Several natural BQP-Complete problems*

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Abstract

A central problem in quantum computing is to identify computational tasks which can be solved substantially faster on a quantum computer than on any classical computer. By studying the hardest such tasks, known as BQP-complete problems, we deepen our understanding of the power and limitations of quantum computers. We present several BQP-complete problems, including Phase Estimation Sampling and Local Hamiltonian Eigenvalue Sampling. Different than the previous known BQP complete problems (the Quadratically Signed Weight Enumerator problem [22] and the Approximation of Jones Polynomials [12, 13, 2]), our problems are of a basic linear algebra nature and are closely related to the well-known quantum algorithm and quantum complexity theories.

1 Introduction

The last decade has witnessed a great surge of fruitful studies in the new paradigm of quantum computing, especially after Shor discovered the celebrated quantum algorithms for factoring and discrete logarithm [26]. While many other areas like quantum complexity theory, quantum cryptography and quantum error correction have been rapidly developed, the progress in quantum algorithm design, one of the most central tasks of quantum computing, appears much slower than what people had expected. Especially, designing quantum algorithms that have super-polynomial speedup over their classical counterparts seems very hard, and we have only succeeded on few problems, including Hallgren’s polynomial time algorithm for Pell’s equation and class groups [11], van Dam, Hallgren and Ip’s polynomial time algorithm for some hidden shift problems [29], Kuperberg’s subexponential time algorithm for HSP over the dihedral group [23], and some others. In a recent survey by Shor [27], two major possible reasons are proposed to explain the difficulty. One is that we have no good intuitions to design quantum algorithms due to our lack of quantum experience. The other is rather pessimistic: there may actually be only a few problems for which quantum computers have significant advantages over classical computers, and probably we have already found almost all of them.

Considering the enormous payoff of efficient quantum algorithms and these possible reasons for the difficulties to discover them, it is central to identify the class of problems that quantum computers can have substantial speedup over classical computers. Stated in the language of complexity theory, the task amounts to pinning down BQP, the class of languages decidable by a uniform family of polynomial-size quantum circuits with bounded error. While the class could be equivalently characterized by various models, including the quantum Turing machine [5], quantum circuits [32] and quantum adiabatic computation [11, 14], identifying it is difficult,

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just as it is difficult to characterize other important classes such as \( \text{NP} \). Nevertheless, it was recently found that the Quadratically Signed Weight Enumerator problem \[22\] and the problem of approximately evaluating the Jones polynomial \[12, 13, 2\] are \( \text{BQP} \)-complete\(^1\). Such problems are the hardest problems in \( \text{BQP} \). Consequently, the study of \( \text{BQP} \)-complete problems is important as it helps us to deepen our understanding of \( \text{BQP} \) by fully capturing the power of quantum computation. This is similar to the study of \( \text{NP} \)-complete problem which aims at understanding the power of nondeterminism.

In this paper, we provide several other \( \text{BQP} \)-complete problems, including the Local Hamiltonian Eigenvalue Sampling (LHES) problem and the Phase Estimation Sampling (PES) problem, which are (roughly) to sample an eigenvalue of a given Local Hamiltonian or a unitary matrix. Both problems are of an elementary linear algebra nature, which may make them accessible to more computer scientists. More importantly, these two problems are very closely related to well-known quantum algorithm and quantum complexity theories. First, the Local Hamiltonian problem, which basically estimates the minimal eigenvalue of the given local Hamiltonian, is well known to be \( \text{QMA} \)-complete \[21, 19, 18\]\(^2\). Our result on LHES says that if we do not aim at estimating the minimal eigenvalue, but at sampling an eigenvalue according to a very natural distribution, then the problem becomes \( \text{BQP} \)-complete. Second, Phase Estimation is a general framework to design and study quantum algorithms. Many known quantum algorithms that have exponential speedup over their classical counterparts can be described in terms of the phase estimation algorithm \[20, 9\]. Now our result implies that this is not an accident; actually all efficient quantum algorithms can be done in this framework.

Measuring the energies of a quantum observable — or in a mathematical language, measuring eigenvalues of a Hamiltonian — is one of the most important tasks in quantum physics. The problems related to estimating/approximating eigenvalues of Hamiltonians or unitaries has been considered in the literature, including how to make the measurement for special cases \[11, 10, 13\], or using the measurement to solve some computational tasks \[30, 8\]. In this paper, we provide a precise complexity-theoretic framework for studying these problems, and show that the sampling versions of these two basic problems are actually \( \text{BQP} \)-complete.

The remainder of this paper is organized as follows. Section 2 is devoted to basic notations used in the paper, and the definitions of the three problems we are studying in this paper. In Section 3 we prove that the three problems are \( \text{BQP} \)-hard. In Section 4 we show that the problems are in \( \text{BQP} \). The paper concludes with Section 5 which mentions some open problems for future work.

## 2 Preliminaries and definitions

A quantum register consisting of \( n \) qubits is described mathematically by a tensor product Hilbert space \( \mathcal{H} = (\mathbb{C}^2)^\otimes n \). A state of the quantum register is given by a unit vector \( |\psi\rangle \). Transformations of the states are described by unitary operations acting on \( \mathcal{H} \). Every unitary operation has to be composed out of elementary gates for implementation purposes. A measurement with respect to the orthogonal subspaces \( S_1, S_2 \) (where \( S_1 \oplus S_2 = \mathcal{H} \)) causes the system to collapse to \( P_1 |\psi\rangle / \| P_1 |\psi\rangle \| \) or \( P_2 |\psi\rangle / \| P_2 |\psi\rangle \| \), with probability \( \| P_1 |\psi\rangle \|^2 \) and \( \| P_2 |\psi\rangle \|^2 \), respectively, where \( P_i \) is the projector onto the subspace \( S_i \). For a comprehensive introduction to quantum computing, please refer to the textbooks \[23, 21\].

