W_{k,\ell}^{2j}$ using Suzuki’s splitting formulas of order $2k + 1$ with simulation error $\varepsilon_{j,\ell}^S = 2^{j-q} \cdot (Cd)^{-2/(1-\eta)}$, for $j = 0, 1, \ldots, q - 1$, $\ell = 1, 2, \ldots, L$.

approximates the ground state energy $E_0$ with relative error $O(\varepsilon)$, as $d\varepsilon \to 0$, using a number of bit queries proportional to

$$c(k) \cdot \varepsilon^{-(3 + \frac{1}{2k})} \cdot C \left( \frac{4 - 2\eta}{1 - \eta} + \frac{5 - 2\eta}{2k(1 - \eta)} \right) \cdot d^{1 + \frac{4 - 2\eta}{1 - \eta} + \frac{3}{2k(1 - \eta)}}$$

and a number of quantum operations proportional to

$$c(k) \cdot \varepsilon^{-(3 + \frac{1}{2k})} \cdot C \left( \frac{4 - 2\eta}{1 - \eta} + \frac{5 - 2\eta}{2k(1 - \eta)} \right) \cdot d^{1 + \frac{4 - 2\eta}{1 - \eta} + \frac{3}{2k(1 - \eta)}},$$

where $c(k) := \frac{80c}{3} \cdot (\frac{2\pi}{3})^{k-1} \cdot (\frac{8\pi}{3})^{1/2k} \cdot (24\pi)^{1+\frac{1}{2k}}$, with constant probability of success.

Finally, observe that at the end of the algorithm the state in the bottom register $|\psi_{out,L}\rangle$ satisfies

$$|\langle \psi_{out,L}|u_{0,L}\rangle|^2 \geq 1 - O \left((Cd)^{-\frac{\eta}{1-\eta}}\right),$$

where $|u_{0,L}\rangle$ denotes the ground state eigenvector of $M_h$. This observation motivates the algorithm in the next section.
3.3 An algorithm preparing a quantum state approximating the ground state eigenvector

In Section 3.2 we exhibited a quantum algorithm, based on repeated applications of phase estimation, approximating the ground state energy of the Hamiltonian $H$ (eq. (1) and (2)). It turns out we can use the same algorithm with different values of its parameters, to prepare a quantum state overlapping with the ground state eigenvector of the discretized Hamiltonian $M_h$.

In particular in this section we show an algorithm that:

1. estimates the ground state energy of the Hamiltonian $H$ with relative error $\varepsilon$,
2. approximates the ground state $|u_{0,L}\rangle$ of the discretized Hamiltonian $M_h$ by a state $|\psi\rangle$ such that 
   \[ |\langle u_{0,L}|\psi \rangle|^2 \geq 1 - O(\delta), \]
   where $\delta \in (0,1)$.  

We remark that for $\delta = \Omega \left( (Cd)^{-\frac{2-\eta}{3}} \right)$ we can use the algorithm in Section 3.2. From now on we assume that $\delta = o \left( (Cd)^{-\frac{2-\eta}{3}} \right)$.

3.3.1 Error analysis

We work exactly like in Section 3.2.1 to get the same number of qubits $b$ for the top register of phase estimation (see (8)), namely,
\[ b = \left\lceil \log \frac{2R\pi}{dh} \right\rceil = \left\lceil \log(6\pi h^{-3}) \right\rceil = \log \Theta\left(h^{-3}\right). \]

3.3.2 Success probability

Equations (14), (15) remain the same. What changes is the number of stages $L$. Since we require 
\[ |\langle \psi_{\text{out},L}|u_0 \rangle|^2 \geq 1 - O(\delta), \]
we set
\[ (Cd/L)^{2-\eta} = \delta \Rightarrow L = Cd/\delta^{1/(2-\eta)}. \]  

Just as before, the success probability of the algorithm after $L$ stages is
\[ P_{\text{total}} \geq \left( 1 - \frac{(Cd)^{2-\eta}/L^{1-\eta}}{L} \right)^2 \cdot e^{-\kappa_2(Cd)^{2-\eta}/L^{1-\eta}} = \left( 1 - \frac{o(1)}{L} \right) \cdot e^{-o(1)} \geq 3/4, \]
according to our choice of $L$ in (18) and the fact that $\delta = o \left( (Cd)^{-\frac{2-\eta}{3}} \right)$, since for larger $\delta$ we can use the algorithm in Section 3.2 as we pointed out.

\(^5\)In this section $\delta$ is an input parameter to the algorithm, and is slightly different from $\delta$ as used in sections 3.2.2–3.2.4
3.3.3 Matrix exponential error

Just like before, we approximate $W_{h,\ell}$ with error

$$
\varepsilon_{j,\ell}^S := 2^{j-(b+t_0)}/(L/Cd)^2,
$$

which according to our choice of $L$ becomes

$$
\varepsilon_{j,\ell}^S = 2^{j-(b+t_0)}\delta^{2/(2-\eta)}.
$$

Note that the total error of phase estimation at each stage is $2 \cdot \sum_{j=0}^{b+t_0-1} \varepsilon_{j,\ell}^S = 2 \cdot \delta^{2/(2-\eta)}$, which is asymptotically smaller than $(C\delta)^{2-\eta} = \delta$.

3.3.4 Cost

We work as before. Using the bounds on the number of exponentials [11] required to simulate $W_{h,\ell}^{2^j}$, we have

$$
N_{\ell} = \sum_{j=0}^{t_0+b-1} N_{j,\ell} \leq \sum_{j=0}^{t_0+b-1} 2 \cdot 5 \cdot 5^{k-1} \cdot \|\Delta_h/R\|_2 \cdot 2^j \left( \frac{4e \cdot 2 \cdot 2^j \|\ell \cdot V_h\|_2}{\varepsilon_{j,\ell}^S} \right)^{1/(2k)} \cdot \frac{4e \cdot 2}{3} \left( \frac{5}{3} \right)^{k-1},
$$

where the order of the splitting formula is $2k+1$, $k \geq 1$. Since $\|\Delta_h/R\|_2 \leq 1$ and $\|\ell \cdot V_h\| \leq \frac{C}{3dh}$, we have

