Quantum Phase Processing: Transform and Extract Eigen-Information of Quantum Systems

Xin Wang,¹, ⋆ Youle Wang,¹, † Zhan Yu,¹, ‡ and Lei Zhang¹, §

¹Institute for Quantum Computing, Baidu Research, Beijing 100193, China

(Dated: September 29, 2022)

Quantum computing can provide speedups in solving many problems as the evolution of a quantum system is described by a unitary operator in an exponentially large Hilbert space. Such unitary operators change the phase of their eigenstates and make quantum algorithms fundamentally different from their classical counterparts. Based on this unique principle of quantum computing, we develop a new algorithmic framework “Quantum phase processing” that can directly apply arbitrary trigonometric transformations to eigenphases of a unitary operator. The quantum phase processing circuit is constructed simply, consisting of single-qubit rotations and controlled-unitaries, typically using only one ancilla qubit. Besides the capability of phase transformation, quantum phase processing in particular can extract the eigen-information of quantum systems by simply measuring the ancilla qubit, making it naturally compatible with indirect measurement. Quantum phase processing complements another powerful framework known as quantum singular value transformation and leads to more intuitive and efficient quantum algorithms for solving problems that are particularly phase-related. As a notable application, we propose a new quantum phase estimation algorithm without quantum Fourier transform, which requires the least ancilla qubits and matches the best performance so far. We further exploit the power of our QPP framework by investigating a plethora of applications in Hamiltonian simulation, entanglement spectroscopy, and quantum entropies estimation, demonstrating improvements or optimality for almost all cases.

I. INTRODUCTION

Quantum computer provides a computational framework that can solve certain problems dramatically faster than classical machines. Quantum computing has been applied in many important tasks, including breaking encryption [1], searching databases [2], and simulating quantum evolution [3]. Recent advances in quantum computing show that quantum singular value transformation (QSVT) introduced by Gilyén et al. [4] has led to a unified framework of the most known quantum algorithms [5], including amplitude amplification [4], quantum walks [4], phase estimation [5, 6], and Hamiltonian simulations [7–10]. This framework can further be used to develop new quantum algorithms such as quantum entropies estimation [11–13], fidelity estimation [14], ground state preparation and ground energy estimation [15–17].

Although powerful, the current QSVT may not naturally and intuitively unify quantum algorithms related to phase processing, as its main principle is to apply singular value transformations to a linear operator embedded in a larger unitary. However, the ability of processing phase indeed plays a central role in many quantum algorithms. For example, the trick of phase kickback, where the phase of the target qubits is kicked back to the ancilla qubit, is intensively used almost everywhere in quantum computing. With the aid of controlled-unitary gates, many quantum algorithms utilize phase kickback to extract information of large unitary operations from phases of ancilla qubits, including the quantum phase estimation [18, 19], the swap test [20, 21], the Hadamard test [22], and the one-clean-qubit model [23]. Hence, it is of great interest and necessity to explore a generalized framework that could interpret those phase-related quantum algorithms in a different formalism compared to QSVT, which may further leads to improved performances or new quantum algorithms and help us better exploit the power of quantum computing.

The framework of QSVT was originated from a technique called quantum signal processing (QSP) [24, 25]. By interleaving single-qubit signal unitaries and signal processing unitaries, QSP is able to implement a transformation of the signal in $SU(2)$. There are several conventions of QSP varied by choosing different signal unitaries. In the construction of QSVT, Gilyén et al. [4] chose the signal unitary to be a reflection, then extended the signal unitary to a multi-qubit block encoding with the idea of qubitization [7], which naturally leads to a polynomial transformation on the singular values of a block-encoded linear operator. The achievable polynomial transformations in QSVT are decided by reflection-based QSP, which has parity constraints or limitations, i.e., it can implement either an even polynomial or an odd one. Thus, to achieve a general transformation in QSVT, one might have to apply techniques such as linear-combination-of-unitaries [26] and amplitude amplification [27, 28], which take extra resources. In recent work, Yu et al. [29] developed a new convention of QSP that overcomes the parity limitation by choosing the signal unitary as a $z$-rotation and adding an extra signal processing unitary. Such a modified QSP could implement arbitrary complex trigonometric polynomials. Consequently, it is natural to investigate and develop the multi-qubit extension of this trigonometric QSP in [29].

* wangxin73@baidu.com
† youle.wang92@gmail.com
‡ yuzh.james@gmail.com
§ leizhang116.4@gmail.com

The authors are listed in alphabetical order. Part of this work was done when Y. W., Z. Y., and L. Z. were research interns at Baidu Research.
In this work, we generalize the trigonometric QSP and propose a novel algorithmic framework called quantum phase processing (QPP). This framework has the ability to apply arbitrary trigonometric transformations to eigenphases of a unitary operator. Besides achieving the eigenphases transformation, QPP is also natively compatible with indirect measurements, enabling it to extract the eigen-information of quantum systems by measuring a single ancilla qubit. We further employ this framework to design efficient quantum algorithms for solving various problems. First, we use the idea of binary search to develop an efficient phase estimation algorithm without using quantum Fourier transform, requiring only one ancilla qubit. Such an algorithm can be applied to solve factoring problems and amplitude estimations. Second, we show that QPP can be applied to simulate the time evolution under a Hamiltonian \( H \) with access to a block encoding of \( H \). This method is in the same spirit as QSP-based Hamiltonian simulation [7, 25], which also matches the optimal query complexity. Third, we propose a generic method to estimate quantum entropies, including the von Neumann entropy, the quantum relative entropy and the family of quantum Rényi entropies [30]. Despite the fact that QPP could be combined with amplitude estimation to achieve a quadratic speedup, we present algorithms that repeatedly measured the single ancilla qubit to estimate entropies rather than using amplitude estimation, demonstrating its compatibility with indirect measurements. Overall, QPP provides a powerful algorithmic framework to exploit quantum applications and delivers a new perspective on understanding and designing quantum algorithms.

The structure of this paper is presented as follows. Section II introduces the structure and principal capability of quantum phase processing. In Section III, we propose the novel quantum phase search algorithm, then we analyze the performance of the algorithm and make a brief comparison with previous works. Section IV interprets the method of Hamiltonian simulation in the QPP framework. In Section V, we develop a generic approach for quantum entropies estimation and further showcase the methods of estimating von Neumann entropies, quantum relative entropies and quantum Rényi entropies, then we compare our algorithms with prior methods. Proofs and further discussions of this work are left in the appendix.

II. THE FRAMEWORK OF QUANTUM PHASE PROCESSING

A. Trigonometric quantum signal processing

The concept of quantum signal processing (QSP) was introduced by Low et al. [24], who showed how to transform a \( 2 \times 2 \) signal unitary \( R_x(x) = e^{i x \sigma_z} \) into a target unitary whose entries are some transformations of the signal \( x \). The approach is to apply the signal unitary \( R_x(x) \) interleaved with some signal processing unitaries \( R_z(\phi) \), i.e.

\[
R_z(\phi_0) R_z(x) R_z(\phi_1) R_z(x) \cdots R_z(x) R_z(\phi_k).
\]

Gilyén et al. [4] slightly modified the signal unitary as a reflection and explicitly showed that the transformation corresponds to a Chebyshev polynomial of the signal \( x \). Another common convention of QSP is to choose the signal unitary to be a \( z \)-rotation \( R_z(x) \) with signal processing unitaries being \( x \)-rotations \( R_x(\phi) \) [31, 32], which corresponds to a trigonometric polynomial of the signal \( x \). Different conventions of QSP and their relationships are summarized by Martyn et al. [5]. Observe that both of these two conventions of QSP have constraints on the achievable polynomials: for the Chebyshev QSP, each entry is a polynomial with either even or odd parity; for the trigonometric QSP, each entry is a trigonometric polynomial (in the exponential form) with either real or imaginary coefficients. As a result, the technique of linear-combination-of-unitaries [26] is necessary for these conventions of QSP to implement a general polynomial transformation, which requires extra ancilla qubits. In a recent work, Yu et al. [29] overcame the constraints by adding an extra signal processing unitary in each iteration so that one could implement arbitrary complex trigonometric polynomial transformation in a single QSP. Our work is heavily based on this improved trigonometric QSP, which is defined as

\[
W_{\omega, \theta, \phi}^L(x) := R_z(\omega) R_y(\theta_0) R_z(\phi_0) \prod_{l=1}^L R_z(x) R_y(\theta_l) R_z(\phi_l),
\]

where \( L \in \mathbb{N} \) is the number of layers, \( \omega \in \mathbb{R} \), \( \theta = (\theta_0, \theta_1, \ldots, \theta_L) \in \mathbb{R}^{L+1} \) and \( \phi = (\phi_0, \phi_1, \ldots, \phi_L) \in \mathbb{R}^{L+1} \) are parameters. The quantum circuit of \( W_{\omega, \theta, \phi}^L(x) \) is illustrated in Fig. 1.

\[
\begin{align*}
|0\rangle \rightarrow R_z(\phi_L) R_y(\theta_L) R_z(x) \cdots R_z(\phi_0) R_y(\theta_0) R_z(\omega)
\end{align*}
\]

Fig 1: Circuit of \( W_{\omega, \theta, \phi}^L(x) \), where the signal block is \( R_z(\cdot) \), and the signal processing block is composed of \( R_y(\cdot) \) and \( R_z(\cdot) \).

The following theorem characterizes the correspondence between QSP and complex trigonometric polynomials.
Theorem 1 (Trigonometric quantum signal processing [29]) There exist $\omega \in \mathbb{R}$, $\theta = (\theta_0, \theta_1, \ldots, \theta_L) \in \mathbb{R}^{L+1}$ and $\phi = (\phi_0, \phi_1, \ldots, \phi_L) \in \mathbb{R}^{L+1}$ such that

$$
W_{\omega, \theta, \phi}(x) = \begin{bmatrix}
P(x) & -Q(x)
\end{bmatrix}
\begin{bmatrix}
P^*(x) \\
Q^*(x)
\end{bmatrix}
$$

(3)

if and only if Laurent polynomials $P, Q \in \mathbb{C}[e^{ix/2}, e^{-ix/2}]$ satisfy

1. $\deg(P) \leq L$ and $\deg(Q) \leq L$,

2. $P$ and $Q$ have parity $L$ mod 2,

3. $\forall x \in \mathbb{R}$, $|P(x)|^2 + |Q(x)|^2 = 1$.

The initial version of Theorem 1 first introduced in [29] is in the form of quantum neural networks. Here we restate the theorem in the formalism of QSP without changing the principle. Theorem 1 demonstrates a decomposition of QSP $W_{\omega, \theta, \phi}(x)$ into complex Laurent polynomials, as well as a construction of QSP from complex Laurent polynomials. From the second condition of Theorem 1, it seems that $P$ and $Q$ still have parity constraints, i.e. either have parity 0 or 1, but in fact Laurent polynomials in $\mathbb{C}[e^{ix/2}, e^{-ix/2}]$ with parity 0 are essentially complex trigonometric polynomials in $\mathbb{C}[e^{ix}, e^{-ix}]$ without parity constraints. The proof of this theorem also provides an algorithm that calculates angles $\omega, \theta$ and $\phi$ in $O(\text{poly}(L))$ operations, one can refer to Algorithm 3 in Appendix A1 for more details. There are also many other methods to compute the angles (see, e.g., [31–34]). It can be inferred from Theorem 1 that if $P(x)$ satisfies the parity constraint and $|P(x)| \leq 1$ for all $x \in \mathbb{R}$, then there exists a corresponding $Q(x)$ satisfying the three conditions. The detailed analysis can be found in Appendix A1.