### 2.1 Definition of the problems

The standard definition of Local Hamiltonian and Phase Estimation, two problems extensively studied in quantum complexity theory and in quantum algorithm engineering, are as follows.

\(^1\)Strictly speaking, approximation of the Jones polynomial is neither a language nor a decision problem. Here the concept of completeness is generalized in both their and our work: A computational task is \( \text{BQP} \)-complete if it can be solved by a polynomial time quantum computer, and any \( \text{BQP} \) problem can be reduced to this problem.

\(^2\)Recently another problem (Consistency of Local Density Matrices) is showed to be also \( \text{QMA} \)-complete \[24\].
Local Hamiltonian Minimal Eigenvalue (LH)

**Input:** 1) Two numbers $a$ and $b$ such that $a < b$ and the gap $b - a = \Omega(1/poly(n))$. 2) A Hamiltonian $H = \sum_j H_j$ operating on $n$ qubits, where $j$ ranges over a set of size polynomial in $n$, and each $H_j$ operates on a constant number of qubits. It is promised that either $\lambda(H) < a$ or $\lambda(H) > b$, where $\lambda(H)$ is the minimal eigenvalue of $H$.

**Output:** 0 if $\lambda(H) < a$, and 1 if $\lambda(H) > b$.

Phase Estimation (PE)

**Input:** A unitary matrix $U$, given by black-boxes of controlled-$U$, controlled-$U^2$, ..., controlled-$U^{2^{j-1}}$ operations, and an eigenvector $|u\rangle$ of $U$ with eigenvalue $e^{2\pi i \varphi}$ with the value of $\varphi \in [0,1)$ unknown.

**Output:** An $n$-bit estimation of $\varphi$.

The paper will study several average and sampling variants of them. For the sampling versions, we need a notion of the approximation of a probability distribution. Suppose there is a probability distribution $p$ on the sample space $X = \{x_1, \ldots, x_M\}$, on which a distance function $d$ has been defined. Then a probability distribution $q$ on $X$ is said to $(\epsilon, \delta)$-approximate $p$ if there is a decomposition $q_i = \sum_j q_j$ s.t. each $q_{ij} \geq 0$ and $\forall j, \sum_{i \in d(x_i, x_j) \leq \varepsilon} q_{ij} \geq (1 - \delta)q_j$. Intuitively, this means that if we draw a sample according to $q$, then it will be $\epsilon$-close to $x_j$ with probability at least $(1 - \delta)p_j$. Sometimes we also say that a sample drawn according to the probability distribution $q$ is an estimation of $x_j$ up to $\epsilon$ with probability at least $(1 - \delta)p_j$.

**Comment.** Note that because of the $\epsilon$-approximation (induced by the distance $d$), the standard distance measures between two probability distributions, such as total variance (or any $p$-norm generalization of it), Hellinger distance, or Kullback-Leibler distance, do not qualify for our purpose. For example, suppose $X = \{0.01, 0.02, \ldots, 1\}$, $p(x) = 0.1$ if $x \in \{0.1, 0.2, \ldots, 1\}$, and $q(x) = 0.1$ if $x \in \{0.09, 0.19, \ldots, 0.99\}$. Then intuitively these two distributions are very close to each other. But the total variance between them is $\frac{1}{2} \sum x |p(x) - q(x)| = 1$, the maximal possible distance. (In this example, the Hellinger distance is 1, and the Kullback-Leibler distance is infinity. All of these are not desired because they treat different samples in the sample space as totally different objects. But in many applications such as those in this paper, the sample space has a natural distance measure on it.)

Now we are ready to define the sampling versions of LH and PE as follows. Note that they are sampling problems rather than the standard decision or searching problems: on every input, a sampling problem is required to output some value with some probability.

Local Hamiltonian Eigenvalue Sampling (LHES)

**Input:** 1) Hamiltonian $H = \sum_j H_j$ operating on $n$ qubits, where $j$ ranges over a set of size polynomial in $n$, and each $H_j$ operates on a constant number of qubits. Suppose the eigenvalues and the corresponding eigenvectors of $H$ are $\{\lambda_k, |\eta_k\rangle\}_{k}$ satisfying $|\lambda_k| < poly(n)$ for each $k$. 2) An estimation precision $\epsilon = \Omega(1/poly(n))$. 3) A sampling error probability $\delta = \Omega(1/poly(n))$. 4) A classical $n$-bit string $b \in \{0,1\}^n$.

**Output:** An estimation of $\lambda_k$ up to $\epsilon$ with probability at least $(1 - \delta)|\langle b | \eta_k \rangle|^2$.

Phase Estimation Sampling (PES)

**Input:** 1) $\langle U \rangle$, the description of a $2^n \times 2^n$ unitary matrix $U$ (which is a $poly(n)$-size quantum circuit). Suppose the eigenvalues of $U$ are $\{\lambda_j = e^{2\pi i \varphi_j}\}_{j=1,\ldots,2^n}$ (where $\varphi_j \in [0,1)$ for each $j$), with the corresponding eigenvectors $\{|\eta_j\rangle\}_{j=1,\ldots,2^n}$. 2) An estimation precision $\epsilon = \Omega(1/poly(n))$. 3) A sampling error probability $\delta = \Omega(1/poly(n))$. 4) A classical $n$-bit string $b \in \{0,1\}^n$.

**Output:** An estimation of $\varphi_j$ up to $\epsilon$ with probability at least $(1 - \delta)|\langle b | \eta_j \rangle|^2$. 