$$
N_{\ell} \leq \frac{80e}{3} \cdot 5^{k-1} \cdot \left( \frac{8e}{3} \right)^{1/2k} \cdot \left( \frac{5}{3} \right)^{k-1} \cdot 2^{(b+t_0)/(2k)} \cdot \left( \frac{\ell}{L} \right)^{1/2k} \cdot \left( \frac{C/(dh^{-2})}{\delta^{2/(2-\eta)}} \right)^{1/(2k)}
\leq \frac{80e}{3} \cdot 5^{k-1} \cdot \left( \frac{8e}{3} \right)^{1/2k} \cdot \left( \frac{5}{3} \right)^{k-1} \cdot \frac{b+t_0}{2k} (1+\frac{1}{2\pi}) \cdot \left( \frac{\ell}{L} \right)^{1/2k} \cdot C^{1/(2k)} \cdot d^{-1/(2k)}
\leq \frac{80e}{3} \cdot 5^{k-1} \cdot \left( \frac{8e}{3} \right)^{1/2k} \cdot \left( \frac{5}{3} \right)^{k-1} \cdot (24\pi)^{1+\frac{1}{2k}} \cdot \left( \frac{\ell}{L} \right)^{1/2k} \cdot C^{1/(2k)} \cdot d^{-1/(2k)}
\leq \frac{80e}{3} \cdot 5^{k-1} \cdot \left( \frac{8e}{3} \right)^{1/2k} \cdot \left( \frac{5}{3} \right)^{k-1} \cdot (24\pi)^{1+\frac{1}{2k}} \cdot \left( \frac{\ell}{L} \right)^{1/2k} \cdot C^{1/(2k)} \cdot d^{-1/(2k)}
$$

since $2^b \leq 12\pi h^{-3}$ and $2^t_0 \leq 2^\delta$. Once again, let $c(k) := \frac{80e}{3} \cdot \left( \frac{25}{3} \right)^{k-1} \cdot \left( \frac{8e}{3} \right)^{1/(2k)} \cdot (24\pi)^{1+\frac{1}{2k}}$. The total number of exponentials required is

$$
N = \sum_{\ell=1}^{L} N_{\ell} \leq c(k) \cdot C^{1/(2k)} \cdot d^{-1/(2k)} \cdot h^{-(3+\frac{1}{2k})} \cdot \delta^{-\frac{1}{\eta(2-\eta)}} \cdot \sum_{\ell=1}^{L} \left( \frac{\ell}{L} \right)^{1/(2k)}
\leq c(k) \cdot C^{1/(2k)} \cdot d^{-1/(2k)} \cdot h^{-(3+\frac{1}{2k})} \cdot \delta^{-\frac{1}{\eta(2-\eta)}} \cdot L
\leq c(k) \cdot C^{1+\frac{1}{2k}} \cdot d^{1+\frac{1}{2k}} \cdot h^{-(3+\frac{1}{2k})} \cdot \delta^{-1-\frac{1}{2k}-\frac{1}{2\pi} \cdot \frac{1}{\eta(2-\eta)}}
$$
For relative error $O(\varepsilon)$, it suffices to set $h \leq \varepsilon$. In that case

$$N \leq c(k) \cdot C^{1+\frac{1}{2k}} \cdot d^{1-\frac{1}{2k}} \cdot \varepsilon^{-(3+\frac{1}{2k})} \cdot \delta^{-1-\frac{1}{2k}-\frac{1}{2d-1}}$$

(19)

The analysis above leads to the following theorem.

**Theorem 3.** Consider the ground state energy and ground state eigenvector estimation problem for the time-independent Schrödinger equation (1),(2) with a convex potential. Let $\delta = o((Cd)^{-\frac{2}{2-d}})$. The quantum algorithm that applies $L = Cd \cdot \delta^{-1/(2-\eta)}$ stages of repeated phase estimation with

- **Number of qubits:** The top register has $q := b + t_0 = 3 \log \varepsilon^{-1} + \log \delta^{-1} + O(1)$ qubits, and the bottom register has $\Theta(d \log \varepsilon^{-1})$ qubits.

- **Input state:** The top register is always initialized to $|0\rangle^{\otimes q}$. The bottom register in the first stage is initialized to $|u_0,0\rangle$. Thereafter, the bottom register is set according to $|\psi_{in,\ell}\rangle := |\psi_{out,\ell-1}\rangle$ for $\ell = 2, 3, \ldots, L$.

- **Implementation of exponentials:** Implement each exponential $W_{j,l}^{2^j}$ using Suzuki splitting formulas of order $2k+1$ with simulation error $\varepsilon_{j,l}^S = 2^{j-q} \cdot \delta^{2/(2-\eta)}$, for $j = 0, 1, \ldots, q-1$.

approximates the ground state energy $E_0$ with relative error $O(\varepsilon)$, for $\varepsilon = o(d^{-2})$, using a number of bit queries proportional to

$$c(k) \cdot C^{1+\frac{1}{2k}} \cdot d^{1-\frac{1}{2k}} \cdot \varepsilon^{-(3+\frac{1}{2k})} \cdot \delta^{-1-\frac{1}{2k}-\frac{1}{2d-1}}$$

and a number of quantum operations proportional to

$$c(k) \cdot C^{1+\frac{1}{2k}} \cdot d^{2-\frac{1}{2k}} \cdot \varepsilon^{-(3+\frac{1}{2k})} \cdot \delta^{-1-\frac{1}{2k}-\frac{1}{2d-1}}$$

where $c(k) = \frac{80e}{3} \cdot 5^{k-1} \cdot \left(\frac{8e}{3}\right)^{1/2k} \cdot \left(\frac{5}{3}\right)^{k-1} \cdot (24\pi)^{1+\frac{1}{2k}}$. The final state on the lower register $|\psi_{out,L}\rangle$ satisfies

$$|\langle u_0 | \psi_{out,L} \rangle|^2 \geq 1 - O(\delta),$$

where $|u_0\rangle$ is the ground state eigenvector of $M_h$. The algorithm succeeds with probability at least $3/4$.

### 4 Acknowledgements

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5 Appendix

We derive some useful intermediate results for the analysis in Section 3.1.

Proposition 1. Consider phase estimation with initial state $|0\rangle^\otimes b \otimes |\psi_m\rangle$ and the unitaries $\hat{U}_t$, $t = 0, 1, \ldots, 2^b - 1$. Let $m$ be the measurement outcome of phase estimation and let $|\psi_m\rangle$ be the state after the measurement in the bottom register. Let $c_0 = \langle \psi_m | u_0 \rangle$ and $c'_0 = \langle \psi_m | u_0 \rangle$, where $|u_0\rangle$ is ground state eigenvector. If

- $b$ is such that the phases satisfy $|\phi_j - \phi_0| > \frac{5}{2^b}$ for all $j = 1, 2, \ldots, n^d - 1$.
- $|c_0|^2 \geq \frac{n^2}{16}$.