Other than decomposing and constructing QSP, we are also interested in how to represent the trigonometric polynomial transformation. One way is to project out $P(x)$ from $W_{\omega, \theta, \phi}$, i.e., the $\langle 0 | \cdot | 0 \rangle$ entry:

Corollary 2 For any complex-valued trigonometric polynomial $F(x) = \sum_{j=-L}^{L} c_j e^{ixj}$ with $\|c\|_1 \leq 1$, there exist $\omega \in \mathbb{R}$ and $\theta, \phi \in \mathbb{R}^{2L+1}$ such that for all $x \in \mathbb{R}$,

$$
\langle 0 | W^{2L}_{\omega, \theta, \phi}(x) | 0 \rangle = F(x).
$$

(4)

Moreover, based on the fact that any non-negative real-valued trigonometric polynomial is a product between a Laurent polynomial in $\mathbb{C}[e^{ix/2}, e^{-ix/2}]$ and its complex conjugate, as proved in Appendix A1, the trigonometric polynomial can be represented by the expectation value of measuring a Pauli-Z observable with respect to the state $W_{\omega, \theta, \phi}(0)$.

Corollary 3 For any real-valued trigonometric polynomial $F(x) = \sum_{j=-L}^{L} c_j e^{ixj}$ with $\|c\|_1 \leq 1$, there exist $\omega \in \mathbb{R}$ and $\theta, \phi \in \mathbb{R}^{L+1}$ such that for all $x \in \mathbb{R}$, $f_{W}(x) := \langle 0 | W^{L}_{\omega, \theta, \phi}(x) | 0 \rangle = F(x)$.

(5)

The idea of this corollary is that, for a real-valued trigonometric polynomial $F(x)$ with degree $L$ and satisfies $\|F(x)\| \leq 1$, we could find a Laurent polynomial $P \in \mathbb{C}[e^{ix/2}, e^{-ix/2}]$ with degree $L$ such that $PP^* = (F(x) + 1)/2$, then the expectation value of measuring $Z$ observable turns to be $F(x)$. The detailed proofs are deferred to Appendix A2.

B. Framework of Quantum Phase Processing

Although the model of QSP provides a systematical method to make arbitrary polynomial transformations, it only works on a qubit-like quantum system. Gilyén et al. [4] proposed a multi-qubit lifted version of the Chebyshev QSP, called quantum singular value transformation (QSVT), which could efficiently apply Chebyshev polynomial transformations to the singular values of a linear operator embedded in a larger unitary. In this work, we consider a similar extension of the trigonometric QSP and establish a quantum phase processing (QPP) algorithmic framework that could apply arbitrary trigonometric transformations to eigenphases of a unitary matrix $U$. The framework of QPP generalizes the trigonometric QSP by replacing the input signal

\[1\] For a Laurent polynomial $P \in \mathbb{C}[z, z^{-1}]$, $P$ has parity 0 if all coefficients corresponding to odd powers of $z$ are 0, and similarly $P$ has parity 1 if all coefficients corresponding to even powers of $z$ are 0.
Lemma with Corollary 4 shows that the eigenspace of QPP trivially follows from combining Lemma 4 (Eigenspace Decomposition of QPP) we analyze the eigenspace decomposition of QPP: analogs of could perform a trigonometric polynomial transformation on the eigenphase of the unitary $U$ where $R_{y}^{(0)}$ and $R_{z}^{(0)}$ are rotation gates applied on the first qubit. For an odd $L \in \mathbb{N}$, we apply an extra layer

$$
\begin{bmatrix}
U^\dagger & 0 \\
0 & I
\end{bmatrix} R_{y}^{(0)}(\theta_L) R_{z}^{(0)}(\phi_L)
$$

to $V_{\omega, \theta, \phi}^{L-1}(U)$. The quantum circuit of $V_{\omega, \theta, \phi}^{L}(U)$ is shown as in Fig. 2.

![Fig 2: General circuit for quantum phase processing $V_{\omega, \theta, \phi}^{L}(U)$, here the number of layers $L$ is an even integer.](image)

One could find that QPP simply replaces the signal unitary $R_{s}(x)$ in QSP with interleaved unitaries controlled-$U$ and controlled-$U^\dagger$. We note that such a construction of using controlled-unitaries was common and frequently used in previous works [7, 17, 25, 33]. The intuition lying behind the extension is that controlled-$U$ and its inverse are naturally multi-qubit analogs of $R_{s}$ gates. To better understand how rotation gates in the first ancilla qubit process the phase of the target unitary $U$, we analyze the eigenspace decomposition of QPP:

**Lemma 4 (Eigenspace Decomposition of QPP)** Suppose $U$ is an $n$-qubit unitary with spectral decomposition

$$
U = \sum_{j=0}^{2^{n}-1} e^{i\tau_j} |\chi_j\rangle \langle \chi_j|.
$$

For all $L \in \mathbb{N}$, $\omega \in \mathbb{R}$ and $\theta, \phi \in \mathbb{R}^{L+1}$, we have

$$
V_{\omega, \theta, \phi}^{L}(U) = \bigoplus_{j=0}^{2^{n}-1} (e^{-i\tau_j/2})^{L \mod 2} \cdot W_{\omega, \theta, \phi}(\tau_j) \mathbb{B}_j
$$

where $\mathbb{B}_j := \{|0, \chi_j\rangle, |1, \chi_j\rangle\}$.

The proof of this lemma is deferred to Appendix A.3. Lemma 4 shows that the eigenspace of QPP $V_{\omega, \theta, \phi}(U)$ coincides with that of the unitary $U$. Using this property, we generalize the single-qubit trigonometric QSP to the multi-qubit QPP that could perform a trigonometric polynomial transformation on the eigenphase of the target unitary $U$. Similar to QSP, there are two ways to perform the transformation. We could measure the first ancilla qubit and achieve an evolution of the input state upon post-selection of the measurement result being $|0\rangle$, as shown in the follow theorem:

**Theorem 5 (Quantum phase evolution)** Given an $n$-qubit unitary $U = \sum_{j=0}^{2^{n}-1} e^{i\tau_j} |\chi_j\rangle \langle \chi_j|$ and an $n$-qubit quantum state $|\psi\rangle = \sum_{j=0}^{2^{n}-1} \alpha_j |\chi_j\rangle$, for any trigonometric polynomial $F(x) = \sum_{j=-L}^{L} c_j e^{i\lambda_x}$ with $\|c\|_1 \leq 1$, there exist $\omega \in \mathbb{R}$ and $\theta, \phi \in \mathbb{R}^{2L+1}$ such that

$$
\langle 0 | \otimes I^\otimes n \rangle V_{\omega, \theta, \phi}^{2L}(U) |0, \psi\rangle = \sum_{j=0}^{2^{n}-1} \alpha_j F(\tau_j) |\chi_j\rangle.
$$

The proof of Theorem 5 trivially follows from combining Lemma 4 with Corollary 2, which we defer to Appendix A.4. The other way is to evaluate trigonometric polynomial on the eigenphases and represent the result by the expectation value of measuring an observable on the first qubit:
Theorem 6 (Quantum phase evaluation) Given an $n$-qubit unitary $U = \sum_{j=0}^{2^n-1} e^{i\tau_j} |\chi_j\rangle \langle \chi_j|$ and an $n$-qubit quantum state $\rho$, for any real-valued trigonometric polynomial $F(x) = \sum_{j=-L}^{L} c_j e^{ijx}$ with $\|c\|_1 \leq 1$, there exist $\omega \in \mathbb{R}$ and $\theta, \phi \in \mathbb{R}^{L+1}$ such that $\tilde{\rho} = V_{\omega, \theta, \phi}(U) \left( |0\rangle \langle 0| \otimes \rho \right) V_{\omega, \theta, \phi}(U) \dagger$ satisfies

$$f_V(U) := \text{tr} \left[ (Z^{(0)} \otimes I) \cdot \tilde{\rho} \right] = \sum_{j=0}^{2^n-1} p_j F(\tau_j),$$

where $p_j = \langle \chi_j | \rho | \chi_j \rangle$ and $Z^{(0)}$ is a Pauli-Z observable acting on the first qubit.

Theorem 6 is proved by combining Lemma 4 and Corollary 3, as shown in Appendix A 4. Theorem 6 shows that QPP is natively compatible with indirect measurements, which could represent the target trigonometric polynomial by probabilities of measuring the ancilla qubit. Such a property does not emerge in QSVT, since QSVT typically represent the target polynomial transformation in amplitudes. Chebyshev’s inequality dictates that an estimate of the expectation value within an additive error $\delta$ can be obtained by measuring the ancilla qubit for $O(1/\delta^2)$ times. Alternatively, one could apply amplitude estimation [27] to estimate the value by calling the QPP circuit for $O(1/\delta)$ times, which is quadratically more efficiently than classical sampling but with a larger circuit depth. In particular, since the ancilla qubit in QPP naturally works as a flag qubit, we could directly apply the iterative amplitude estimation [35] on QPP without using extra qubits.

Theorem 5 and Theorem 6 lie in the heart of QPP algorithmic framework, together demonstrating that QPP is a versatile and flexible framework for phase-related problems. First, QPP could act in a similar manner to QSVT but transforming eigenphases but with a larger circuit depth. In particular, since the ancilla qubit in QPP naturally works as a flag qubit, we could directly estimate the value by calling the QPP circuit for $O(1/\delta^2)$ times. Alternatively, one could apply amplitude estimation [27] to estimate the value by calling the QPP circuit for $O(1/\delta)$ times, which is quadratically more efficiently than classical sampling but with a larger circuit depth. In particular, since the ancilla qubit in QPP naturally works as a flag qubit, we could directly apply the iterative amplitude estimation [35] on QPP without using extra qubits.

Theorem 5 and Theorem 6 lie in the heart of QPP algorithmic framework, together demonstrating that QPP is a versatile and flexible framework for phase-related problems. First, QPP could act in a similar manner to QSVT but transforming eigenphases but with a larger circuit depth. In particular, since the ancilla qubit in QPP naturally works as a flag qubit, we could directly apply the iterative amplitude estimation [35] on QPP without using extra qubits.

For the sake of notation simplicity, we omit the parameters $L, \omega, \theta$ and $\phi$, writing QSP as $W(x)$ and QPP as $V(U)$ in the rest of this paper. Next we will show that framework of QPP is a powerful tool for designing efficient and intuitive quantum algorithms for solving various problems, including quantum phase estimation, Hamiltonian simulation, and quantum entropies estimation.

III. QUANTUM PHASE ESTIMATION

Quantum phase estimation is one of the most important and useful subroutines in quantum computing. The problem of phase estimation is formally defined as follows: Given a unitary $U$ and an eigenstate $|\chi\rangle$ of $U$ with eigenvalue $e^{i\tau}$, estimate the eigenphase $\tau$ up to an additive error $\delta$. In this section, we will develop an efficient algorithm for quantum phase estimation based on QPP. Before proceeding, let us do a little warming up to get familiar with the QPP framework. We start by considering a simple method of Hadamard test.

A. Warm-up example: the Generalized Hadamard test

A common method to estimate the phase of a unitary is the Hadamard test, which solves the following problem: Given a unitary $U$ and a state $|\chi\rangle$, estimate $\langle \chi | U | \chi \rangle$. The Hadamard test uses the measurement result of the ancillary qubit as a random variable whose expected value is the real part $\Re \{ \langle \chi | U | \chi \rangle \}$. It also estimates the imaginary part $\Im \{ \langle \chi | U | \chi \rangle \}$ by adding a phase gate. We now show that QPP is a generalization of the Hadamard test.