One could also consider to estimate the average phase instead of sampling the phase. One caveat here is that in the Phase Estimation and the PES problems, it is implicitly assumed that the estimation is in a circular sense, i.e. if the \( \varphi_u \) is very close to 1, then an answer very close to 0 is considered correct.\(^3\) But when we consider the average phase, this becomes a problem: if we have two unitary matrices, one with all eigenvalues close to -1 and another with all eigenvalues close to 1, then we may not be able to distinguish them since the average phase of the second matrix could also be close to 1/2 due to the cancellation of those small and large phases. For this reason, it is more natural to consider the average eigenvalue of a unitary matrix. We define the Local Unitary matrix Average Eigenvalue (LUAE) as follows.

**Local Unitary matrix Average Eigenvalue (LUAE)**

**Input:** The same as that of PES.

**Output:** An estimation of the average eigenvalue \( \lambda = \sum_{j=1}^{2^n} |\langle b|\eta_j\rangle|^2 \lambda_j \) up to precision \( \epsilon \) with probability at least \( 1 - \delta \).

The main theorem of this paper can be written as

**Theorem 1** LHES, PES and LUAE are all \( \text{BQP} \)-complete.

### 3 BQP-hardness of the problems

In this section we will show that the three problems LHES, PES and LUAE are all \( \text{BQP} \)-hard.

#### 3.1 LHES is \( \text{BQP} \)-hard

**Theorem 2** \( \text{BQP} \subseteq \text{BPP}^{\text{LHES}} \)

**Proof** For any \( L \in \text{BQP} \), there is a uniform family of polynomial size quantum circuits with \( \epsilon \)-bounded error (for a small constant \( \epsilon \)) that decides if \( x \in L \) or \( x \notin L \) as depicted in Figure 1. For \( n \)-bit inputs, denote by \( U \) the corresponding quantum circuit and suppose the size of \( U \) is \( M \), which is bounded by a polynomial in \( n \). Further suppose that the computation is described by \( U|x,0\rangle = \alpha_{x,0}|0\rangle|\psi_{x,0}\rangle + \alpha_{x,1}|1\rangle|\psi_{x,1}\rangle \), where \( 0 \) is the initial state of the ancillary qubits, and \( |\psi_{x,0}\rangle \) and \( |\psi_{x,1}\rangle \) are pure states. After the \( U \) transform, the first qubit is measured and the algorithm outputs the result based on the outcome of the measurement. As the requirement of correctness, we have \( |\alpha_{x,0}|^2 < \epsilon \) if \( x \in L \), and \( |\alpha_{x,1}|^2 < \epsilon \) if \( x \notin L \).

\[
\begin{align*}
|x_1\rangle & \\
|x_2\rangle & \\
\vdots & U \quad \vdots \\
|x_n\rangle & \\
|0\rangle & \\
\end{align*}
\]

**Figure 1:** Circuit U

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\(^3\)This can be seen from the analysis of the Phase Estimation algorithm; see, for example, [25].
We now construct a local Hamiltonian $H$ encoding the circuit $U$ and binary strings $b$ encoding the inputs $x$ such that eigenvalue sampling applied to $H$ and $b$ yields significantly different probability distributions for the two cases of $x \in \mathcal{L}$ and $x \notin \mathcal{L}$. To this end, we construct the circuit $V$ in Figure 2, where we add a qubit $|r\rangle$ to store a copy of the output of $U$.

![Figure 2: Circuit V](image)

Suppose the circuit is decomposed as $U = U_M \cdots U_1$, where each $U_j$ an elementary gate. Then $U^\dagger = U_1^\dagger \cdots U_M^\dagger$. Let $V_j$ be the $j$-th gate in $V$, i.e. $V_j = U_j$ for $j = 1, \ldots, M$, $V_{M+1}$ be the CNOT gate, and $V_j = U_{2M+2-j}^\dagger$ for $j = M+2, \ldots, 2M+1$. Let $N = 2M+1$, the number of gates in $V$. Attach a clock register $|\rangle_t$ to the system. Define the operator

$$F = \sum_{j=1}^{N-1} V_j \otimes |j\rangle_t \langle j-1|_t + V_N \otimes |0\rangle_t \langle N-1|_t.$$  

(1)

Note that $F$ is an $O(\log N)$-local operator; we will remark how to slightly modify it to be a 4-local operator at the end of the proof. Define

$$|\varphi_{x,j}\rangle = F^j(|0\rangle|x,0\rangle|0\rangle_t)$$  

(2)

for $j \geq 0$, where $F^j$ means that $F$ is applied $j$ times. Then for $j = 0, \ldots, 2N-1$,

$$|\varphi_{x,j}\rangle = \begin{cases} 
|0\rangle \otimes U_j \cdots U_1|x,0\rangle \otimes |j\rangle_t & j = 0, \ldots, M \\
|0\rangle \otimes U_{2M+2-j}^\dagger \cdots U_{M}^\dagger P_U \cdots U_1|x,0\rangle \otimes |j\rangle_t & j = M+1, \ldots, 2M \\
|0\rangle \otimes U_{j-2M}^\dagger \cdots U_{M}^\dagger P_U \cdots U_1|x,0\rangle \otimes |j-N\rangle_t & j = 2M+1, \ldots, 3M+1 \\
|0\rangle \otimes U_{2N-j} \cdots U_1|x,0\rangle \otimes |j-N\rangle_t & j = 3M+2, \ldots, 4M+1 
\end{cases}$$  

(3)

where $P_0$ and $P_1$ are the projectors onto the subspaces of the first output qubit of $U$ being 0 and 1, respectively. It is also easy to see that $|\varphi_{x,j}\rangle = |\varphi_{x,j \mod 2N}\rangle$ for $j \geq 2N$.