Then, with probability $p \geq |c_0|^2 \cdot \left( \frac{4}{\pi^2} - 2 \sum_{j=0}^{b-1} \| U^{2^j} - \tilde{U}_2 \| \right)$, we get an outcome $m$ such that

- $|\phi_0 - \frac{m}{2^b}| \leq \frac{1}{2^{b+1}}$

and

- if $1 - |c_0|^2 \leq \gamma \varepsilon_H$ then $1 - |c'_0|^2 \leq (\gamma + 14)\varepsilon_H$
- if $1 - |c_0|^2 \geq \gamma \varepsilon_H^{-\eta}$, for $\eta \in (0, 1)$, then $|c'_0| \geq |c_0|$

where $\gamma$ is a positive constant.

Proof. After the application of $H^\otimes b$ on the top in phase estimation the state becomes

$$
\frac{1}{2^{b/2}} \sum_{k=0}^{2^b-1} |k\rangle \sum_{j=0}^{n^d-1} c_j |u_j\rangle
$$

The state of the system after the application of the controlled $\tilde{U}_2$, $t = 0, 1, \ldots, b - 1$ is

$$
\sum_{j=0}^{n^d-1} c_j \frac{1}{2^{b/2}} \sum_{k=0}^{2^b-1} |k\rangle \tilde{U}_k |u_j\rangle = \frac{1}{2^{b/2}} \sum_{j=0}^{n^d-1} c_j \sum_{k=0}^{2^b-1} |k\rangle \left( U^k |u_j\rangle + D_k |u_j\rangle \right),
$$

where $D_k = \tilde{U}_k - U^k$. Then $\|D_k\| \leq \varepsilon_H$. Since $|u_j\rangle$, $j = 0, 1, \ldots, n^d - 1$, are the eigenvectors of $U$, the state can be written as $|\psi_1\rangle + |\psi_2\rangle$, where

$$
|\psi_1\rangle = \frac{1}{2^{b/2}} \sum_{j=0}^{n^d-1} c_j \sum_{k=0}^{2^b-1} |k\rangle U^k |u_j\rangle = \frac{1}{2^{b/2}} \sum_{j=0}^{n^d-1} c_j \sum_{k=0}^{2^b-1} |k\rangle e^{2\pi i k \phi_j} |u_j\rangle,
$$

and

$$
|\psi_2\rangle = \frac{1}{2^{b/2}} \sum_{j=0}^{n^d-1} c_j \sum_{k=0}^{2^b-1} |k\rangle D_k |u_j\rangle = \frac{1}{2^{b/2}} \sum_{j=0}^{n^d-1} c_j \sum_{k=0}^{2^b-1} |k\rangle |x_{j,k}\rangle,
$$

where $|x_{j,k}\rangle := D_k |u_j\rangle$. Clearly $\| |x_{j,k}\rangle \| \leq \varepsilon_H$, for all $k = 0, 1, \ldots, 2^b - 1$ and $j = 0, 1, \ldots, n^b - 1$. 

20
The next step in phase estimation is to apply $\mathbb{F}^H \otimes I$, where $\mathbb{F}^H$ is the inverse Fourier transform. The state becomes $|\psi_{\mathbb{F}^H u}\rangle = |\psi_{1,\mathbb{F}^H u}\rangle + |\psi_{2,\mathbb{F}^H u}\rangle$, where

$$
|\psi_{1,\mathbb{F}^H u}\rangle = \frac{1}{2^b/2} \sum_{j=0}^{n^d-1} c_j \sum_{k=0}^{2^b-1} \mathbb{F}^H |k\rangle e^{2\pi ik\phi_j} |u_j\rangle
$$

$$
= \frac{1}{2^b} \sum_{j=0}^{n^d-1} c_j \sum_{k,\ell=0}^{2^b-1} e^{2\pi ik(\phi_j - \frac{\pi i}{2^b})} |\ell\rangle |u_j\rangle
$$

$$
= \sum_{j=0}^{n^d-1} c_j \sum_{\ell=0}^{2^b-1} \alpha(\ell, \phi_j) |\ell\rangle |u_j\rangle
$$

where

$$
\alpha(\ell, \phi_j) := \frac{1}{2^b} \sum_{k=0}^{2^b-1} e^{2\pi ik(\phi_j - \frac{\pi i}{2^b})} \quad (20)
$$

and

$$
|\psi_{2,\mathbb{F}^H u}\rangle = \sum_{j=0}^{n^d-1} c_j \frac{1}{2^b/2} \sum_{k=0}^{2^b-1} \mathbb{F}^H |k\rangle |x_{j,k}\rangle = \sum_{j=0}^{n^d-1} c_j \frac{1}{2^b} \sum_{k,\ell=0}^{2^b-1} e^{-2\pi ik/2^b} |\ell\rangle |x_{j,k}\rangle.
$$

Finally we measure the top register on the computational basis, and denote the outcome by $m$. The resulting state is $|m, \psi_m\rangle = \frac{|m,\psi_{1,m}\rangle + |m,\psi_{2,m}\rangle}{||m,\psi_{1,m}\rangle + ||m,\psi_{2,m}\rangle||}$ where

$$
|m, \psi_{1,m}\rangle = \frac{1}{2^b} \sum_{j=0}^{n^d-1} c_j \sum_{k=0}^{2^b-1} e^{2\pi ik(\phi_j - \frac{\pi i}{2^b})} |m\rangle |u_j\rangle = \sum_{j=0}^{n^d-1} c_j \alpha(m, \phi_j) |m\rangle |u_j\rangle,
$$

and

$$
|m, \psi_{2,m}\rangle = \frac{1}{2^b} \sum_{j=0}^{n^d-1} c_j \sum_{k=0}^{2^b-1} e^{-2\pi imk/2^b} |m\rangle |x_{j,k}\rangle \quad (21)
$$

We now consider the magnitude of the projection of the resulting state $|m, \psi_m\rangle$ on $|m, u_0\rangle$, namely $|c_0'|^2 = |\langle m, u_0 | m, \psi_m \rangle| = |\langle u_0 | \psi_m \rangle|$. We have

$$
|c_0'|^2 = \frac{|c_0\alpha(m, \phi_0) + \frac{1}{2^b} \sum_{j=0}^{n^d-1} c_j \sum_{k=0}^{2^b-1} e^{-2\pi imk/2^b} \langle u_0 | x_{j,k} \rangle|^2}{||\psi_{1,m}\rangle + ||\psi_{2,m}\rangle||^2} \quad (22)
$$

If we did not have the matrix exponential approximation error, then with probability at least $|c_0|^2 \cdot \frac{8}{\pi^2}$ the measurement yields an outcome $m$ such that $|\phi_0 - \frac{m}{2^b}| < \frac{1}{2^b}$, see [3, Thm. 11]. There are at most two such outcomes. The one that has the highest probability among them leads to an estimate that is closest to the phase. From now on let $m$ denote the outcome for which $m/2^b$ is closest to the phase. Then its probability is $|c_0|^2 \cdot |\alpha(m, \phi_0)|^2 \geq |c_0|^2 \cdot \frac{1}{\pi^2} \cdot \frac{8}{\pi^2}$ and the error satisfies $|\phi_0 - \frac{m}{2^b}| \leq \frac{1}{2^b + \pi^2}$.