Given a unitary $U$ and a quantum state $|\chi\rangle$ such that $U |\chi\rangle = e^{i\tau} |\chi\rangle$, let $F(x) = \cos(x)$ be the target trigonometric polynomial for QPP. By Theorem 6, there exists a single-layer QPP $V(U)$ such that

$$f_V(U) = \text{tr} \left[ |0, \chi\rangle \langle 0, \chi| \left( Z^{(0)} \otimes I \right) V(U) \right] = \cos(\tau) = \Re \{ \langle \chi | U | \chi \rangle \},$$

Specifically, by computing the angles $\omega, \theta$ and $\phi$, one can find that the two rotation gates in the first ancilla qubit are essentially Hadamard gates, which means that QPP implements the Hadamard test. Similarly, let the target trigonometric polynomial be $F(x) = \sin(x)$, then QPP can estimate $\sin(\tau) = \Im \{ \langle \chi | U | \chi \rangle \}$. The phase $\tau$ could be obtained from $\cos(\tau)$ and $\sin(\tau)$. Furthermore, one can select trigonometric polynomials other than $\sin(x)$ and $\cos(x)$, which yields a generalization of the Hadamard test. For example, QPP with a trigonometric polynomial $F(x)$ that approximates the function $f(x) = x/2\pi$ could directly estimate the phase $\tau$.

Although QPP can implement a generalized Hadamard test to estimate the phase, the input state $|\chi\rangle$ is required to be an eigenstate of target unitary. However, quite often we are given a superposition of eigenstates instead of a pure eigenstate, such
as in the factoring problem. In addition, measuring the ancilla qubit for $O(1/\delta^2)$ times are necessary to estimate the expected value with an additive error $\delta$, despite the fact that the complexity can be improved via amplitude estimation. Can we do better? As demonstrated in the following section, we can further employ QPP to construct a more efficient phase estimation algorithm that accepts a superposition of eigenstates, without using amplitude estimation.

## B. Quantum phase searching

As introduced in Section II, QPP can directly process the eigenphases of the target unitary, which allows us to classify the eigenphases. The main idea is to use a trigonometric polynomial to approximate a step function, so that we could utilize QPP to locate the eigenphases by a binary search procedure. We first show that QPP can classify the eigenphases of $U$.

**Lemma 7 (Phase classification)** Given a unitary $U = \sum_{j=0}^{2^n-1} e^{i\tau_j} |\chi_j\rangle \langle \chi_j|$, then for any $\Delta \in (0, \pi)$ and $\varepsilon \in (0, 1)$, there exists a QPP circuit $V(U)$ of $L = O\left(\frac{1}{\Delta} \log \frac{1}{\varepsilon}\right)$ layers such that

$$V(U) |0, \chi_k\rangle = \begin{cases} \sqrt{1 - \varepsilon_k} |0, \chi_k\rangle + \sqrt{\varepsilon_k} |1, \chi_k\rangle & \text{if } \tau_k \in [\Delta, \pi - \Delta), \\ \sqrt{\varepsilon_k} |0, \chi_k\rangle + \sqrt{1 - \varepsilon_k} |1, \chi_k\rangle & \text{if } \tau_k \in (-\pi + \Delta, -\Delta], \end{cases}$$

for $0 \leq k < 2^n$, where $\varepsilon_k \in (0, \varepsilon)$.

The proof of Lemma 7 is deferred to Appendix B.1. By phase kickback, measuring measuring the ancilla qubit decides which subinterval the eigenphase $\tau$ belongs to with probability at least $1 - \varepsilon$. Next we apply a phase shift $e^{i\zeta}$ to $U$ to move to the middle point of the designated subinterval, so that $V(e^{i\zeta}U)$ determines the next subinterval. Using this fascinating property, repeating the binary search procedure shrinks the phase interval until QPP cannot decide next subintervals, i.e. $\tau \in [\zeta_l, \zeta_r]$ and $|\zeta_r - \zeta_l| \approx 2\Delta$. See the phase interval search (PIS) procedure in Algorithm 1 for details.

### Algorithm 1 Phase Interval Search (PIS)

**Require**: A unitary $U$, an eigenstate $|\chi\rangle$ of $U$ with eigenvalue $e^{i\tau}$, an interval $[\zeta_l, \zeta_r]$, a $\Delta \in (0, \frac{1}{2})$, an $\varepsilon \in (0, 1)$, and an integer $Q$.

**Ensure**: An updated interval $[\zeta_l, \zeta_r]$ such that $\tau \in [\zeta_l, \zeta_r]$ and $
|\zeta_r - \zeta_l| = 2(\Delta + \frac{\varepsilon}{Q})$

1: for $j = 0 \ldots Q - 1$ do  
2: Set the middle point $\zeta_m = \frac{\zeta_l + \zeta_r}{2}$.
3: Construct QPP circuit $V_{\omega, \theta, \phi}(e^{-i\zeta_m}U)$ in Lemma 7 according to $\Delta$ and $\varepsilon$.
4: Apply the circuit to the state $|0, \chi\rangle$ and measure the ancilla qubit. If $\zeta_r - \zeta_l > 2\pi - 2\Delta$, update

$$[\zeta_l, \zeta_r] \leftarrow \begin{cases} [\zeta_m - \Delta, \zeta_r + \Delta], & \text{if the outcome is 0} \\ [\zeta_l - \Delta, \zeta_m + \Delta], & \text{if the outcome is 1} \end{cases}$$

otherwise

$$[\zeta_l, \zeta_r] \leftarrow \begin{cases} [\zeta_m - \Delta, \zeta_r], & \text{if the outcome is 0} \\ [\zeta_l, \zeta_m + \Delta], & \text{if the outcome is 1} \end{cases}$$

5: end for
6: Output the interval $[\zeta_l, \zeta_r]$.

By Lemma 7, the phase interval search procedure shrinks the phase interval to a length $2(\Delta + \frac{\varepsilon}{Q})$ with probability at least $(1 - \varepsilon)^Q$. Now that the phase interval is too narrow for phase classification, we apply QPP on $(e^{i\zeta}U)^d$ for some appropriate integer $d$ so that the binary search procedure can continue to locate the amplified phase $d\tau \in [d\zeta_l, d\zeta_r]$. Repeating the entire procedure gives an estimation of phase $\tau$ up to required precision $\delta$, as shown in Algorithm 2.
Algorithm 2 Quantum Phase Search Algorithm (QPS)

Require: A unitary $U$, an eigenstate $|\chi\rangle$ of $U$ with eigenvalue $e^{i\tau}$, a $\Delta \in (0, \frac{1}{2})$, an $\varepsilon \in (0, 1)$ and a $\delta \in (0, 1)$.
Ensure: A phase $\tau \in \mathbb{R}$ such that $|\tau - \tau| < \delta$.
1: Set $Q \leftarrow [\log \frac{\pi}{\Delta}]$, $\Delta \leftarrow \Delta + \frac{1}{2Q\pi}$, $T \leftarrow \lfloor \frac{\log \delta}{\log \Delta} \rfloor$ and $d \leftarrow \lfloor 1/\Delta \rfloor$. Initialize the interval $[\zeta_l, \zeta_r] \leftarrow [\pm \pi]$. 
2: for $t = 0, \ldots, T - 1$ do
3: Update the interval by the phase interval search procedure,
4: Store the middle point of interval $\zeta_m^{(t)} \leftarrow \frac{\zeta_l^{(t)} + \zeta_r^{(t)}}{2}$.
5: Update $U \leftarrow e^{-i\zeta_m^{(t)} U}$ and $[\zeta_l, \zeta_r] \leftarrow [d(\zeta_l - \zeta_m^{(t)}), d(\zeta_r - \zeta_m^{(t)})]$. 
6: end for
7: Output $\hat{\tau} \leftarrow \sum_{t=0}^{T-1} \zeta_m^{(t)} d^{-t}$.

Note that Algorithm 2 could accept a superposition of eigenstates as the input, since eigenstates whose eigenvalues disagree with measurement results of the ancilla qubit will be filtered out, and finally the state in the main register converges to a single eigenstate of $U$ at the end of the quantum phase search algorithm. A more detailed analysis of the quantum phase search algorithm can be found Appendix B 2. Observe that Algorithm 2 queries controlled-$U^j$ for $LTQ$ times, we have the following analysis on the complexity of the algorithm:

Theorem 8 (Complexity of Quantum Phase Search) Given an $n$-qubit unitary $U$ and an eigenstate $|\chi\rangle$ of $U$ with eigenvalue $e^{i\tau}$, Algorithm 2 can use one ancilla qubit and $O\left(\frac{1}{\varepsilon} \log \left(\frac{1}{\varepsilon} \log \frac{1}{\Delta}\right)\right)$ queries to controlled-$U$ and its inverse to obtain an estimation of $\tau$ up to $\delta$ precision with probability at least $1 - \varepsilon$.

The proof of this theorem is deferred to Appendix B 4. We can see that the quantum phase search algorithm provides a nearly quadratic speedup compared to the Hadamard test method in Section III A. More importantly, the phase search algorithm does not require the input state being an eigenstate of $U$, making it more versatile for solving specific problems like the factoring problem. We discuss two important applications of quantum phase search, factoring and amplitude estimation, in Appendix B 5 and B 6.

C. Comparison to related works

The quantum phase estimation method originally purpose to solve the Abelian Stabilizer Problem [18, 36] was found to work for general unitaries. The most well-known version of phase estimation method [18] queries the controlled-$U$ for $O(\frac{1}{\delta})$ times and applies the inverse quantum Fourier transform (QFT) [37] to estimate the eigenphase of a unitary $U$ with precision $\delta$ and success probability at least $4/\pi^2$. The success probability can be boosted to $1 - \varepsilon$ by using additional $O(\log \frac{1}{\delta})$ ancilla qubits [19]. Introducing classical feed-forward process [18, 38] can further reduce the number of ancilla to one without increase of circuit depth. Recent studies [5, 6] utilize the structure of QSVT to reinterpret phase estimation methods, bringing potential trade-offs among precision, query complexity and number of ancilla qubits. The quantum phase search method proposed in this work is based on the intuitive idea of binary search, which is fundamentally different from the previous QFT-based algorithms. Here we compare our phase search method to some previous quantum phase estimation algorithms with respect to the query complexity and number of ancilla qubits under the same precision and success probability, which is shown in Table I. One can see that the quantum phase search method achieves the best query complexity while requiring the least ancilla qubits, turning out to be an efficient phase estimation algorithm.

| Methods for QPE                      | Queries to controlled-$U$                      | # of ancilla qubits | Success probability | Precision |
|-------------------------------------|------------------------------------------------|---------------------|---------------------|-----------|
| QFT-based [18, 19, 39]              | $O\left(\frac{1}{\varepsilon} \left(1 + \frac{1}{\tau}\right)\right)$ | $\left[\log \frac{1}{\delta} + \log (2 + \frac{1}{\varepsilon})\right]$ |                     |           |
| Semi-classical QFT-based [18, 38]   | $O\left(\frac{1}{\delta} \left(1 + \frac{1}{\tau}\right)\right)$ | 1                   |                     |           |
| QSVT-based [5, 6]                   | $\tilde{O}\left(\frac{1}{\delta} \log \left(\frac{1}{\varepsilon}\right)\right)$ | $\left[\log \frac{1}{\delta}\right] + 3$ (or 3) | $1 - \varepsilon$  | $\delta$ |
| QPP-based (in Theorem 8)            | $\tilde{O}\left(\frac{1}{\delta} \log \left(\frac{1}{\varepsilon}\right)\right)$ | 1                   |                     |           |

TABLE I: Comparison of QPE Algorithms. In the query complexity, the $\tilde{O}$ notation omits $\log \log$ factors. The number of ancilla qubits is the total number of qubits used other for the system of $U$. 
IV. HAMILTONIAN PROBLEMS

To demonstrate that QPP is a versatile framework, we utilize it to solve Hamiltonian simulation problems. Notice that QPP may not be directly applied to a Hamiltonian, as its input must be a unitary matrix. Therefore, we must address the issue before proceeding to the algorithm design. Fortunately, a handy technique known as block encoding [7, 40] could assist us in encoding a general matrix into a unitary.