Note that for different $j$ and $j'$ in $\{0, \ldots, 2N-1\}$, $|\varphi_{x,j}\rangle$ and $|\varphi_{x,j'}\rangle$ are orthogonal if $|j-j'| \neq N$ due to the clock register. Also note that $U_M \cdots U_1|x,0\rangle = U|x,0\rangle = \alpha_{x,0}|0\rangle|\psi_{x,0}\rangle + \alpha_{x,1}|1\rangle|\psi_{x,1}\rangle$ by definition. Therefore, we have $\langle \varphi_{x,j}| \varphi_{x,N+j}\rangle = \langle x,0|U_1^\dagger \cdots U_{M}^\dagger P_U \cdots U_1|x,0\rangle = |\alpha_{x,0}|^2$ for $j = 0, \ldots, N-1$. To summarize, we have

$$\langle \varphi_{x,j}| \varphi_{x,j'}\rangle = \begin{cases} 
0 & |j-j'| \neq N \\
|\alpha_{x,0}|^2 & |j-j'| = N 
\end{cases}$$  

(4)

Define the subspace $S_x = \text{span}\{ |\varphi_{x,j}\rangle : j = 0, \ldots, 2N-1 \}$. The key point here is that though $F$ has an exponentially large dimension, $F|_{S_x}$ is of only polynomial dimension. Now
if \( \alpha_{x,0} = 1 \), then \( S_x \) has dimension of \( N \), and \( F \) has a period of \( N \) on \( S_x \). Actually, \( F|_{S_x} \) is just a shift operator on the basis \( \{ |\varphi_{x,i}\rangle \}_{i=0,\ldots,N-1} \), i.e. \( F|_{S_x} |\varphi_{x,i}\rangle = |\varphi_{x,(i+1) \mod N}\rangle \). It is not hard to see that this operator has eigenvalues \( \lambda_k = e^{2\pi i/N} \) with corresponding eigenvectors \( |\xi_k\rangle = \frac{1}{\sqrt{N}} \sum_{j=0}^{N-1} e^{-kj/N} |\varphi_{x,j}\rangle \), where \( e^{2\pi i/N} = \cos(2\pi k/N) + i\sin(2\pi k/N) \).

Also note the fact that

\[
|\langle \varphi_{x,0} | \xi_k \rangle|^2 = \frac{1}{N}
\]

for any \( k = 0,\ldots, N-1 \).

Now we consider the general case of \( \alpha_{x,0} \neq 1 \), in which case \( S_x \) has dimension \( 2N \) and \( F \) has period of \( 2N \). Note that if \( x \notin L \), then \( |\varphi_{x,N+j}\rangle \) is very close to \( |\varphi_{x,j}\rangle \); if \( x \in L \), then \( |\varphi_{x,N+j}\rangle \) is almost orthogonal to \( |\varphi_{x,j}\rangle \). See Figure 3 for an illustration.

To find the eigenvalues and eigenvectors of \( F|_{S_x} \), define

\[
|\phi_{x,j}\rangle = \frac{|\varphi_{x,j}\rangle + |\varphi_{x,N+j}\rangle}{\||\varphi_{x,j}\rangle + |\varphi_{x,N+j}\rangle\|}, \quad |\gamma_{x,j}\rangle = \frac{|\varphi_{x,j}\rangle - |\varphi_{x,N+j}\rangle}{\||\varphi_{x,j}\rangle - |\varphi_{x,N+j}\rangle\|}
\]

for \( j = 0,\ldots, N-1 \). Then first, because \( \langle \varphi_{x,j} | \varphi_{x,N+j} \rangle = |\alpha_{x,0}|^2 \) is a real number, we have \( \langle \varphi_{x,j} | \gamma_{x,j} \rangle = 0 \). Together with Equality \( 4 \), we know that \( \{ |\phi_{x,0}\rangle, \ldots, |\phi_{x,N-1}\rangle, |\gamma_{x,0}\rangle, \ldots, |\gamma_{x,N-1}\rangle \} \) form an orthonormal basis of \( S_x \). Second, since

\[
|\varphi_{x,0}\rangle \xrightarrow{F} |\varphi_{x,1}\rangle \xrightarrow{F} \ldots \xrightarrow{F} |\varphi_{x,2N-1}\rangle \xrightarrow{F} |\varphi_{x,0}\rangle,
\]

we observe that

\[
|\phi_{x,0}\rangle \xrightarrow{F} |\phi_{x,1}\rangle \xrightarrow{F} \ldots \xrightarrow{F} |\phi_{x,2N-1}\rangle \xrightarrow{F} |\phi_{x,0}\rangle
\]

and

\[
|\gamma_{x,0}\rangle \xrightarrow{F} |\gamma_{x,1}\rangle \xrightarrow{F} \ldots \xrightarrow{F} |\gamma_{x,2N-1}\rangle \xrightarrow{F} -|\gamma_{x,0}\rangle.
\]