If we account for the error, the probability of $m$ becomes at least $|c_0|^2 \cdot \frac{1}{\pi^2} - 2 \sum_{j=0}^{b-1} ||U^{2^j} - \tilde{U}_2||$; see [8, pg. 195].
From Lemma 3 we have \( \|\psi_{2,m}\| \leq \varepsilon_H \). In addition \( \langle m, \psi_{2,m}|m, u_0 \rangle \leq \|\psi_{2,m}\| \cdot \|u_0\| \leq \varepsilon_H \). Using Lemma 2 and for \( \varepsilon_H < \sqrt{8/\pi^2} \), equation (22) becomes

\[
|c'_0| > |c_0| \left( \frac{\left|\alpha(m, \phi_0)\right|}{\sqrt{\sum_{j=0}^{n(d-1)} |c_j|^2 \cdot |\alpha(m, \phi_j)|^2}} - 7 \frac{\varepsilon_H}{|c_0|} \right)
\]

\[
= |c_0| \left( \frac{1}{\sqrt{\sum_{j=0}^{n(d-1)} |c_j|^2 \cdot |\alpha(m, \phi_j)|^2}} - 7 \frac{\varepsilon_H}{|c_0|} \right)
\]

\[
= |c_0| \left( \frac{1}{\sqrt{|c_0|^2 + \sum_{j=1}^{n(d-1)} |c_j|^2}} - 7 \frac{\varepsilon_H}{|c_0|} \right)
\]  

(23)

Let \( k \) be such that \( |\alpha(m, \phi_k)|^2 = \max_{i \geq 1} |\alpha(m, \phi_i)|^2 \). Then using the assumption \( |\phi_k - \phi_0| > 5/2^b \) we have that \( |\phi_k - m/2^b| > 4/2^b \). From [3, Thm. 11] we get that \( |\alpha(m, \phi_k)|^2 \leq \frac{1}{(2^{2b} - 2^{b+2})^2} = \frac{1}{64} \). Combine this with \( |\alpha(m, \phi_0)|^2 \geq \frac{8}{25\pi^2} = \frac{4}{\pi^2} \) to obtain

\[
|c'_0| > |c_0| \left( \frac{1}{\sqrt{|c_0|^2 + \frac{\pi^2}{256} \cdot \sum_{j=1}^{n(d-1)} |c_j|^2}} - 7 \frac{\varepsilon_H}{|c_0|} \right)
\]

\[
= |c_0| \left( \frac{1}{\sqrt{|c_0|^2 + \frac{\pi^2}{256} \cdot (1 - |c_0|^2)}} - 7 \frac{\varepsilon_H}{|c_0|} \right)
\],  

(24)

since \( \sum_{j=0}^{n(d-1)} |c_j|^2 = 1 \).

Now examine the different cases, depending on the magnitude of \( |c_0| \).

Case 1: \( 1 - |c_0|^2 \leq \gamma \varepsilon_H \), for a constant \( \gamma \). Then (24) becomes

\[
|c'_0| > |c_0| \left( \frac{\varepsilon_H}{\sqrt{1 - \gamma \varepsilon_H}} \right),
\]

because \( f(x) = \frac{1}{\sqrt{x + \frac{\pi^2}{256}(1-x)}} \) is a monotonically decreasing function for \( x \in [0, 1] \). Hence

\[
|c'_0|^2 > |c_0|^2 \left( 1 - \frac{14}{\sqrt{1 - \gamma \varepsilon_H}} \varepsilon_H + \frac{49}{1 - \gamma \varepsilon_H} \varepsilon_H^2 \right)
\]

\[
\geq (1 - \gamma \varepsilon_H) \cdot \left( 1 - \frac{14}{\sqrt{1 - \gamma \varepsilon_H}} \varepsilon_H + \frac{49}{1 - \gamma \varepsilon_H} \varepsilon_H^2 \right)
\]

\[
= 1 - \gamma \varepsilon_H - 14 \varepsilon_H \sqrt{1 - \gamma \varepsilon_H} + 49 \varepsilon_H^2
\]

\[
\geq 1 - \gamma \varepsilon_H - 14 \varepsilon_H + 49 \varepsilon_H^2 \geq 1 - (\gamma + 14) \varepsilon_H,
\]

where the second from last inequality holds because \( 1 - \gamma \varepsilon_H < 1 \). This concludes the first part of the theorem.
Case 2: $1 - |c_0|^2 \geq \gamma \varepsilon_H^{1-\eta}$, for $\eta \in (0,1)$ and $\gamma > 0$. Then (24) becomes

$$|c'_0| > |c_0| \left( \frac{1}{\sqrt{1 - (1 - \frac{\pi^2}{256}) \gamma \varepsilon_H^{1-\eta}}} - 7 \frac{\varepsilon_H}{\pi/4} \right),$$

because $f(x) = \frac{1}{\sqrt{x + \frac{\pi^2}{256} (1-x)}}$ is a monotonically decreasing function for $x \in [0,1 - \gamma \varepsilon_H^{1-\eta}]$ and $|c_0|^2 \geq \frac{\pi^2}{16}$.

Note that $\frac{1}{\sqrt{1-a}} \geq \sqrt{1+a}$, for $|a| \leq 1$. Hence

$$|c'_0|^2 > |c_0|^2 \left( 1 + \frac{\gamma \varepsilon_H^{1-\eta} - 56 \pi \varepsilon_H}{\pi/4} \right)\sqrt{1 + \left( \frac{\gamma \varepsilon_H^{1-\eta} + 28 \pi^2 \varepsilon_H^2}{\pi^2} \right)} > |c_0|^2,$$

for $\varepsilon_H$ sufficiently small. \hfill \Box

**Lemma 2.** For $0 \leq \varepsilon_H < \frac{\pi^2}{256}$, $|c_0|^2 \geq \frac{\pi^2}{16}$ and assuming the measurement outcome $m$ in phase estimation satisfies $\left| \frac{m}{2^6} - \phi_0 \right| \leq 2^{-(b+1)}$ we have

$$\frac{|\alpha(m, \phi_0) - \varepsilon_H|}{\sqrt{\sum_{j=0}^{n-1} |c_j|^2 |\alpha(m, \phi_j)|^2 + \varepsilon_H}} > \frac{|\alpha(m, \phi_0)|}{\sqrt{\sum_{j=0}^{n-1} |c_j|^2 |\alpha(m, \phi_j)|^2}} - 7 \varepsilon_H,$$

where $c_0$ and $\alpha(m, \phi_0)$ are defined in (6) and (20), respectively.