A. Block Encoding

A block encoding of a matrix $A \in \mathbb{C}^{2^n \times 2^n}$ with spectral norm $\|A\| \leq 1$ is a unitary matrix $U_A$ such that the upper-left block of $U$ is $A$, i.e.

$$U = \begin{bmatrix} A & \cdot \\ \cdot & \cdot \end{bmatrix}. \quad (16)$$

Then we can write $A = \langle 0^\otimes m | U_A | 0^\otimes m \rangle$, where $m$ denotes the number of ancilla qubits in the block encoding. In other words, for any state $|\psi \rangle \in \mathbb{C}^N$, we have $\left( (0^\otimes m) \otimes I^\otimes n \right) U_A |0^\otimes m, \psi \rangle = A |\psi \rangle$. In particular, let $|\psi_\lambda \rangle$ be an eigenvector of $A$ with an eigenvalue $\lambda$, then we will have a state

$$U_A |0^\otimes m, \psi_\lambda \rangle = \sqrt{\lambda^2 + 1} |\psi_\lambda \rangle + \sqrt{1 - \lambda^2} |\perp_\lambda \rangle,$$

where $|\perp_\lambda \rangle$ denotes a state orthogonal to $|0^\otimes m, \psi_\lambda \rangle$. In the above equation, we absorb the relative phase into states and ignore the global phase. To associate the spectrum of $A$ and its block encoding $U_A$, it has to be ensured that the subspace span$\{ |0^\otimes m, \lambda \rangle, U_A |0^\otimes m, \lambda \rangle \}$ is invariant under $U_A$. However, this is generally not true for an arbitrary block encoding. To resolve this issue, Low and Chuang [7] proposed a so-called “qubitization” technique that uses controlled-$U_A$ and controlled-$U_A^\dagger$ once to implement a qubitized block encoding $\hat{U}_A$ preserving the subspace span$\{ |0^\otimes (m+1), \lambda \rangle, \hat{U}_A |0^\otimes (m+1), \lambda \rangle \}$. Write

$$\hat{U}_A |0^\otimes (m+1), \psi_\lambda \rangle = \sqrt{\lambda^2 + 1} |\psi_\lambda \rangle + \sqrt{1 - \lambda^2} |\perp_\lambda \rangle,$$

where $|\perp_\lambda \rangle$ denotes a state orthogonal to $|0^\otimes (m+1), \psi_\lambda \rangle$. Then

$$|\chi^\pm_\lambda \rangle = \frac{1}{\sqrt{2}} (|0^\otimes (m+1), \psi_\lambda \rangle \pm i |\perp_\lambda \rangle)$$

are eigenstates of $\hat{U}_A$ with eigenphases $\pm \tau_\lambda = \pm \arccos \lambda$. Now the spectrum of $A$ and that of $\hat{U}_A$ are associated, which allows us to process and extract the spectrum of an arbitrary matrix $A$ by applying QPP on $\hat{U}_A$. More details of qubitization are discussed in Appendix C.1. In the next section, we will show how to use QPP to solve the Hamiltonian simulation problem.

B. Hamiltonian simulation

In the Hamiltonian simulation problem, given a Hamiltonian $H$, a time $t$ and a simulation error $\varepsilon$, the goal is to approximate the time-evolution operator $e^{-iHt}$ to error $\varepsilon$, i.e. produce a unitary $U$ such that $\|U - e^{-iHt}\| \leq \varepsilon$. In quantum computing, this is accomplished by designing a quantum circuit that approximates the operator $e^{-iHt}$ with high precision. Low and Chuang [7] proposes an adaptive Hamiltonian simulation algorithm based on block encoding that reaches the optimal query complexity. Here we show that our results also match the optimal query complexity. In particular, compared to the Hamiltonian simulation based on QSVT [4, 5, 9], our approach does not need the implementation of linear-combination-of-unitaries [26] and amplitude amplification [27, 41].

In this setup of the Hamiltonian simulation problem, the task is to use a block encoding of the rescaled Hamiltonian $H/\Lambda$ for some constant $\Lambda \geq \|H\|$ to simulate the operator $e^{-iHt}$. With out loss of generality, we may assume $\|H\| \leq 1$ and $\Lambda = 1$, since for $\|H\| > 1$ the problem can be considered as simulating evolution under the rescaled Hamiltonian $H/\Lambda$ for time $\Lambda t$. Recall that the qubitization establishes the relation between the eigenvalues of the Hamiltonian $H$ and eigenphases of its qubitized block encoding $\hat{U}_H$, i.e. $\tau_\lambda = \arccos(\lambda)$. Since the time-evolution operator $e^{-iHt}$ can be decomposed as $e^{-i\lambda t}$, the main idea is to use QPP to transform eigenphases of $\hat{U}_H$ by Theorem 5 as $\tau_\lambda \mapsto e^{-i\lambda t}$. We select a trigonometric polynomial $F(x)$ that approximates the function $f(x) = e^{-i\cos(x)t}$ with desired precision. Then applying the trigonometric polynomial $F(x)$ on each eigenphase $\tau_\lambda$ approximates

$$f(\tau_\lambda) = e^{-i\cos(\tau_\lambda)t} = e^{-i\lambda t}, \quad (20)$$
which provides a precise approximation of the time-evolution operator $e^{-iHt}$. The query complexity of Hamiltonian simulation by QPP is analyzed in the following theorem, and the detailed proof is deferred to Appendix D.

**Theorem 9** Given a block encoding $U_H$ of $H/\Lambda$ for some $\Lambda \geq \|H\|$, there exists an algorithm that simulates evolution under the Hamiltonian $H$ for time $t \in \mathbb{R}$ within precision $\delta > 0$, using two ancilla qubits and querying controlled-$U_H$ and controlled-$U_H^\dagger$ for a total number of times in

$$\Theta \left( \Lambda |t| + \frac{\log(2/\delta^2)}{\log\left(e + \frac{\log(2/\delta^2)}{\Lambda |t|}\right)} \right).$$

We point out that one could post-select the ancilla qubit after applying QPP circuit. In this case, we can relax the function approximation error. As a result, the output final state approximates the target state with an error of $\delta$, succeeding with a probability at least $1 - 2\delta$. By contrast, the circuit depth can be reduced. From the result, we conclude that QPP solves Hamiltonian simulation problems with the access to block encoding, and the query complexity matches the optimal results as in [7]. We notice that QPP could also solve other Hamiltonian problems like spectrum estimation, ground state energy estimation, and ground state preparation. We defer the discussion of those applications to Appendix D.

V. QUANTUM ENTROPY ESTIMATION

Quantum entropy is used to characterize the randomness and disorder of a quantum system, which has various theoretical and experimental applications of relevance. Estimating the entropy of a quantum system is an important problem in quantum information science. Classical methods of estimating the quantum entropies require the density matrix of a quantum state, which is costly, especially when the size of system is large. Recent works proposed quantum algorithms that could efficiently estimate quantum entropies [11–13], showing potential quantum speedups over the classical methods. The motivating idea behind these quantum approaches is the purified quantum query model [7], which prepares a purification of a mixed state $\rho$. Formally, the purified quantum query oracle of a mixed state $\rho$ is a unitary $U_\rho$ acting as

$$U_\rho |0\rangle_A |0\rangle_B = |\Psi_\rho\rangle_{AB} = \sum_{j=0}^{2^{n-1}} \sqrt{p_j} |\psi_j\rangle_A |\phi_j\rangle_B,$$

(21)

such that $\text{tr}_B(|\Psi_\rho\rangle\langle\Psi_\rho|) = \rho$, where $\{|\psi_j\rangle\}$ and $\{|\phi_j\rangle\}$ are sets of orthonormal states on the system $A$ and $B$ respectively. Using the qubitization method in [7], such an oracle model can be used to build a qubitized block encoding $\tilde{U}_\rho$ of the target state $\rho$. We show the detailed construction of $\tilde{U}_\rho$ in Appendix C 2.

Consequently, it is reasonable and compelling to investigate whether QPP, the structure designed for unitary phase processing, could contribute to the improvement of quantum algorithms for quantum entropy estimation. Note that quantum entropies of a quantum state $\rho$ can be interpreted as the corresponding classical entropies of the eigenvalues of $\rho$. If one could find trigonometric polynomials $F(x)$ that approximate the classical entropic functions, then quantum entropies can be naturally estimated via phase evaluation of $\tilde{U}_\rho$ in Theorem 6 by the spectral correspondence between $\rho$ and $\tilde{U}_\rho$. Specifically, the following theorem is the basic principle of the QPP-based quantum entropies estimation, and the proof of which is deferred to Appendix E 1.

**Theorem 10** Let $|\Psi_\rho\rangle_{AB}$ be a purification of an $n$-qubit state $\rho$ and $\tilde{U}_\sigma$ be a qubitized block encoding of an $n$-qubit state $\sigma$ with $m$ ancilla qubits. For any real-valued polynomial $f(x) = \sum_{k=0}^{L} c_j x^k$ with $\|c\|_1 \leq 1$, there exists a QPP circuit $V(\tilde{U}_\sigma)$ of $L$ layers such that

$$\langle Z^{(0)} | \Phi \rangle = \text{tr}(\rho f(\sigma)),$$

(22)

where $|\Phi\rangle = \left( V(\tilde{U}_\sigma) \otimes I_B \right) |0^{\otimes(m+1)}\rangle |\Psi_\rho\rangle_{AB}$ and the polynomial on a quantum state is defined as $f(\sigma) = \sum_{k=0}^{L} c_j \sigma^k$.

Theorem 10 shows that one could measure the value of $\text{tr}(\rho f(\sigma))$ as the $Z$ expectation value of the ancilla qubit. An estimate of the expectation value within an additive error $\delta$ can be obtained by measuring the ancilla qubit for $O(1/\delta^2)$ times. Moreover, we could directly apply the iterative amplitude estimation [35] on QPP to achieve a quadratic speedup without using extra qubits. For clarity, we present the QPP circuit of quantum entropy estimation in Figure 3. We also note that Theorem 10 can be applied to extract many information-theoretic properties of quantum states other than quantum entropies.
In this section, to demonstrate the power of QPP, we utilize the generic method in Theorem 10 to estimate the most fundamental entropic functionals for quantum systems, including the von Neumann entropy, the quantum relative entropy, and the family of quantum Rényi entropies.

### A. von Neumann and quantum relative entropy estimation

The von Neumann entropy [42] is a generalization of the Shannon entropy from the classical information theory to quantum information theory. For an $n$-qubit quantum state $\rho$, the von Neumann entropy is defined as follows

$$S(\rho) = - \text{tr}(\rho \ln \rho).$$  \hfill (23)

Let $\{p_j\}$ be the eigenvalues of $\rho$, then the von Neumann entropy is the same as the Shannon entropy of the probability distribution $\{p_j\}$,

$$S(\rho) = \sum_{j=0}^{2^n-1} p_j \ln p_j.$$  \hfill (24)

Recall from the qubitization technique that partial eigenphases of the qubitized block encoding $\hat{U}_\rho$ are given by $\pm \tau_j = \pm \arccos(p_j)$, then we have $p_j = \cos(\pm \tau_j) \in [0, 1]$. Here we assume the non-zero eigenvalues are lower bounded by some $\gamma > 0$. Then by Theorem 10, the main idea of using QPP to estimate the von Neumann entropy is to find a polynomial $f(x)$ that approximates the function $\ln(x)$ with some appropriate scale on the interval $[\gamma, 1]$, and $|f(x)| \leq 1$ for $x \in [-1, 1]$. Particularly, the polynomial $f(x)$ could be obtained from the Taylor series of $\ln(x)$. The overall result is stated in the following theorem.