Therefore \( F|_{S_x} = F_1 \oplus F_2 \), where \( F_1 \) and \( F_2 \) act on \( S_{x,+} = \text{span}\{ |\phi_{x,0}\rangle, \ldots, |\phi_{x,N-1}\rangle \} \) and \( S_{x,-} = \text{span}\{ |\gamma_{x,0}\rangle, \ldots, |\gamma_{x,N-1}\rangle \} \), respectively, with the matrix representations (in the basis \( \{ |\phi_{x,j}\rangle \} \) and \( \{ |\gamma_{x,j}\rangle \} \), respectively) as follows:

\[
F_1 = \begin{pmatrix}
0 & 0 & 0 & \ldots & 0 & 1 \\
1 & 0 & 0 & \ldots & 0 & 0 \\
0 & 1 & 0 & \ldots & 0 & 0 \\
\vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\
0 & 0 & 0 & \ldots & 1 & 0
\end{pmatrix}, \quad F_2 = \begin{pmatrix}
0 & 0 & 0 & \ldots & 0 & -1 \\
1 & 0 & 0 & \ldots & 0 & 0 \\
0 & 1 & 0 & \ldots & 0 & 0 \\
\vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\
0 & 0 & 0 & \ldots & 1 & 0
\end{pmatrix}.
\]
So \( F_1 \) is just a shift operator we mentioned before, which has eigenvalues \( \mu_k = \omega_N^k \) and eigenvectors \( |\eta_k\rangle = \frac{1}{\sqrt{N}} \sum_{j=0}^{N-1} w_N^{-kj} |\phi_{x,j}\rangle \). It is also not hard to find that \( F_2 \) has the eigenvalues \( \nu_k = \omega_N^{k+1/2} \) with the eigenvectors \( |\varsigma_k\rangle = \frac{1}{\sqrt{N}} \sum_{j=0}^{N-1} w_N^{-(k+1/2)j} |\gamma_{x,j}\rangle \). Let \( P_+ \) and \( P_- \) be the projectors onto \( S_+ \) and \( S_- \), respectively. Note that

\[
\|P_-|\varphi_{x,0}\rangle\|^2 = \|\frac{|\varphi_{x,0}\rangle - |\varphi_{x,N}\rangle}{2}\|^2 = \frac{2 - \langle \varphi_{x,0} | \varphi_{x,N} \rangle - \langle \varphi_{x,N} | \varphi_{x,0} \rangle}{4} = \frac{1 - |\alpha_{x,0}|^2}{2} = \frac{|\alpha_{x,1}|^2}{2}.
\]

Thus \( \|P_+|\varphi_{x,0}\rangle\|^2 = 1 - \|P_-|\varphi_{x,0}\rangle\|^2 = (1 + |\alpha_{x,0}|^2)/2 \). By this, we can derive that

\[
|\langle \varphi_{x,0} | \eta_k \rangle|^2 = \frac{1}{2N} (1 + |\alpha_{x,0}|^2), \quad |\langle \varphi_{x,0} | \varsigma_k \rangle|^2 = \frac{1}{2N} |\alpha_{x,1}|^2.
\]

for any \( k = 0, \ldots, N - 1 \).

Now the local Hamiltonian is constructed as \( H = F + F^\dagger \). It is easy to verify that \( H \) is a local Hamiltonian. And further, suppose the eigenvalues of \( F \) are \( \{\kappa_j\} \) with the eigenvectors \( \{|\psi_j\rangle\} \), then the eigenvalues of \( H \) are just \( \{\kappa_j + \kappa_j^*\} \) with the same corresponding eigenvectors. Now the \textbf{BPP} algorithm with the LHES oracle is as follows.

On input \( x \),

1. Feed \((H, 1/4N, 1/100, 0x00)\) as input to the LHES oracle, getting an output \( a \)
2. If \( |a| > 1 \),
   go back to Step 1
3. If \( \min_{k=0, \ldots, N-1} |a - 2 \cos \frac{2\pi(k+1/2)}{N}| < \min_{k=0, \ldots, N-1} |a - 2 \cos \frac{2\pi k}{N}| \)
   output "\( x \in L \)"
   else
   output "\( x \notin L \)"

The algorithm is correct with probability at least \( \frac{1}{2}(1 - \delta)(1 - \epsilon) \) for \( x \in L \), and correct with probability at least \( (1 - \delta)(1 - \frac{\epsilon}{2}) \) for \( x \notin L \). Actually, in Step 1, the oracle will output an estimation of \( 2 \cos \frac{2\pi k}{N} \) (up to an additive \( \frac{1}{4N} \)) with probability at least \( \frac{1}{2N} (1 - \delta)(1 + |\alpha_{x,0}|^2) \), and output an estimation of \( 2 \cos \frac{2\pi(k+1/2)}{N} \) (up to an additive \( \frac{1}{4N} \)) with probability at least \( \frac{1}{2N} (1 - \delta)|\alpha_{x,1}|^2 \), for any \( k = 0, \ldots, N - 1 \). Note that now the case of \( \alpha_{x,0} = 1 \) can be consistently viewed as a special case of \( \alpha_{x,0} \neq 1 \) by comparing Equality (5) and (9).

If \( k \in [N/6, N/3) \cup [2N/3, 5N/6] \), which happens with probability \( 1/3 \) for a uniformly random \( k \in \{0, \ldots, N - 1\} \), then the algorithm will proceed to the outer "else" branch in Step 2. Note that for \( \theta, \theta' \in [\pi/3, 2\pi/3] \cup [4\pi/3, 5\pi/3] \) and \( |\theta - \theta'| = \frac{1}{2N} \), we have \( |2 \cos \theta - 2 \cos \theta'| \geq \frac{\gamma_k}{2N} > \frac{1}{2N} \).

So if \( x \in L \), then with at least probability \( \frac{1}{2}(1 - \delta)|\alpha_{x,1}|^2 \geq \frac{1}{2}(1 - \delta)(1 - \epsilon) \), we can get a value \( " \leq \frac{1}{4N} \)-close" to \( 2 \cos \frac{2\pi(k+1/2)}{N} \) for some \( k \), but \( \" > \frac{1}{4N} \)-far" from any \( 2 \cos \frac{2\pi k}{N} \), so the last step will catch this and output the correct answer.

The case of \( x \notin L \) can be similarly analyzed. Also, it is easy to see that the expected running time of the algorithm is polynomial in the input size, which completes the proof for the \( O(\log n) \)-local LHES reduction.