**Proof.** We first show

$$\frac{|\alpha(m, \phi_0)|}{\sqrt{\sum_{j=0}^{n-1} |c_j|^2 |\alpha(m, \phi_j)|^2 + \varepsilon_H}} > \frac{|\alpha(m, \phi_0)|}{\sqrt{\sum_{j=0}^{n-1} |c_j|^2 |\alpha(m, \phi_j)|^2}} - \gamma \varepsilon_H$$

for $\gamma > 4$. We have

$$\frac{|\alpha(m, \phi_0)|}{\sqrt{\sum_{j=0}^{n-1} |c_j|^2 |\alpha(m, \phi_j)|^2 + \varepsilon_H}} > \frac{|\alpha(m, \phi_0)|}{\sqrt{\sum_{j=0}^{n-1} |c_j|^2 |\alpha(m, \phi_j)|^2}} - \gamma \varepsilon_H$$

$$\Leftrightarrow \gamma > \frac{\sum_{j=0}^{n-1} |c_j|^2 |\alpha(m, \phi_j)|^2 \left( \frac{|\alpha(m, \phi_0)|}{\sqrt{\sum_{j=0}^{n-1} |c_j|^2 |\alpha(m, \phi_j)|^2}} - 2 \varepsilon_H \right)}{\sqrt{\sum_{j=1}^{n-1} |c_j|^2 |\alpha(m, \phi_j)|^2}} - \gamma \varepsilon_H,$$

Then

$$\frac{|\alpha(m, \phi_0) - \varepsilon_H|}{\sqrt{\sum_{j=0}^{n-1} |c_j|^2 |\alpha(m, \phi_j)|^2 + \varepsilon_H}} > \frac{|\alpha(m, \phi_0)|}{\sqrt{\sum_{j=1}^{n-1} |c_j|^2 |\alpha(m, \phi_j)|^2}} - 2 \varepsilon_H$$

for $\gamma > 4$. Taking $\gamma = 5$ completes the proof. \hfill \Box
Lemma 3. Consider $|m, \psi_{2,m}\rangle$ as defined in (21). Then $\|\psi_{2,m}\| \leq \varepsilon_H$.

Proof. We have

$$
\|\psi_{2,m}\| = \left\| \frac{1}{2^b} \sum_{j=0}^{n^d-1} c_j \sum_{k=0}^{2^b-1} e^{-2\pi i mk/2^b} |m\rangle |x_{j,k}\rangle \right\|
$$

$$
\leq \frac{1}{2^b} \sum_{k=0}^{2^b-1} \left| e^{-2\pi i mk/2^b} \right| \left\| |m\rangle \right\| \cdot \left\| \sum_{j=0}^{n^d-1} c_j |x_{j,k}\rangle \right\|
$$

$$
= \frac{1}{2^b} \sum_{k=0}^{2^b-1} \left\| D_k \right\| \cdot \left\| \sum_{j=0}^{n^d-1} c_j |u_j\rangle \right\|
$$

$$
\leq \frac{1}{2^b} \sum_{k=0}^{2^b-1} \left\| D_k \right\| \leq \varepsilon_H,
$$

where $D_k = U_k - \tilde{U}_k$ and since $\|D_k\| \leq \varepsilon_H$ due to (5), and $\|\sum_{j=0}^{n^d-1} c_j |u_j\rangle\| = 1$. □

Lemma 4. Under the conditions of Theorem 1, i.e. $m'$ is the result of phase estimation for which $\left| \frac{m'}{2^{a+b}} - \phi_0 \right| \leq \frac{1}{2^b}$, $|\phi_j - \phi_0| > \frac{5}{2}$ for all $j = 1, 2, \ldots, n^d - 1$ and $|c_0|^2 \geq \pi^2/16$, we have

$$
\frac{|\alpha(m', \phi_j)|^2}{|\alpha(m', \phi_0)|^2} \leq \frac{\pi^2}{32}
$$

with probability $p(t_0) \geq |c_0|^2 \left( 1 - \frac{1}{2^{2(a+b-1)}} \right) - \left( \frac{5\pi^2}{2} + \frac{1 - \pi^2}{2^{2a+b}} \right) \cdot \frac{1}{2^b}$.

Proof. Let $M_2 = 2^{a+b}$ and $\Delta_j = \left| \frac{m'}{M_2} - \phi_j \right|$, $i = 0, \ldots, n^d - 1$. For $j \geq 1$ we have [3]

$$
|\alpha(m', \phi_j)|^2 \leq \frac{1}{4(M_2 \Delta_j)^2} \leq \frac{1}{2^{2a+b+6}}.
$$

Observe that $\Delta_j = \left| \frac{m'}{M_2} - \phi_j \right| = \phi_j - \frac{m'}{M_2} \geq \frac{1}{2^b}$, since $\phi_j > m'/M_2$. Also

$$
|\alpha(m', \phi_0)|^2 = M_2^{-2} \cdot \frac{\sin^2(M_2 \Delta_0 \pi)}{\sin^2(\Delta_0 \pi)} \geq \frac{\sin^2(M_2 \Delta_0 \pi)}{(M_2 \Delta_0 \pi)^2} = \sin^2(M_2 \Delta_0 \pi) = \frac{\sin^2(M_2 \phi_0 \pi)}{M_2^2 (\Delta_0 \pi)^2}
$$

where the inequality follows from $\Delta_0 \pi < \pi 2^{-b} \leq \pi/2$. Hence,

$$
\frac{|\alpha(m', \phi_j)|^2}{|\alpha(m', \phi_0)|^2} \leq \frac{\pi^2}{4} \left( \frac{\Delta_0}{\Delta_j} \right)^2 \frac{1}{\sin^2(M_2 \phi_0 \pi)}.
$$
Note that $\Delta_j \geq 4/2^b$ which yields

$$\frac{|\alpha(m', \phi_j)|^2}{|\alpha(m', \phi_0)|^2} \leq \frac{\pi^2}{2^b} \cdot \frac{1}{\sin^2(M_2 \phi_0 \pi)} \quad (27)$$

Note that the upper bound in (27) depends on how close $M_2 \phi_0$ is to an integer or, equivalently, on the fractional part of $m' - M_2 \phi_0$ for $m' \in \mathcal{G}$. We remark that if $M_2 \phi_0$ is an integer then $|\alpha(m', \phi_0)|^2 = 1$ and the lemma statement holds trivially.