**Theorem 11 (von Neumann entropy estimation)** Given a purified quantum query oracle $U_\rho$ of a state $\rho$ whose non-zero eigenvalues are lower bounded by $\gamma > 0$, there exists an algorithm that estimates $S(\rho)$ up to precision $\varepsilon$ with high probability by measuring a single qubit, querying $U_\rho$ and $U_\rho^\dagger$ for $O\left(\frac{1}{\gamma^2} \log^2 \left(\frac{1}{\gamma^2} \log \left(\frac{\log(1/\gamma)}{\varepsilon}\right)\right)\right)$ times. Moreover, using amplitude estimation improves the query complexity to $O\left(\frac{1}{\gamma^2 \varepsilon^2} \log \left(\frac{1}{\gamma^2} \log \left(\frac{\log(1/\gamma)}{\varepsilon}\right)\right)\right)$.

In particular, the dependence on $\gamma$ can be translated to the rank (or dimension) of the density matrix, from which we have the following corollary.

**Corollary 12** Given a purified quantum query oracle $U_\rho$ of a state $\rho$ whose rank is $\kappa \leq 2^n$, there exists an algorithm that estimates $S(\rho)$ up to precision $\varepsilon$ with high probability by measuring a single qubit, querying $U_\rho$ and $U_\rho^\dagger$ for $O\left(\frac{\kappa^2}{\varepsilon} \log^3 \left(\frac{1}{\gamma^2} \log \left(\frac{1}{\gamma^2}\right)\right)\right)$ times. Moreover, using amplitude estimation improves the query complexity to $O\left(\frac{\kappa^2}{\varepsilon^2} \log \left(\frac{1}{\gamma^2} \log \left(\frac{1}{\gamma^2}\right)\right)\right)$.

We defer the proofs to Appendix E 2. Note that the estimation of the quantum relative entropy between states $\rho$ and $\sigma$, i.e.

$$D(\rho \parallel \sigma) = - \text{tr}(\rho \ln \sigma) - S(\rho),$$  \hfill (25)

immediately follows from the above analysis. In particular, we only need to apply QPP on a qubitized block encoding of $\sigma$ to estimate $\text{tr}(\rho \ln \sigma)$. The result of quantum relative entropy estimation is shown in Theorem 13.

**Theorem 13 (Quantum relative entropy estimation)** Given purified quantum query oracles $U_\rho$ and $U_\sigma$ of states $\rho$ and $\sigma$, respectively, whose non-zero eigenvalues are lower bounded by $\gamma > 0$, there exists an algorithm that estimates $D(\rho \parallel \sigma)$ up to precision $\varepsilon$ with high probability, querying $U_\rho$, $U_\sigma$ and their inverses for $O\left(\frac{1}{\gamma^2 \varepsilon^2} \log^2 \left(\frac{1}{\gamma^2} \log \left(\frac{\log(1/\gamma)}{\varepsilon}\right)\right)\right)$ times. Moreover, using amplitude estimation improves the query complexity to $O\left(\frac{1}{\gamma^2 \varepsilon^2} \log \left(\frac{1}{\gamma^2} \log \left(\frac{\log(1/\gamma)}{\varepsilon}\right)\right)\right)$.
B. Quantum Rényi entropy estimation

The quantum Rényi entropy [30] is a quantum version of the classical Rényi entropy that was first introduced in [43]. For \( \alpha \in (0, 1) \cup (1, \infty) \), the quantum \( \alpha \)-Rényi entropy of an \( n \)-qubit quantum state \( \rho \) is defined as follows:

\[
S_\alpha(\rho) = \frac{1}{1-\alpha} \log \text{tr}(\rho^\alpha).
\]  

(26)

Let \( \{p_j\}_j \) be the eigenvalues of \( \rho \), then the quantum \( \alpha \)-Rényi entropy reduces to the \( \alpha \)-Rényi entropy of the probability distribution \( \{p_j\}_j \),

\[
S_\alpha(\rho) = \frac{1}{1-\alpha} \log \left( \sum_{j=0}^{2^n-1} p_j^\alpha \right).
\]  

(27)

Similarly, we assume all non-zero eigenvalues are greater than some \( \gamma > 0 \). The method of Rényi entropy estimation, based on Theorem 10, is in the same spirit of estimating the von Neumann entropy; the only difference is that we now aim to find a polynomial \( f(x) \) that approximates the function \( x^{\alpha-1} \) for any \( \alpha > 0 \) and \( \alpha \neq 1 \) on the interval \([\gamma, 1]\). The exponent is \( \alpha - 1 \) because we can write \( \text{tr}(\rho^\alpha) = \text{tr}(\rho \cdot \rho^{\alpha-1}) \), and the isolated \( \rho \) comes from the input state of QPP.

When \( \alpha > 0 \) is a non-integer, the polynomial could be given by separately considering the integer part and decimal part of \( \alpha - 1 \). Thus we only need to find a polynomial that approximates \( x^{\alpha-1} \) for \( \alpha \in (0, 1) \) on the interval \( x \in [\gamma, 1] \), which could be obtained from the Taylor series of \( x^{\alpha-1} \). We present the results in the following theorem and more discussions in Appendix E 3.

**Theorem 14 (Quantum Rényi entropy estimation for real \( \alpha \))** Given a purified quantum query oracle \( U_\rho \) of a state \( \rho \) whose non-zero eigenvalues are lower bounded by \( \gamma > 0 \), there exists an algorithm that estimates \( S_\alpha(\rho) \) up to precision \( \varepsilon \) with high probability by measuring a single qubit, querying \( U_\rho \) and \( U_\rho^\dagger \) for a total number of times of

\[
\tilde{O} \left( \frac{1}{\gamma^3 - 2\alpha\varepsilon^2} \cdot \frac{\eta^2}{\alpha} \right), \quad \text{if } \alpha \in (0, 1);
\]

\[
\tilde{O} \left( \frac{\alpha\gamma + 1}{\gamma\varepsilon^2} \cdot \frac{\eta^2}{\alpha} \right), \quad \text{if } \alpha \in (1, \infty);
\]

where \( \eta = \frac{\text{tr}(\rho^\alpha)}{1 - \alpha} \). Moreover, using quantum amplitude estimation improves the query complexity to

\[
\tilde{O} \left( \frac{1}{\gamma^2 - \alpha\varepsilon} \cdot \eta \right), \quad \text{if } \alpha \in (0, 1);
\]

\[
\tilde{O} \left( \frac{\alpha\gamma + 1}{\gamma\varepsilon} \cdot \eta \right), \quad \text{if } \alpha \in (1, \infty).
\]

(28)

(29)

Here the \( \tilde{O} \) notation omits logarithmic factors.

Similarly, we provide a method to estimate \( S_\alpha(\rho) \) without information of \( \gamma \) in Appendix E 3. When \( \alpha \) is an integer, the function \( x^{\alpha-1} \) naturally turns to be a normalized polynomial so that approximation error does not exist by Theorem 10. In this case, the dependence on the threshold \( \gamma \) can be further improved.

**Theorem 15 (Quantum Rényi entropy estimation for integer \( \alpha \))** Suppose \( \alpha > 1 \) is a positive integer, there exists an algorithm that estimates \( S_\alpha(\rho) \) up to precision \( \varepsilon \) with high probability by measuring a single qubit, querying \( U_\rho \) and \( U_\rho^\dagger \) for \( O \left( \frac{\alpha\text{tr}(\rho^\alpha)}{\varepsilon} \cdot \frac{\eta^2}{\alpha} \right) \) times. Moreover, using amplitude estimation improves the query complexity to \( O \left( \frac{\alpha\text{tr}(\rho^\alpha)}{\varepsilon} \right) \).

Note that this method of computing \( S_\alpha(\rho) \) for \( \alpha \in \mathbb{N}_+ \) naturally establishes an efficient algorithm for entanglement spectroscopy, a task of obtaining the entanglement of a quantum state. Consider a bipartite pure state \( |\Psi_\rho\rangle_{AB} \) in Eq. (21), the entanglement between systems \( A \) and \( B \) can be characterized by the eigenvalues of the reduced density operator \( \rho = \text{tr}_B(|\Psi_\rho\rangle\langle\Psi_\rho|) \). Specifically, one needs to compute the \( \text{tr}(\rho^k) \) for \( k = 1, \ldots, k_{\text{max}} \) to estimate \( k_{\text{max}} \) largest eigenvalues of \( \rho \) by the Newton-Girard method [44–46].
C. Comparison to related works

As introduced above, we utilize the framework of QPP to estimate quantum entropies based on the purified quantum query model. Here we briefly mention some closely related works on quantum entropy estimation under a similar setting. For von Neumann entropy $S(\rho)$, Gilyén and Li [11] proposed an efficient quantum algorithm based on QSVT and amplitude estimation that achieves a near-linear query complexity and an additive error $\varepsilon$. Another work by Gur et al. [13] utilized the quantum singular value estimation [47] and amplitude estimation to implement an algorithm with a sublinear query complexity up to a multiplicative error bound. By contrast, our algorithm could estimate the result by measuring the first ancilla qubit, which has a slightly worse query complexity in the worst case but a smaller circuit size. Nevertheless, by Corollary 12, our complexity can depend on the rank of the density matrix, which will be further improved for low-rank cases. Note that one could apply amplitude estimation on QPP without using extra qubits, which might be required for previous QSVT-based algorithms. As a result, the QPP-based algorithms allow us to flexibly consider the trade-off between the query complexity and the circuit depth in practical applications.

| Methods for $S(\rho)$ estimation | Total queries to $U_\rho$ and $U_\rho^+$ | Queries per use of circuit |
|----------------------------------|--------------------------------------|-----------------------------|
| QSVT-based with QAE ([11])       | $\tilde{O}(\frac{d}{\varepsilon^2})$ | $\tilde{O}(\frac{d}{\varepsilon^2})$ |
| QPP-based (assumes rank, in Corollary 12) | $\tilde{O}(\frac{d}{\varepsilon^2})$ | $\tilde{O}(\frac{d}{\varepsilon^2})$ |
| QPP-based with QAE (assumes rank, in Corollary 12) | $\tilde{O}(\frac{d}{\varepsilon^2})$ | $\tilde{O}(\frac{d}{\varepsilon^2})$ |
| QPP-based (in Theorem 11)        | $\tilde{O}(\frac{d}{\varepsilon^2})$ | $\tilde{O}(\frac{d}{\varepsilon^2})$ |
| QPP-based with QAE (in Theorem 11) | $\tilde{O}(\frac{d}{\varepsilon^2})$ | $\tilde{O}(\frac{d}{\varepsilon^2})$ |

TABLE II: Comparison of algorithms on estimating von Neumann entropy within additive error. Here the $\tilde{O}$ notation omits log factors, $\gamma > 0$ is the lower bound of eigenvalues, $\kappa > 0$ is the rank of the state $\rho \in \mathbb{C}^{d \times d}$, and $\varepsilon$ is the additive error of estimating $S(\rho)$. QAE is short for quantum amplitude estimation.