Finally, to obtain a 4-local LHES, we replace \(|i\rangle\) by \(|e_i\rangle = |0..010100..0\rangle\) for \( i = 0, \ldots, N - 1 \), where the only 1 appears at coordinate \( i \). Modify the operator \( F \) to be

\[
F = \sum_{j=1}^{N-1} V_j \otimes |e_j\rangle\langle e_{j-1}| + V_N \otimes |e_0\rangle\langle e_{N-1}|.
\]

Note that \(|e_j\rangle\langle e_{j-1}|\) and \(|e_0\rangle\langle e_{N-1}|\) are 2-local. The remaining proof passes through. □
3.2 PES and LUAE are BQP-hard

Theorem 3 BQP $\subseteq$ BPP$^{\text{PES}}$, BQP $\subseteq$ BPP$^{\text{LUAE}}$.

Proof For any $L \in \text{BQP}$, there is a uniform family of polynomial size quantum circuits with $\epsilon$-bounded error (for a small constant $\epsilon$) that decides if $x \in L$ or $x \notin L$ as in Figure 4. For any input $x \in \{0,1\}^n$, suppose the corresponding circuit $U$ operates on $N = \text{poly}(n)$ qubits, taking $x$ and some ancillary bits $0 = 0^{N-n}$ as the input. After the circuit computation, measuring the first qubit of the output $U|x⟩|0⟩$ give the correct result with probability greater than $1 - \epsilon$. Suppose $U|x⟩|0⟩ = \alpha_{x,0}|0⟩|\psi_{x,0}⟩ + \alpha_{x,1}|1⟩|\psi_{x,1}⟩$, then $|\alpha_{x,0}|^2 < \epsilon$ if $x \in L$, and $|\alpha_{x,1}|^2 < \epsilon$ if $x \notin L$.

Now we construct another circuit $V$ as in Figure 4, where $Z$ is the Pauli-Z matrix

$$Z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}.$$ 

Figure 4: Circuit V

It is easy to see that

$$V|x, 0⟩ = U^†(\alpha_{x,0}|0⟩|\psi_{x,0}⟩ - \alpha_{x,1}|1⟩|\psi_{x,1}⟩)$$

$$= \begin{cases} |x, 0⟩ - 2\alpha_{x,1}U^†|1⟩|\psi_{x,1}⟩ \\ - |x, 0⟩ + 2\alpha_{x,0}U^†|0⟩|\psi_{x,0}⟩ \end{cases}$$

(11)

(12)

Therefore, $|x, 0⟩$ is almost an eigenvector of the eigenvalue $-1$ or $1$, depending on whether $x \in L$ or not. So we can use the PES or LUAE oracle to distinguish between these two cases.

1. BQP $\subseteq$ BPP$^{\text{PES}}$: We run the PES oracle on input $(V, 1/8, 1/100, x0^{N-n})$, and the oracle outputs a (sampled) value $\theta$. Accept if $1/4 \leq \theta \leq 3/4$, and reject otherwise.

To see why this is correct, write $V$ as $V = \sum_j \lambda_j |\eta_j⟩⟨\eta_j|$ where $\lambda_j = e^{2\pi i \omega_j}$ are eigenvalues and $|\eta_j⟩$ are the corresponding eigenvectors. Consider $x \notin L$ first, and the other case $x \in L$ is symmetric. Denote $x0^{N-n}$ by $b$ and decompose it as $|b⟩ = \sum_j \beta_j |\eta_j⟩$. Then $V|b⟩ - |b⟩ = \sum_j (\lambda_j - 1)\beta_j |\eta_j⟩$. By (12), this implies

$$\sum_j (\lambda_j - 1)\beta_j |\eta_j⟩ = -2\alpha_{x,1}U^†|1⟩|\psi_{x,1}⟩.$$ (13)
Since the PES oracle outputs an estimation of $\varphi_j$ up to 1/8 with probability at least $(1 - \delta)|\langle b|\eta_j \rangle|^2$ with $\delta = 1/100$, the success probability of our algorithm is

$$\Pr[\theta < 1/4 \text{ or } \theta > 3/4] \geq \sum_{j:|\varphi_j| < 1/8 \text{ or } |\varphi_j| > 7/8} (1 - \delta)|\langle b|\eta_j \rangle|^2$$

$$= (1 - \delta) \sum_{j:|\lambda_j| - 1 < 2 \sin(\pi/8)} |\beta_j|^2$$

$$= (1 - \delta)(1 - \sum_{j:|\lambda_j - 1| \geq 2 \sin(\pi/8)} |\beta_j|^2)$$

$$\geq (1 - \delta)(1 - \sum_{j:|\lambda_j - 1| \geq 2 \sin(\pi/8)} \frac{|\lambda_j - 1|^2}{4 \sin^2(\pi/8)} |\beta_j|^2)$$

$$\geq (1 - \delta)(1 - \frac{1}{4 \sin^2(\pi/8)} \|\sum_j (\lambda_j - 1)\beta_j|\eta_j\|)^2$$

$$= (1 - \delta)(1 - \frac{1}{4 \sin^2(\pi/8)} \|2\alpha_{x,1}U|1\rangle|\psi_{x,1}\|)^2$$

$$= (1 - \delta)(1 - \frac{|\alpha_{x,1}|^2}{\sin^2(\pi/8)})$$

$$= (1 - \delta)(1 - \frac{\epsilon}{\sin^2(\pi/8)})$$

where (20) is because of equality (13). Therefore the error probability is less than $O(\epsilon)$. The same arguments can show the correctness for the case of $x \in L$, which completes our proof for the first part.