Consider, without loss of generality, the closest result $m_0$ to $M_2 \phi_0$ such that $m_0 - M_2 \phi_0 = Y \cdot 2^{-q} \leq 1/2$, $0 < Y \leq 1$, i.e., $m_0 > M_2 \phi_0$. (The case $m_0 < M_2 \phi_0$ is dealt with similarly and we omit it.)

Denote by $m_\ell$, for $\ell = -2^{t_0}, -2^{t_0} + 1, \ldots, 2^{t_0} - 1$, the measurement result such that $m_\ell - M_2 \phi_0 = \ell + Y \cdot 2^{-q}$. These are all the elements of $\mathcal{G}$, the set defined in Theorem 1.

Case 1: Let $1/2 \geq Y \cdot 2^{-q} \geq 1/4$. Then

$$\sin^2(M_2 \phi_0 \pi) = \sin^2(m_\ell \pi - M_2 \phi_0 \pi) = \sin^2(Y \cdot 2^{-q} \pi) \geq \sin^2(\pi/4) \geq 1/2,$$

which according to equation (27) implies

$$\frac{|\alpha(m_\ell, \phi_j)|^2}{|\alpha(m_\ell, \phi_0)|^2} \leq \frac{\pi^2}{32}, \quad (28)$$

for all $m_\ell \in \mathcal{G}$.

Case 2: We now examine the case where $Y \cdot 2^{-q} < 1/4$, i.e. $q \geq 2$. In this case we deal with results $m_\ell$ in the set $\mathcal{G}$ for which the bound for $|\alpha(m_\ell, \phi_j)|^2$ may become greater than $\frac{\pi^2}{32}$.

We show that these results occur with probability at most $\left(\frac{5\pi^2}{2^5} + \frac{1-\pi^2}{2^5}\right)2^{-t_0}$.

Using equation (26) for $m_0$ we obtain

$$|\alpha(m_0, \phi_0)|^2 \geq \frac{\sin^2(Y \cdot 2^{-q} \pi)}{(Y \cdot 2^{-q} \pi)^2} = \sin^2(Y \cdot 2^{-q} \pi).$$

Note that $Y \cdot 2^{-q} < 1/4$, hence $\text{sinc}(\cdot)$ is decreasing. As a result

$$|\alpha(m_0, \phi_0)|^2 \geq \sin^2(2^{-q} \pi) \geq \left(2^{-q} \pi - \frac{(2^{-q} \pi)^3}{6}\right)^2 = \left(1 - \frac{\pi^2}{6 \cdot 2^{2q}}\right)^2,$$

since $\sin(x) \geq x - \frac{x^3}{3!}$, for $x < 1$. Furthermore, since $q \geq 2$ using equation (25) we get

$$\frac{|\alpha(m_0, \phi_j)|^2}{|\alpha(m_0, \phi_0)|^2} \leq \frac{1}{4 \cdot 2^{2(t_0+2)}} \cdot \left(1 - \frac{\pi^2}{6 \cdot 2^{2q}}\right)^{-2} < \frac{1}{28} \cdot \left(1 - \frac{\pi^2}{6 \cdot 2^4}\right) < \frac{\pi^2}{32}, \quad (29)$$

since $t_0 \geq 1$ and $q \geq 2$.

We now examine the remaining results $m_\ell$ for $\ell = \pm 1, \pm 2, \ldots, \pm (2^{t_0} - 1), -2^{t_0}$. From equation (26) we have

$$|\alpha(m_\ell, \phi_0)|^2 \geq \sin^2((\ell + Y \cdot 2^{-q}) \pi) = \frac{\sin^2(Y \cdot 2^{-q} \pi)}{((\ell + Y \cdot 2^{-q} \pi)^2} \geq \frac{2^{-2(q+1)} \cdot 8}{((\ell + Y \cdot 2^{-q} \pi)^2},$$

25
since $1/4 > Y \cdot 2^{-q} \geq 2^{-(q+1)}$ and $\sin x \geq \frac{2\sqrt{3}}{\pi} x$, for $x < \pi/4$. From equation (25) we have

$$\frac{|\alpha(m_\ell, \phi_j)|^2}{|\alpha(m_\ell, \phi_0)|^2} \leq \frac{\pi^2}{8} \cdot \frac{(\ell + Y \cdot 2^{-q})^2 \cdot 2^{2(q+1)}}{2^{2t_0+6}}$$

which for $\ell \geq 1$ implies

$$\frac{|\alpha(m_\ell, \phi_j)|^2}{|\alpha(m_\ell, \phi_0)|^2} \leq \frac{\pi^2}{2^9} \cdot \frac{(\ell + 1)^2 \cdot 2^{2(q+1)}}{2^{2t_0}} =: \beta(\ell, q, t_0) \quad (30)$$

and for $\ell \leq -1$ implies

$$\frac{|\alpha(m_\ell, \phi_j)|^2}{|\alpha(m_\ell, \phi_0)|^2} \leq \frac{\pi^2}{2^9} \cdot \frac{\ell^2 \cdot 2^{2(q+1)}}{2^{2t_0}} =: \beta(\ell, q, t_0) \quad (31)$$

If $q$ is relatively large, although $M_2 \phi_0$ is very close to $m_0$, we might have $\beta(\ell, q, t_0) > \pi^2/32$, for some results $m_\ell$. Let $B = \{\ell \in \{-2^{t_0}, -2^{t_0} + 1, \ldots, 2^{t_0} - 1\} : \beta(\ell, q, t_0) > \pi^2/32\}$ the set of the indices of those results, with $B_- = \{\ell \in B : \ell < 0\}$ and $B_+ = \{\ell \in B : \ell > 0\}$. In addition, let $\ell_1$ be the minimum element of the set $B_+$ and $\ell_2$ be the maximum element of $B_-$. For any $\ell \in B_+$ we have

$$\frac{\pi^2}{2^9} \cdot \frac{(\ell + 1)^2 \cdot 2^{2(q+1)}}{2^{2t_0}} > \pi^2/32 \Leftrightarrow (\ell + 1)^2 2^{2q} > \frac{2^7 \cdot 2^{2t_0} \pi^2}{2^5 \pi^2} = 4 \cdot 2^{2t_0}. \quad (32)$$

Similarly, for any $\ell \in B_-$ we have

$$\frac{\pi^2}{2^9} \cdot \frac{\ell^2 \cdot 2^{2(q+1)}}{2^{2t_0}} > \pi^2/32 \Leftrightarrow \ell^2 2^{2q} > \frac{2^7 \cdot 2^{2t_0} \pi^2}{2^5 \pi^2} = 4 \cdot 2^{2t_0}. \quad (33)$$