With regard to the family of quantum $\alpha$-Rényi entropies $S_\alpha(\rho)$, when $\alpha$ is an integer, QPP establishes an efficient algorithm for entanglement spectroscopy. Compared to previous algorithms for entanglement spectroscopy [44, 45], the QPP-based algorithm significantly reduces the circuit width from $O(n\alpha)$ to $4n + 1$ without using qubit resets as in [46]. For a more general case that $\alpha$ is not an integer, Subramanian and Hsieh [12] introduced a quantum algorithm that combines the QSVT technique and the DQC1 (Deterministic Quantum Computation with one clean qubit) method. Their algorithm estimates $S_\alpha(\rho)$ with an additive error by measuring a single qubit, using an expected total number $\tilde{O}(d^2/\gamma^2)$ queries to the purified quantum oracle, where $d = 2^n$ is the dimension of $\rho$. Our QPP-based approaches improve the results in [12] in terms of the dependence on the dimension. For instance, for $\alpha > 1$, our algorithms based on single-qubit measurement require a query complexity of $\tilde{O}(d^2/\gamma^2)$. The main reason there is a speedup factor of $d^2$ is that the DQC1 method requires a maximally mixed state $\frac{1}{n}I$ as the input state, whereas the QPP-based method uses $\rho$ as the input state. Moreover, as we mention before, QSVT is not natively compatible with indirect measurement, one needs to utilize an extra ancilla qubit to control the QSVT circuit in order to implement indirect measurement, as shown in [12]. Similar to the earlier description, we could leverage quantum amplitude estimation to achieve a better query complexity. More detailed comparisons are shown in Table III.

| Methods for $S_\alpha(\rho)$ estimation | Total queries to $U_\rho$ and $U_\rho^+$ | $\alpha \in (0, 1)$ | $\alpha \in (1, \infty)$ | $\alpha \in \mathbb{N}_+$ |
|---------------------------------------|--------------------------------------|-----------------|-----------------|-----------------|
| QSVT-based with DQC1 ([12])           | $\tilde{O}\left(\frac{d^2}{\gamma^2} \cdot \eta^2\right)$ | $\tilde{O}\left(\frac{d^2}{\gamma^2} \cdot \eta^2\right)$ | $\tilde{O}\left(\frac{d^2}{\gamma^2} \cdot \eta^2\right)$ | $\tilde{O}\left(\frac{d^2}{\gamma^2} \cdot \eta^2\right)$ |
| QPP-based (in Theorem 14 and 15)      | $\tilde{O}\left(\frac{1}{\gamma^2} \cdot \eta^2\right)$ | $\tilde{O}\left(\frac{1}{\gamma^2} \cdot \eta^2\right)$ | $\tilde{O}\left(\frac{1}{\gamma^2} \cdot \eta^2\right)$ | $\tilde{O}\left(\frac{1}{\gamma^2} \cdot \eta^2\right)$ |
| QPP-based with QAE (in Theorem 14 and 15) | $\tilde{O}\left(\frac{1}{\gamma^2} \cdot \eta\right)$ | $\tilde{O}\left(\frac{1}{\gamma^2} \cdot \eta\right)$ | $\tilde{O}\left(\frac{1}{\gamma^2} \cdot \eta\right)$ | $\tilde{O}\left(\frac{1}{\gamma^2} \cdot \eta\right)$ |

TABLE III: Comparison of algorithms on estimating quantum $\alpha$-Rényi entropies within additive error for different $\alpha$. Here the $\tilde{O}$ notation omits log factors, $\gamma > 0$ is the lower bound of eigenvalues of a mixed state $\rho \in \mathbb{C}^{d \times d}$, $\eta := \frac{\text{tr}(\rho^{\alpha-1})}{\text{tr}(\rho)}$ is the quantity depending on $\alpha$ and $\rho$, and $\varepsilon$ is the additive error of estimating $S_\alpha(\rho)$. QAE is short for quantum amplitude estimation.

The polynomial transformation implemented by QSVT lies in amplitudes of the outcome state, which could not be obtained by indirect measurements of the ancilla qubit in QSVT, thus most QSVT-based entropies estimation algorithms estimate the value
either by applying amplitude estimation or combining with the DQC1 model, and both of these methods increase the circuit size. Another approach is using a polynomial to estimate the square root of the function \( \sqrt{f(x)} \), as shown by Wang et al. [48]. This approach makes QSVT compatible with indirect measurements, since the approximated function now can be represented by the probability of measuring, which is similar as in QPP. However, the problem is that sometimes \( \sqrt{f(x)} \) could be more difficult to approximate than \( f(x) \). For example, \( f(x) = x \) is just a simple one-term polynomial, whereas \( \sqrt{x} \) takes much more terms to precisely approximate. Thus such a method presented in [48] may lead to even worse complexity than previous ones in [11–13]. We defer further discussion and comparison to Appendix E4.

VI. CONCLUDING REMARKS

In this paper, we introduce a new quantum phase processing (QPP) algorithmic framework based on applying trigonometric transformations to eigenphases of a unitary operator. The framework allows us to implement a desired evolution to the input state and, more interestingly, to extract the eigen-information of quantum systems by simply measuring the ancilla qubit. We demonstrate the capability of this framework by developing QPP-based algorithms for solving a variety of problems. Owing to the capability of QPP to directly process eigenphases, we design an efficient and intuitive phase estimation algorithm purely based on the idea of binary search, which uses only one ancilla qubit and matches the best prior performance. Utilizing block encoding and qubitization, we show that QPP could reproduce and even improve previous quantum algorithms based on the framework of QSVT, such as Hamiltonian simulation and quantum entropies estimation.

Our results show that QPP is a powerful framework for developing quantum algorithms related to eigenphase transformation and processing, which in particular complements the existing QSVT framework. QPP generalizes the trigonometric QSP by extending the \( R_\pi \) rotation instead of the reflection in the Chebyshev QSP as QSVT did, which introduces a new method in terms of lifting QSP to multiple qubits. On one hand, QPP implements arbitrary complex trigonometric polynomial, which overcomes the parity constraints in QSVT and thus exempts the use of linear-combination-of-unitaries in certain cases. On the other hand, QPP is natively compatible with indirect measurements, which could extract eigen-information of the main system via measuring the single ancilla qubit. Notably, QPP could work without amplitude estimation, which requires shorter circuits and less coherence time than QSVT, and hence might be more friendly to near-term quantum hardware. QPP natively inherits the trick of phase kickback, and thus it is particularly suitable to develop phase-related quantum algorithms. Other than applications mentioned in this paper, QPP can be potentially applied to other problems, including but not limited to Rényi divergence estimation, unitary trace estimation, and quantum Monte Carlo method. Moreover, considering the connections between quantum signal processing and single-qubit quantum neural networks [29, 49], our results may be lead to applications of QSVT and QPP in the area of quantum machine learning. Overall, we believe that the QPP algorithmic framework would deepen our understanding of quantum algorithm design and shed light on the search for quantum applications in quantum physics, quantum chemistry, machine learning, and beyond.

[1] Peter W. Shor, “Polynomial-Time Algorithms for Prime Factorization and Discrete Logarithms on a Quantum Computer,” SIAM J. Comput. 26, 1484–1509 (1997).
[2] Lov K. Grover, “A fast quantum mechanical algorithm for database search,” in Proceedings of the Twenty-Eighth Annual ACM Symposium on Theory of Computing, STOC ’96 (Association for Computing Machinery, New York, NY, USA, 1996) pp. 212–219.
[3] Seth Lloyd, “Universal Quantum Simulators,” Science 273, 1073–1078 (1996).
[4] András Gilyén, Yuan Su, Guang Hao Low, and Nathan Wiebe, “Quantum singular value transformation and beyond: Exponential improvements for quantum matrix arithmetic,” in Proceedings of the 51st Annual ACM SIGACT Symposium on Theory of Computing (2019) pp. 193–204, arXiv:1806.01838 [quant-ph].
[5] John M. Martyn, Zane M. Rossi, Andrew K. Tan, and Isaac L. Chuang, “A Grand Unification of Quantum Algorithms,” PRX Quantum 2, 040203 (2021), arXiv:2105.02859.
[6] Patrick Rall, “Faster Coherent Quantum Algorithms for Phase, Energy, and Amplitude Estimation,” Quantum 5, 566 (2021).
[7] Guang Hao Low and Isaac L. Chuang, “Hamiltonian Simulation by Qubitization,” Quantum 3, 163 (2019), arXiv:1610.06546 [quant-ph].
[8] Seth Lloyd, Bobak T. Kiani, David R. M. Arvidsson-Shukur, Samuel Bosch, Giacomo De Palma, William M. Kaminsky, Zi-Wei Liu, and Milad Marvian, “Hamiltonian singular value transformation and inverse block encoding,” (2021), arXiv:2104.01410 [quant-ph].
[9] John M. Martyn, Yuan Liu, Zachary E. Chin, and Isaac L. Chuang, “Efficient Fully-Coherent Quantum Signal Processing Algorithms for Real-Time Dynamics Simulation,” (2022), arXiv:2110.11327 [quant-ph].
[10] Andrew M Childs, Dmitri Maslov, Yunseong Nam, Neil J Ross, and Yuan Su, “Toward the first quantum simulation with quantum speedup,” Proceedings of the National Academy of Sciences 115, 9456–9461 (2018).
[11] András Gilyén and Tongyang Li, “Distributional property testing in a quantum world,” in 11th Innovations in Theoretical Computer Science Conference, ITCS 2020, January 12-14, 2020, Seattle, Washington, USA (2020) pp. 25:1–25:19.
[12] Sathyawageeswar Subramanian and Min-Hsiu Hsieh, “Quantum algorithm for estimating α-Rényi entropies of quantum states,” Physical Review A 104, 022428 (2021).
[13] Tom Gur, Min-Hsuan Hsieh, and Sathyawageeswar Subramanian, “Sublinear quantum algorithms for estimating von Neumann entropy,” (2021), arXiv:2111.11139 [quant-ph].

[14] András Gilyén and Alexander Poremba, “Improved Quantum Algorithms for Fidelity Estimation,” (2022), arXiv:2203.15993 [quant-ph].

[15] Lin Lin and Yu Tong, “Near-optimal ground state preparation,” Quantum 4, 372 (2020).

[16] Lin Lin and Yu Tong, “Heisenberg-limited ground-state energy estimation for early fault-tolerant quantum computers,” PRX Quantum 3, 010318 (2022).

[17] Yulong Dong, Lin Lin, and Yu Tong, “Ground state preparation and energy estimation on early fault-tolerant quantum computers via quantum eigenvalue transformation of unitary matrices,” arXiv preprint arXiv:2204.05955 (2022).

[18] A. Yu Kitaev, “Quantum measurements and the Abelian Stabilizer Problem,” (1995), arXiv:quant-ph/9511026.

[19] R. Cleve, A. Ekert, C. Macchiavello, and M. Mosca, “Quantum algorithms revisited,” Proceedings of the Royal Society of London. Series A: Mathematical, Physical and Engineering Sciences 454, 339–354 (1998).

[20] Adrian Barenco, André Berthiaume, David Deutsch, Artur Ekert, Richard Jozsa, and Chiara Macchiavello, “Stabilization of Quantum Computations by Symmetrization,” SIAM Journal on Computing 26, 1541–1557 (1997).

[21] Harry Buhrman, Richard Cleve, John Watrous, and Ronald de Wolf, “Quantum Fingerprinting,” Physical Review Letters 87, 167902 (2001).

[22] Dorit Aharonov, Vaughan Jones, and Zeph Landau, “A Polynomial Quantum Algorithm for Approximating the Jones Polynomial,” Algorithmica 55, 395–421 (2009).

[23] E. Knill and R. Laflamme, “Power of One Bit of Quantum Information,” Physical Review Letters 81, 5672–5675 (1998).

[24] Guang Hao Low, Theodore J. Yoder, and Isaac L. Chuang, “Methodology of Resonant Equiangular Composite Quantum Gates,” Physical Review X 6, 041067 (2016).

[25] Guang Hao Low and Isaac L Chuang, “Optimal hamiltonian simulation by quantum signal processing,” Physical review letters 118, 010501 (2017).