2. **BQP \subseteq BPP_{LUAE}**: For the circuit $V$ in Figure 4, it is easy to show that $\bar{x}$ is close to $-1$ (and 1) if $x \in L$ (and $x \notin L$). First observe that for any $b$, we have $\bar{x} = \langle b|U|b\rangle$, which can be shown by writing both $U$ and $b$ in terms of $|\eta_j\rangle$'s. Now for $b = x0$, if $x \notin L$, then $|\bar{x} - 1| = ||\langle b|U|b\rangle - 1| = ||\langle b|U|b\rangle - |b\rangle| = \frac{2|\alpha_{x,1}|}{\sqrt{\epsilon}} \leq 2\sqrt{\epsilon}$. Similarly if $x \in L$, then $|\bar{x} + 1| \leq 2\sqrt{\epsilon}$. Thus a good estimation to $\bar{x}$ suffices to distinguish between $x \in L$ and $x \notin L$. □

## 4 The problems are in BQP

In this section, we will prove that LHES, PES and LUAE are all in BQP. We will first review the standard algorithm for Phase Estimation, then observe that the same algorithm actually gives the desired PES solution. We then use it to show an algorithm for LHES. Finally, we prove that LUAE is in BQP.

### 4.1 Phase Estimation and an efficient quantum algorithm for PES

Phase Estimation can be solved by a quantum algorithm as follows (see, for example, [25]). The working space has two registers. The first register consists of $t = n + \lceil \log(2 + 1/2\delta) \rceil$ qubits and is prepared in $|0\ldots0\rangle$. The second register contains the eigenvector $|u\rangle$. Measuring $\hat{\varphi}$ in the first register after carrying out the transformations described below gives the desired $n$-bit
estimation of $\varphi$ with probability of at least $1 - \delta$.

$$|0\rangle^{\otimes t}|u\rangle$$

$$-\frac{1}{\sqrt{2^t}} \sum_{j=0}^{2^t-1} |j\rangle|u\rangle$$  \hspace{1cm} \text{// apply the Fourier transform (24)}

$$-\frac{1}{\sqrt{2^t}} \sum_{j=0}^{2^t-1} |j\rangle U^j |u\rangle$$  \hspace{1cm} \text{// apply the controlled powers of $U$ (25)}

$$= \frac{1}{\sqrt{2^t}} \sum_{j=0}^{2^t-1} e^{2\pi i j \varphi} |j\rangle |u\rangle$$

$$\rightarrow |\tilde{\varphi}\rangle |u\rangle$$  \hspace{1cm} \text{// apply the inverse Fourier transform (27)}

The following observation says that the same algorithm actually works for PES.

**Fact.** If we feed $|0\rangle b\rangle$ instead of $|0\rangle u\rangle$ as input to the above algorithm for the Phase Estimation problem and let $t = [\log \frac{1}{\epsilon}] + [\log(2+\frac{1}{\delta})]$, then the measurement of the first register gives the desired sampling output. This implies that PES can be solved by a BQP machine.

This actually holds not only for $|b\rangle$ but also for a general state $|\eta\rangle$. To see why this is true, write $|\eta\rangle$ as $\sum_{j=1}^n \alpha_j |\eta_j\rangle$, then by the linearity of the operations, the final state is $\alpha_j |\tilde{\varphi}_j\rangle |\eta_j\rangle$. For more details, we refer the readers to [24] (Chapter 5). Note that to implement the controlled-$U^{2^j}$ operations for $j = 0, \ldots, 2^t - 1$ in the above algorithm, we need to run $U$ for $2^t$ times, which can be done efficiently since $t = [\log \frac{1}{\epsilon}] + [\log(2+\frac{1}{\delta})]$ and $\epsilon = \Omega(1/poly(n))$, $\delta = \Omega(1/poly(n))$.

### 4.2 LHES in BQP

**Theorem 4** LHES can be implemented by a uniform family of quantum circuits of polynomial size.

**Proof** By a simple scaling ($H' = H/\Lambda = \sum_j H_j/\Lambda$ where $\Lambda = \max_k \{|\lambda_k| = poly(n)|\}$, we can assume that all the eigenvalues $\lambda_k$ of $H$ satisfy $|\lambda_k| < 1/4$. The basic idea to design the BQP algorithm is to use Phase Estimation Sampling on $e^{2\pi i H'}$. Note that $e^{2\pi i H'}$ is unitary, and if the eigenvalues and eigenvectors of $H$ are $\{\lambda_k, |\eta_k\rangle\}$, then those of $e^{2\pi i H'}$ are just $\{e^{2\pi i \lambda_k}, |\eta_k\rangle\}$. Therefore, it seems that it is enough to run the PES algorithm on $(e^{2\pi i H'}, \epsilon, \delta, b)$, and if we get some $\lambda > 1/2$, then output $\lambda - 1$. However, note that $H$ is of exponential dimension, so $e^{2\pi i H'}$ is not ready to compute in the straightforward way. Fortunately, this issue is well studied in the quantum simulation algorithms, and the standard approach is the following asymptotic approximation by the Trotter formula [28, 13, 26] or its variants. Here using the simulation technique, we obtain

$$\left(e^{2\pi i \sum_j H_j/m}\right)^m = \left(\prod_j e^{2\pi i H_j/m}\right)^m + O(1/m)$$  \hspace{1cm} (28)

Now we run PES on $(b, \epsilon, \delta/2, e^{2\pi i H'})$. Whenever we need to call $e^{2\pi i H'}$, we use $\prod_j e^{2\pi i H_j/m}$ for $m$ times instead. Note that such substitution yields $O(1/m)$ deviation, so $t = \log \frac{1}{2\epsilon} + O(1)$ calls yield $O(\frac{1}{m\epsilon\delta}) \leq \frac{c}{m\epsilon\delta}$ deviation for some constant $c$. Let $m = \frac{2\epsilon}{c\delta^2}$, thus the final error probability is less than $\frac{c}{m\epsilon\delta} = \delta$, achieving the desired estimation and sampling precisions. \(\square\)

**Comment.** From the proof we can see that as long as $e^{2\pi i H'}$ can be simulated efficiently from the description of $H$, we can sample the eigenvalues of $H$ as desired. Since sparse Hamiltonians,
which contains local Hamiltonians as special cases, can be simulated efficiently \[ \mathcal{BQP} \], we know that if we modify the definition of LHES by allowing \( H \) to be sparse, then it is also \( \mathcal{BQP} \)-complete.