From [3, Thm. 11] and for $\ell \in B_+$ we have

$$|\alpha(m_\ell, \phi_0)|^2 = M_2^2 \cdot \frac{\sin^2((\ell + Y \cdot 2^{-p})\pi)}{\sin^2 \left(\frac{\ell + Y \cdot 2^{-q} \pi}{M_2}\right)} \leq \frac{(Y \cdot 2^{-q} \cdot \pi)^2}{\left(\frac{2\sqrt{3}}{\pi}(\ell + Y \cdot 2^{-q})\pi\right)^2} \leq \frac{\pi^2}{2^{2q} \cdot \ell^2 \cdot 2^3} \quad (34)$$

since $Y \cdot 2^{-q} < 1/4$. Similarly for $\ell \in B_-$ we have

$$|\alpha(m_\ell, \phi_0)|^2 \leq \frac{(Y \cdot 2^{-q} \cdot \pi)^2}{\left(\frac{2\sqrt{3}}{\pi}(\ell + Y \cdot 2^{-q})\pi\right)^2} \leq \frac{\pi^2}{2^{2q} \cdot (\ell + 1/4)^2 \cdot 2^3} \quad (35)$$

Let $P_1(B)$ the probability of getting a result $m_\ell \in B$. We have

$$P_1(B) = \sum_{\ell \in B} \sum_{j=0}^{n-1} |c_j|^2 |\alpha(m_\ell, \phi_j)|^2$$

$$= \sum_{\ell \in B_-} \sum_{j=0}^{n-1} |c_j|^2 |\alpha(m_\ell, \phi_j)|^2 + \sum_{\ell \in B_+} \sum_{j=0}^{n-1} |c_j|^2 |\alpha(m_\ell, \phi_j)|^2$$
We can write
\[
\sum_{\ell \in B_-} \sum_{j=0}^{n^d-1} |c_j|^2 |\alpha(m_\ell, \phi_j)|^2 = \sum_{\ell \in B_-} \left( |c_0|^2 |\alpha(m_\ell, \phi_0)|^2 + \sum_{j=1}^{n^d-1} |c_j|^2 |\alpha(m_\ell, \phi_j)|^2 \right)
\]
and
\[
\sum_{\ell \in B_+} \sum_{j=0}^{n^d-1} |c_j|^2 |\alpha(m_\ell, \phi_j)|^2 = \sum_{\ell \in B_+} \left( |c_0|^2 |\alpha(m_\ell, \phi_0)|^2 + \sum_{j=1}^{n^d-1} |c_j|^2 |\alpha(m_\ell, \phi_j)|^2 \right)
\]
Note that \(\sum_{j=1}^{n^d-1} |c_j|^2 = 1 - |c_0|^2 \leq 1 - \frac{\pi^2}{16}\) according to the Lemma’s assumptions, and \(|\alpha(m_\ell, \phi_j)|^2 \leq 2^{-(2t_0+6)}\) from (25). Using the bound from (35) we have
\[
\sum_{\ell \in B_-} \sum_{j=0}^{n^d-1} |c_j|^2 |\alpha(m_\ell, \phi_j)|^2 \leq \sum_{\ell \in B_-} \left( |\alpha(m_\ell, \phi_0)|^2 + \frac{1 - \pi^2/16}{2^{2t_0+6}} \right)
\]
\[
\leq \frac{\pi^2}{22q+3} \sum_{\ell = -2t_0}^{\ell_2} \frac{1}{(\ell + 1/4)^2} + (\ell_2 + 2t_0 + 1) \left( 1 - \frac{\pi^2}{16} \right) \frac{1}{2^{2t_0+6}}
\]
\[
\leq \frac{\pi^2}{22q+3} \sum_{\ell = -2t_0}^{\ell_2} \frac{1}{(\ell + 1/4)^2} + \left( 1 - \frac{\pi^2}{16} \right) \frac{1}{2^{t_0+6}}.
\]
We now take cases in order to calculate \(\sum_{\ell = -2t_0}^{\ell_2} \frac{1}{(\ell + 1/4)^2}\) depending on the value of \(\ell_2\).

**Case 2.1** Let \(\ell_2 = -1\). Then
\[
\sum_{\ell = -2t_0}^{\ell_2} \frac{1}{(\ell + 1/4)^2} = \frac{2^4}{3^2} + \int_{-2t_0}^{-1} \frac{1}{(x + 1/4)^2} dx \leq \frac{2^4}{3^2} + \frac{4}{3} = \frac{28}{9}.
\]
As a result,
\[
\sum_{\ell \in B_-} \sum_{j=0}^{n^d-1} |c_j|^2 |\alpha(m_\ell, \phi_j)|^2 \leq \frac{7}{18} \cdot \frac{\pi^2}{2^{2q}} + \left( 1 - \frac{\pi^2}{16} \right) \frac{1}{2^{t_0+6}}. \tag{36}
\]

**Case 2.2** Let \(\ell_2 < -1\). Then
\[
\sum_{\ell = -2t_0}^{\ell_2} \frac{1}{(\ell + 1/4)^2} \leq \int_{-2t_0}^{\ell_2+1} \frac{1}{(x + 1/4)^2} dx \leq \frac{1}{-\ell_2 - 5/4}.
\]
As a result,
\[
\sum_{\ell \in B_-} \sum_{j=0}^{n^d-1} |c_j|^2 |\alpha(m_\ell, \phi_j)|^2 \leq \frac{\pi^2}{22q+3} \cdot \frac{1}{-\ell_2 - 5/4} + \left( 1 - \frac{\pi^2}{16} \right) \frac{1}{2^{t_0+6}}. \tag{37}
\]
Similarly we examine the probability of the results $m_{\ell}$ for $\ell \in \mathcal{B}_+$. Using the bound from (34) we have

$$\sum_{\ell \in \mathcal{B}_+} \sum_{j=0}^{n^d-1} |c_j|^2 |\alpha(m_{\ell}, \phi_j)|^2 \leq \sum_{\ell \in \mathcal{B}_+} \left( |\alpha(m_{\ell}, \phi_0)|^2 + \frac{1 - \pi^2/16}{2^{2t_0+6}} \right)$$

$$\leq \frac{\pi^2}{2^{2q+3}} \sum_{\ell = \ell_1}^{2^{t_0}-1} \frac{1}{\ell^2} + \left( 2^{t_0} - \ell_1 + 1 \right) \left( 1 - \frac{\pi^2}{16} \right) \frac{1}{2^{2t_0+6}}$$

$$\leq \frac{\pi^2}{2^{2q+3}} \sum_{\ell = \ell_1}^{2^{t_0}-1} \frac{1}{\ell^2} + \left( 1 - \frac{\pi^2}{16} \right) \frac{1}{2^{t_0+6}}.$$

We now consider different values of $\ell_1$, to calculate $\sum_{\ell = \ell_1}^{2^{t_0}-1} \frac{1}{\ell^2}$.