[26] Andrew M. Childs and Nathan Wiebe, “Hamiltonian simulation using linear combinations of unitary operations,” Quantum Inf. Comput. 12, 901–924 (2012).

[27] Gilles Brassard, Peter Høyer, Michele Mosca, and Alain Tapp, “Quantum amplitude amplification and estimation,” Contemporary Mathematics 305, 53–74 (2002).

[28] Dominic W. Berry, Andrew M. Childs, Richard Cleve, Robin Kothari, and Rolando D. Somma, “Exponential improvement in precision for simulating sparse Hamiltonians,” in Proceedings of the Forty-Sixth Annual ACM Symposium on Theory of Computing, STOC ’14 (Association for Computing Machinery, New York, NY, USA, 2014) pp. 283–292.

[29] Zhan Yu, Hongshun Yao, Mujin Li, and Xin Wang, “Power and limitations of single-qubit native quantum neural networks,” (2022), arXiv:2205.07848 [cond-mat, physics:math-ph, physics:quant-ph].

[30] Dénes Petz, “Quasi-entropies for finite quantum systems,” Reports on Mathematical Physics 23, 57–65 (1986).

[31] Jeongwan Haah, “Product Decomposition of Periodic Functions in Quantum Signal Processing,” Quantum 3, 190 (2019), arXiv:1806.10236.

[32] Rui Chao, Dawei Ding, Andras Gilyen, Cupjin Huang, and Mario Szegedy, “Finding Angles for Quantum Signal Processing with Machine Precision,” (2020), arXiv:2003.02831 [quant-ph].

[33] Thais de Lima Silva, Lucas Borges, and Leandro Aolita, “Fourier-based quantum signal processing,” (2022), 10.48550/arXiv.2206.02826.

[34] Yulong Dong, Xiang Meng, K. Birgitta Whaley, and Lin Lin, “Efficient phase-factor evaluation in quantum signal processing, ” Physical Review A 103, 042419 (2021), arXiv:2002.11649 [physics, physics:quant-ph].

[35] Dmitry Grinko, Julien Gacon, Christa Zoufal, and Stefan Woerner, “Iterative quantum amplitude estimation,” npj Quantum Information 7, 1–6 (2021).

[36] A. Kitaev, A. Shen, and M. Vyalyi, Classical and Quantum Computation, Graduate Studies in Mathematics, Vol. 47 (American Mathematical Society, Providence, Rhode Island, 2002) p. 272.

[37] D Coppersmith, An approximate fourier transform useful in quantum computing, Tech. Rep. (1994).

[38] Robert B. Griffiths and Chi-Sheng Niu, “Semiclassical Fourier Transform for Quantum Computation,” Physical Review Letters 76, 3228–3231 (1996), arXiv:quant-ph/9511007.

[39] Michael A Nielsen and Isaac L Chuang, Quantum computation and quantum information (Cambridge university press, 2010).

[40] Shantanav Chakraborty, András Gilyén, and Stacey Jeffery, “The power of block-encoded matrix powers: Improved regression techniques via faster hamiltonian simulation,” in 46th International Colloquium on Automata, Languages, and Programming, ICALP 2019, July 9-12, 2019, Patras, Greece, LIPIcs, Vol. 132 (Schloss Dagstuhl - Leibniz-Zentrum für Informatik, 2019) pp. 33:1–33:14.

[41] Dominic W Berry, Graeme Ahokas, Richard Cleve, and Barry C Sanders, “Efficient quantum algorithms for simulating sparse Hamiltonians,” Communications in Mathematical Physics 270, 359–371 (2007).

[42] John von Neumann, Mathematische Grundlagen der Quantenmechanik, 2nd ed., Die Grundlehren der mathematischen Wissenschaften in Einzeldarstellungen No. 38 (Springer, Berlin Heidelberg, 1996).

[43] Alfréd Rényi, “On measures of entropy and information,” in Proceedings of the Fourth Berkeley Symposium on Mathematical Statistics and Probability, Volume 1: Contributions to the Theory of Statistics (University of California Press, 1961) pp. 547–561.

[44] Sonika Johri, Damian S. Steiger, and Matthias Troyer, “Entanglement spectroscopy on a quantum computer,” Physical Review B 96, 195136 (2017).

[45] Yigit Subasi, Lukasz Cincio, and Patrick J. Coles, “Entanglement spectroscopy with a depth-two quantum circuit,” Journal of Physics A: Mathematical and Theoretical 52, 044001 (2019), arXiv:1806.08865 [cond-mat, physics:quant-ph].

[46] Justin Yirka and Yigit Subasi, “Qubit-efficient entanglement spectroscopy using qubit resets,” Quantum 5, 535 (2021), arXiv:2010.03080 [quant-ph].

[47] Jordanis Kerenidis and Anupam Prakash, “Quantum recommendation systems,” arXiv preprint arXiv:1603.08675 (2016).
[48] Qisheng Wang, Ji Guan, Junyi Liu, Zhicheng Zhang, and Mingsheng Ying, “New Quantum Algorithms for Computing Quantum Entropies and Distances,” (2022), arXiv:2203.13522 [quant-ph].
[49] Adrián Pérez-Salinas, Alba Cervera-Lierta, Elies Gil-Fuster, and José I. Latorre, “Data re-uploading for a universal quantum classifier,” Quantum 4, 226 (2020).
[50] Rich Rines and Isaac Chuang, “High Performance Quantum Modular Multipliers,” (2018), arXiv:1801.01081 [quant-ph].
[51] Seong-Min Cho, Aeyoung Kim, Dooho Choi, Byung-Soo Choi, and Seung-Hyun Seo, “Quantum Modular Multiplication,” IEEE Access 8, 213244–213252 (2020).
[52] Yohichi Suzuki, Shumpei Uno, Rudy Raymond, Tomoki Tanaka, Tamiya Onodera, and Naoki Yamamoto, “Amplitude estimation without phase estimation,” (2020), arXiv:1904.10246 [quant-ph].
[53] Scott Aaronson and Patrick Rall, “Quantum Approximate Counting, Simplified,” (2021), arXiv:1908.10846 [quant-ph].
[54] Patrick Rall and Bryce Fuller, “Amplitude Estimation from Quantum Signal Processing,” (2022), arXiv:2207.08628 [quant-ph].
[55] Daan Camps, Lin Lin, Roel Van Beeumen, and Chao Yang, “Explicit quantum circuits for block encodings of certain sparse matrices,” arXiv preprint arXiv:2203.10236 (2022).
[56] Milton Abramowitz, Irene A Stegun, and Robert H Romer, “Handbook of mathematical functions with formulas, graphs, and mathematical tables,” (1988).
[57] Dominic W. Berry, Andrew M. Childs, and Robin Kothari, “Hamiltonian simulation with nearly optimal dependence on all parameters,” (IEEE, 2015) pp. 792–809.
[58] Daniel S Abrams and Seth Lloyd, “Quantum algorithm providing exponential speed increase for finding eigenvalues and eigenvectors,” Physical Review Letters 83, 5162–5165 (1999).
[59] David Poulin, Alexei Kitaev, Damian S. Steiger, Matthew B. Hastings, and Matthias Troyer, “Quantum algorithm for spectral measurement with a lower gate count,” Phys. Rev. Lett. 121, 010501 (2018).
[60] Youle Wang, Benchi Zhao, and Xin Wang, “Quantum algorithms for estimating quantum entropies,” (2022), arXiv:2203.02386 [quant-ph].
Supplementary Material

In this Supplementary Material, we provide detailed proofs of results stated in this paper, and discuss some further applications of the QPP algorithmic framework.

Appendix A: Theorems of Quantum Phase Processing

1. Existence of Laurent complementary and angle finding

Other than the characterization of trigonometric QSP in Theorem 1, we also need to specify the achievable trigonometric polynomials \( P(x) \) for which there exists a corresponding \( Q(x) \) satisfying the three conditions in Theorem 1. First we prove the following lemma, using similar ideas of root finding from previous works [31–33].

**Lemma S1** Suppose \( A(x) \) is a non-negative real-valued trigonometric polynomial. Then there exists a Laurent polynomial \( Q \in \mathbb{C}[e^{ix/2}, e^{-ix/2}] \) such that \( QQ^* = A \).

**Proof** Denote \( A(x) = \sum_{j=-2L}^{2L} a_j e^{jix/2} \). We can decompose \( A \) by the set of \( 4L \) roots \( \{\xi_k\}_{k=1}^{4L} \) so that

\[
A(x) = a_{2L} e^{-iLx} \prod_{k=1}^{2L} (e^{ix/2} - \xi_k),
\]

where \( \{\xi_k\}_{k=1}^{4L} \) can be efficiently found by computing all roots of a regular complex polynomial

\[
g(\xi) := \prod_{j=0}^{4L} a_j^{-2L} \xi^j.
\]

In particular, since \( A \) is real and non-negative, these roots appear in inverse conjugate pairs i.e. \( \{\xi_k\}_{k=1}^{4L} = \{\xi_k, -\frac{1}{\xi_k}\}_{k=1}^{2L} \). Then \( A \) can be further simplified to

\[
A(x) = a_{2L} e^{-iLx} \left[ \prod_{k=1}^{2L} (e^{ix/2} - \xi_k) \right] \left[ \prod_{k=1}^{2L} (e^{ix/2} - \frac{1}{\xi_k}) \right].
\]

From the fact \( e^{ix/2} - \xi_k = -e^{ix/2} \xi_k (e^{-ix/2} - \frac{1}{\xi_k}) \), we have

\[
A(x) = a_{2L} \left[ \prod_{k=1}^{2L} \xi_k \right] \left[ \prod_{k=1}^{2L} (e^{ix/2} - \frac{1}{\xi_k}) \right] \left[ \prod_{k=1}^{2L} (e^{ix/2} - \frac{1}{\xi_k}) \right].
\]

Let \( q := a_{2L} \prod_{k=1}^{2L} \xi_k \). Note that \( q \) is real since

\[
A(0) = a_{2L} g(0) = a_{2L} \prod_{k=1}^{2L} \xi_k = \frac{a_{2L} \prod_{k=1}^{2L} \xi_k^2}{\prod_{k=1}^{2L} |\xi_k|^2} \quad (A.4)
\]

is real. Define \( Q(x) := \sqrt{q} e^{-iLx/2} \prod_{k=1}^{2L} (e^{ix/2} - \frac{1}{\xi_k}) \) and the result follows.

Using Lemma S1, we show that there exists a \( Q \) such that \( QQ^* = 1 - PP^* \) for any trigonometric series \( P \) satisfying \( |P|^2 \leq 1 \).

**Lemma S2 (Existence of Laurent complementary)** Let \( P \in \mathbb{C}[e^{ix/2}, e^{-ix/2}] \) be a Laurent polynomial with degree no larger than \( L \) and parity \( L \mod 2 \). Then \( |P(x)| \leq 1 \) for all \( x \in \mathbb{R} \) if and only if there exists a Laurent polynomial \( Q \in \mathbb{C}[e^{ix/2}, e^{-ix/2}] \) satisfying

1. \( \deg(Q) \leq L \),
2. \( Q \) has parity \( L \mod 2 \),
3. \( \forall x \in \mathbb{R}, |P(x)|^2 + |Q(x)|^2 = 1 \).