### 4.3 Local unitary matrices average eigenvalue estimation

**Theorem 5** \( \mathcal{LUE} \) is in \( \mathcal{BQP} \).

We can use the \( \mathcal{BQP} \) algorithm for PES to get \( O(1/\epsilon\delta) \) (independent) samples \( \varphi^{(1)}, \ldots, \varphi^{(m)} \) and use the sample mean \( \overline{\lambda} = \frac{1}{m} \sum_{j=1}^{m} e^{2\pi i \varphi^{(j)}} \) as an desired estimation of \( \overline{\lambda} \), which can be proved by studying the Phase Estimation algorithm in more details \(^4\). But here we shall give a different algorithm whose analysis is much simpler. Recall that \( \overline{\lambda} = \langle b | U | b \rangle \). So after we apply the circuit \( U \) to \( | b \rangle \), the problem becomes to estimate the inner product of two quantum states \( | b \rangle \) and \( U | b \rangle \), which can be done by the standard SWAP test. For example, Yao \[^{33}\] gave an estimate of \( | \langle u | v \rangle | \) up to \( \epsilon \) with error probability \( \delta \) by applying the SWAP test in \( O(\frac{1}{\sqrt{\epsilon}} \log \frac{1}{\delta}) \) pairs of \( | u \rangle, | v \rangle \). Here for the special two states \( | b \rangle \) and \( U | b \rangle \), it turns out that we can slightly decrease the cost to \( O(\frac{1}{\sqrt{\epsilon}} \log \frac{1}{\delta}) \), by using the following lemma proved in \[^{31}\]:

**Lemma 6** Let \( U \) be a quantum circuit of length \( O(\text{poly}(n)) \) acting on \( n \) qubits, and let \( | \psi \rangle \) be a pure state of the \( n \) qubits which can be prepared in time \( O(\text{poly}(n)) \). It is then possible to sample from random variables \( X, Y \in \{ -1, +1 \} \) for which

\[
\mathbb{E}[X + i Y] = \langle U | \psi \rangle
\]

in \( O(\text{poly}(n)) \) time.

**Proof** (of Theorem \[^{5}\]) Run the sampling algorithm in the lemma to get \( m = O(\frac{1}{\epsilon} \log \frac{1}{\delta}) \) samples \( (X_1, Y_1), \ldots, (X_m, Y_m) \). Let \( \overline{X} = \frac{1}{m} \sum_{j=1}^{m} X_j \) and \( \overline{Y} = \frac{1}{m} \sum_{j=1}^{m} Y_j \). Use the sample mean \( \overline{\lambda} = \overline{X} + i \overline{Y} \) as an desired estimation of \( \overline{\lambda} \). Noting \( \text{Var}[X] \leq 4 \) and \( \text{Var}[Y] \leq 4 \) (by the definition of variance), we have by Chernoff’s bound that

\[
\Pr[|\overline{\lambda} - \overline{\lambda}| \geq \epsilon] \leq \Pr[|\overline{X} - \text{Re}(\overline{\lambda})| \geq \epsilon/2] + \Pr[|\overline{Y} - \text{Im}(\overline{\lambda})| \geq \epsilon/2] \leq \delta.
\]

as desired. \( \square \)

### 5 Discussions and open problems

One might wonder why not to consider the average eigenvalue of a local Hamiltonian. Actually, since \( \langle b | H | b \rangle = \langle b | \sum_j H_j | b \rangle = \sum_j \langle b | H_j | b \rangle \) and each \( \langle b | H_j | b \rangle \) can be easily computed even deterministically, we can obtain the exact average eigenvalue of a local Hamiltonian deterministically in polynomial time.

However, as shown very recently by Janzing and Wocjan, if we generalize the problem to estimating the average eigenvalue of \( H^m \) where \( m = \text{poly}(n) \) is part of the input, then the problem of estimating \( \langle b | H^m | b \rangle \) is \( \mathcal{BQP} \)-complete \[^{17}\].

We can also consider the complexity of unguided version of the problems studied so far. That is, \( b \) is not part of the input, and we want to sample the eigenvalue/phase with equal probability or estimate the average eigenvalue under the uniform distribution over all the \( 2^n \) eigenvalues. We use \( \text{LHES}_u, \text{PES}_u, \text{LUA}_e \) to denote the corresponding problems. We basically do not know anything about these problems yet, except some trivial facts like \( \text{LUA}_u \in \mathcal{BQP} \) due to the following simple observation: \( \mathbb{E}_b[|\langle b | U | b \rangle|] = \frac{1}{|\psi|^2} \sum_b |\langle b | U | b \rangle|^2 = \frac{1}{|\psi|^2} \sum_b |\langle b | H_j | b \rangle|^2 \lambda_j \). We can just uniformly choose \( b \in \{0, 1\}^n \) and run the algorithm in Lemma \[^{6}\].

\(^4\)Directly applying the definition of the PES problem as a black-box is not enough: the mean of the output of the PES algorithm may be far away from \( \overline{\lambda} \) because of the exponentially many eigenvalues and for each eigenvalue the output probability is \( \epsilon \) away from the correct one.
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