**Case 2.3** Let $\ell_1 = 1$. Then

$$\sum_{\ell = \ell_1}^{2^{t_0}-1} \frac{1}{\ell^2} = 1 + \int_1^{2^{t_0}-1} \frac{1}{x^2} dx \leq 2.$$

As a result,

$$\sum_{\ell \in \mathcal{B}_+} \sum_{j=0}^{n^d-1} |c_j|^2 |\alpha(m_{\ell}, \phi_j)|^2 \leq \frac{\pi^2}{2^{2q+3}} \sum_{\ell = \ell_1}^{2^{t_0}-1} \frac{1}{\ell^2} + \left( 1 - \frac{\pi^2}{16} \right) \frac{1}{2^{t_0+6}}. \quad (38)$$

**Case 2.4** Let $\ell_1 > 1$. Then

$$\sum_{\ell = \ell_1}^{2^{t_0}-1} \frac{1}{\ell^2} \leq \int_{\ell_1-1}^{2^{t_0}-1} \frac{1}{x^2} dx \leq \frac{1}{\ell_1 - 1}.$$

As a result,

$$\sum_{\ell \in \mathcal{B}_+} \sum_{j=0}^{n^d-1} |c_j|^2 |\alpha(m_{\ell}, \phi_j)|^2 \leq \frac{\pi^2}{2^{2q+3}} \cdot \frac{1}{\ell_1 - 1} + \left( 1 - \frac{\pi^2}{16} \right) \frac{1}{2^{t_0+6}}. \quad (39)$$

Let $\ell_1 = 1, \ell_2 = -1$. Then from (36),(38)

$$P_1(\mathcal{B}) \leq \left( \frac{7}{18} + \frac{1}{4} \right) \frac{\pi^2}{2^{2q}} + \frac{1 - \pi^2/16}{2^{5}} \cdot \frac{1}{2^{t_0}}.$$

From (32),(33) we have $2^{2q} > 2^{2t_0+2}$ and $2^{2q} > 2^{2t_0}$. Hence

$$P_1(\mathcal{B}) \leq \left( \frac{7}{18} + \frac{1}{4} \right) \frac{\pi^2}{2^{2t_0+2}} + \frac{1 - \pi^2/16}{2^{5}} \cdot \frac{1}{2^{t_0}} \leq \frac{1 - \pi^2/16}{2^{4}} 2^{-t_0}, \quad (40)$$

for $t_0$ sufficiently large.

Let $\ell_1 = 1, \ell_2 < -1$. From (37),(38)

$$P_1(\mathcal{B}) \leq \frac{\pi^2}{2^{2q+3}} \cdot \frac{1}{-\ell_2 - 5/4} + \frac{\pi^2}{2^{2q+2}} + \frac{1 - \pi^2/16}{2^{5}} \cdot \frac{1}{2^{t_0}}.$$
From (32),(33) we have $2^{2q} > 2^{2t_0}$ and $2^{2q} > \frac{2^{2t_0+2}}{\ell_2^2}$. Hence

$$P_1(B) \leq \frac{\pi^2}{2^q} \cdot \frac{\ell_2^2}{(-\ell_2 - 5/4)^2} \cdot 2^{-(2t_0+2)} + \frac{1 - \pi^2/16}{2^5} \cdot \frac{1}{2t_0} + \frac{\pi^2}{2^{2t_0+2}} \leq \left( \frac{\pi^2}{2^3} + \frac{1 - \pi^2/16}{2^5} \right) 2^{-t_0}, \quad (41)$$

since $\frac{\ell_2^2}{(-\ell_2 - 5/4)^2} \leq 2^{t_0+1}$ for $t_0 \geq 2$.

Let $\ell_1 > 1$, $\ell_2 = -1$. From (36),(39)

$$P_1(B) \leq \frac{7}{18} \cdot \frac{\pi^2}{2^{2q}} + \frac{\pi^2}{2^{2q+3}} \cdot \frac{1}{\ell_1 - 1} + \frac{1 - \pi^2/16}{2^5} \cdot \frac{1}{2t_0}. \quad (42)$$

From (32),(33) we have $2^{2q} > 2^{2t_0+2}$ and $2^{2q} > \frac{2^{2t_0+2}}{(\ell_1+1)^2}$. Hence

$$P_1(B) \leq \frac{7}{18} \cdot \frac{\pi^2}{2^{2t_0+2}} + \frac{1 - \pi^2/16}{2^5} \cdot \frac{1}{2t_0} + \frac{\pi^2}{2^{2t_0+2}} + \frac{\pi^2}{2^{2t_0+5}} \cdot \frac{(\ell_1 + 1)^2}{\ell_1 - 1} \leq \left( \frac{\pi^2}{2^3} + \frac{1 - \pi^2/16}{2^5} \right) 2^{-t_0}, \quad (42)$$

since $\frac{(\ell_1+1)^2}{\ell_1 - 1} \leq 3 \cdot 2^{t_0}$ for $t_0 \geq 1$.

Let $\ell_1 > 1$, $\ell_2 < -1$. From (37),(39)

$$P_1(B) \leq \frac{\pi^2}{2^{2q+3}} \cdot \frac{1}{-\ell_2 - 5/4} + \frac{1 - \pi^2/16}{2^5} \cdot \frac{1}{2t_0} + \frac{\pi^2}{2^{2q+3}} \cdot \frac{1}{\ell_1 - 1}. \quad (42)$$

From (32),(33) we have $2^{2q} > \frac{2^{2t_0+2}}{(\ell_1+1)^2}$ and $2^{2q} > \frac{2^{2t_0+2}}{\ell_2^2}$. Hence

$$P_1(B) \leq \frac{\pi^2}{2^{2t_0+5}} \cdot \frac{(\ell_1 + 1)^2}{\ell_1 - 1} + \frac{1 - \pi^2/16}{2^5} \cdot \frac{1}{2t_0} + \frac{\pi^2}{2^{2t_0+5}} \cdot \frac{\ell_2^2}{-\ell_2 - 5/4} \leq \left( \frac{5\pi^2}{2^5} + \frac{1 - \pi^2/16}{2^5} \right) 2^{-t_0}. \quad (43)$$

Finally, combining the results from (40),(41),(42) and (43) we have

$$P_1(B) \leq \left( \frac{5\pi^2}{2^5} + \frac{1 - \pi^2/16}{2^5} \right) 2^{-t_0}. \quad \blacksquare$$

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