**Proof** \((\Leftarrow)\) The statement trivially holds from the third condition \( |P(x)|^2 + |Q(x)|^2 = 1 \).

\((\Rightarrow)\) Suppose \( P \in \mathbb{C}[e^{ix/2}, e^{-ix/2}] \) is a Laurent polynomial satisfying above requirements. Note that if \( |P(x)| = 1 \) for all \( x \in \mathbb{R} \), then the result follows by setting \( Q = 0 \). Suppose \( |P(x)| < 1 \) for some \( x \in \mathbb{R} \). Then \( A = 1 - PP^* \) is a real and positive Laurent polynomial. By Lemma S1, there exists a Laurent polynomial \( Q \in \mathbb{C}[e^{ix/2}, e^{-ix/2}] \) such that \( QQ^* = 1 - PP^* \) i.e. \( |P(x)|^2 + |Q(x)|^2 = 1 \) for all \( x \in \mathbb{R} \). The first and second conditions follow by the fact that \( \deg(P) \leq L \) and \( P \) has parity \( L \mod 2 \).

Combined with Lemma S2 and Theorem 1, now we can compute the corresponding rotation angles \( \alpha, \theta \) and \( \phi \) of \( W_{\omega, \theta, \phi} \) for a given trigonometric polynomial \( P(x) \), as shown in Algorithm 3.
Algorithm 3 Angle Finding

Require: A Laurent polynomial \( P \in \mathbb{C}[e^{ix/2}, e^{-ix/2}] \) such that \(|P(x)| \leq 1\) for all \( x \in \mathbb{R} \).
Ensure: Rotation parameters \( \omega, \theta, \phi \) such that \( \langle 0| W_{\omega, \theta, \phi}(x)|0 \rangle = P(x) \) for all \( x \in [-\pi, \pi] \).

1. Compute the set of roots \( \{x_k\}_{k=1}^L \) and leading coefficient \( a_{2L} \) from real-valued and non-negative trigonometric polynomial \( A(x) = 1 - P(x)P^*(x) \), where \( L \) is the degree of \( P \). Sort the set by ascending modulus and determine

\[
Q \leftarrow \sqrt{a_{2L} \prod_{k=1}^{2L} \xi_k e^{-iLx/2} \sum_{k=1}^{2L} (e^{ix/2} - \frac{1}{\xi_k})} \quad \text{(A.5)}
\]

2. while \( \deg(P) > 0 \) do
3. \( k \leftarrow \deg(P), p_k \leftarrow P[e^{ikx/2}], p_{-k} \leftarrow P[e^{-ikx/2}] \), \( q_k \leftarrow Q[e^{ikx/2}] \) and \( q_{-k} \leftarrow Q[e^{-ikx/2}] \).
4. Determine \( \theta_k, \phi_k \) such that \( \cos \frac{\theta_k}{2} e^{i\theta_k/2} p_k + \sin \frac{\theta_k}{2} e^{-i\theta_k/2} q_k = 0 \), \( -\sin \frac{\theta_k}{2} e^{i\theta_k/2} p_k + \cos \frac{\theta_k}{2} e^{-i\theta_k/2} q_k = 0 \).
5. Update polynomials (simultaneously) such that

\[
P \leftarrow e^{i\frac{\phi_k}{2}} \cos \frac{\theta_k}{2} e^{i\theta_k/2} p + e^{-i\frac{\phi_k}{2}} \sin \frac{\theta_k}{2} e^{i\theta_k/2} Q, \quad Q \leftarrow e^{-i\frac{\phi_k}{2}} \cos \frac{\theta_k}{2} e^{-i\theta_k/2} Q - e^{i\frac{\phi_k}{2}} \sin \frac{\theta_k}{2} e^{-i\theta_k/2} P \quad \text{(A.6)}
\]
6. end while
7. Determine \( \omega, \theta, \phi \) such that \( R_{\omega}(\theta) R_{\theta}(\phi) R_{\phi}(\omega) = \begin{bmatrix} P & -Q \\ Q & P^* \end{bmatrix}; \theta \leftarrow (\theta_0, ..., \theta_L), \phi \leftarrow (\phi_0, ..., \phi_L). \)
8. Return \( \omega, \theta \) and \( \phi \).

2. Proofs of Corollary 2 and Corollary 3

**Corollary 2** For any complex-valued trigonometric polynomial \( F(x) = \sum_{j=-L}^{L} c_j e^{ijx} \) with \( \|e\|_1 \leq 1 \), there exist \( \omega \in \mathbb{R} \) and \( \theta, \phi \in \mathbb{R}^{2L+1} \) such that for all \( x \in \mathbb{R} \),

\[
\langle 0| W^{2L}_{\omega, \theta, \phi}(x)|0 \rangle = F(x). \quad \text{(A.7)}
\]

**Proof** Note that \( F \) is a Laurent polynomial with degree no larger than \( 2L \). By Lemma S2, there exists a Laurent polynomial \( G \in \mathbb{C}[e^{ix/2}, e^{-ix/2}] \) such that \( \deg(G) \leq 2L \), \( G \) has parity 0 and \( |F(x)|^2 + |G(x)|^2 = 1 \) for all \( x \in \mathbb{R} \). By Theorem 1, there exists \( \omega \in \mathbb{R}, \theta \in \mathbb{R}^{2L+1} \) and \( \phi \in \mathbb{R}^{2L+1} \) such that

\[
W^{2L}_{\omega, \theta, \phi} = \begin{bmatrix} F & -G \\ G^* & F^* \end{bmatrix}. \quad \text{(A.8)}
\]

The result directly follows.

**Corollary 3** For any real-valued trigonometric polynomial \( F(x) = \sum_{j=-L}^{L} c_j e^{ijx} \) with \( \|e\|_1 \leq 1 \), there exist \( \omega \in \mathbb{R} \) and \( \theta, \phi \in \mathbb{R}^{L+1} \) such that for all \( x \in \mathbb{R} \),

\[
f_W(x) := \langle 0| W^{L}_{\omega, \theta, \phi}(x)^\dagger Z^{2L}_{\omega, \theta, \phi}(x)|0 \rangle = F(x). \quad \text{(A.9)}
\]

**Proof** Note that \( (1 \pm F(x))/2 \) are non-negative real-valued trigonometric polynomials. Then by Lemma S1 there exist two Laurent polynomials \( P, Q \) such that for all \( x \in \mathbb{R} \),

\[
P(x)P^*(x) = \frac{1 + F(x)}{2} \quad \text{and} \quad Q(x)Q^*(x) = \frac{1 - F(x)}{2}. \quad \text{(A.10)}
\]

Observe that \( P \) and \( Q \) satisfy the three conditions in Theorem 1, thus there exists \( \omega \in \mathbb{R}, \theta \in \mathbb{R}^{L+1} \) and \( \phi \in \mathbb{R}^{L+1} \) such that

\[
\langle 0| W^{L}_{\omega, \theta, \phi}(x)^\dagger Z^{L}_{\omega, \theta, \phi}(x)|0 \rangle = P(x)P^*(x) - Q(x)Q^*(x) = F(x), \quad \text{(A.11)}
\]

for all \( x \in \mathbb{R} \).
3. Proof of Lemma 4

Lemma 4 (Eigenspace Decomposition of QPP) Suppose $U$ is an $n$-qubit unitary with spectral decomposition

$$U = \sum_{j=0}^{2^n-1} e^{i\tau_j} |\chi_j\rangle |\chi_j\rangle.$$  \hspace{1cm} (A.12)

For all $L \in \mathbb{N}$, $\omega \in \mathbb{R}$ and $\theta, \phi \in \mathbb{R}^{L+1}$, we have

$$V_{\omega, \theta, \phi}^L(U) = \bigoplus_{j=0}^{2^n-1} (e^{-i\tau_j/2})^L \bmod 2 : W_{\omega, \theta, \phi}^L(\tau_j) \mathbb{B}_j,$$  \hspace{1cm} (A.13)

where $\mathbb{B}_j := \{|0, \chi_j\rangle, |1, \chi_j\rangle\}$.

Proof Observe that the decomposition of unitaries is

$$\begin{bmatrix} U^\dagger & 0 \\ 0 & I \end{bmatrix} = \sum_{j=0}^{2^n-1} e^{-i\tau_j} |\theta\rangle_0 \otimes |\chi_j\rangle |\chi_j\rangle + \sum_{j=0}^{2^n-1} |1\rangle_0 \otimes |\chi_j\rangle |\chi_j\rangle \hspace{1cm} (A.14)$$

$$= \sum_{j=0}^{2^n-1} e^{-i\tau_j} \begin{bmatrix} e^{-i\tau_j/2} & 0 \\ 0 & e^{i\tau_j/2} \end{bmatrix} \otimes |\chi_j\rangle |\chi_j\rangle = \sum_{j=0}^{2^n-1} e^{-i\tau_j} R_z(\tau_j) \otimes |\chi_j\rangle |\chi_j\rangle \hspace{1cm} (A.15)$$

$$= \bigoplus_{j=0}^{2^n-1} e^{-i\tau_j} R_z(\tau_j) \mathbb{B}_j, \quad \text{and} \hspace{1cm} (A.16)$$

$$\begin{bmatrix} I & 0 \\ 0 & U \end{bmatrix} = \sum_{j=0}^{2^n-1} |0\rangle_0 \otimes |\chi_j\rangle |\chi_j\rangle + \sum_{j=0}^{2^n-1} e^{i\tau_j} |1\rangle_0 \otimes |\chi_j\rangle |\chi_j\rangle \hspace{1cm} (A.17)$$

$$= \sum_{j=0}^{2^n-1} e^{i\tau_j} \begin{bmatrix} e^{-i\tau_j/2} & 0 \\ 0 & e^{i\tau_j/2} \end{bmatrix} \otimes |\chi_j\rangle |\chi_j\rangle = \sum_{j=0}^{2^n-1} e^{i\tau_j} R_z(\tau_j) \otimes |\chi_j\rangle |\chi_j\rangle \hspace{1cm} (A.18)$$

$$= \bigoplus_{j=0}^{2^n-1} e^{i\tau_j} R_z(\tau_j) \mathbb{B}_j. \hspace{1cm} (A.19)$$

In a similar manner, we can decompose $R_y$ and $R_z$ gates applied on the first qubit, such that for any $\zeta \in \mathbb{R}$,

$$R_y^{(0)}(\zeta) \otimes I = R_y^{(0)}(\zeta) \otimes \sum_{j=0}^{2^n-1} |\chi_j\rangle |\chi_j\rangle = R_y^{(0)}(\zeta) \otimes \bigoplus_{j=0}^{2^n-1} |\chi_j\rangle = \bigoplus_{j=0}^{2^n-1} R_y(\zeta) \mathbb{B}_j \hspace{1cm} (A.20)$$

$$R_z^{(0)}(\zeta) \otimes I = \ldots = \bigoplus_{j=0}^{2^n-1} R_z(\zeta) \mathbb{B}_j$$

For convenience $\mathbb{B}_j$s are omitted in the rest of the proof. From above equations, for all even $L \in \mathbb{N}$ and $\omega \in \mathbb{R}, \theta, \phi \in \mathbb{R}^{L+1},$

$$V_{\omega, \theta, \phi}^L(U) = \bigoplus_{j=0}^{2^n-1} R_z(\omega) R_y(\theta_0) R_z(\phi_0) \prod_{l=1}^{L/2} e^{-i\tau_{2l-1}} R_z(\tau_j) R_y(\theta_{2l-1}) R_z(\phi_{2l-1}) e^{i\tau_{2l}} R_z(\tau_j) R_y(\theta_{2l}) R_z(\phi_{2l}) \hspace{1cm} (A.21)$$

$$= \bigoplus_{j=0}^{2^n-1} R_y(\theta_0) R_z(\phi_0) \prod_{l=1}^{L} R_z(\tau_j) R_y(\theta_l) R_z(\phi_l) = \bigoplus_{j=0}^{2^n-1} W_{\omega, \theta, \phi}(\tau_j). \hspace{1cm} (A.22)$$

Similar statement holds for odd $L \in \mathbb{N}.$
4. Proofs of Theorem 5 and Theorem 6

**Theorem 5 (Quantum phase evolution)** Given an \( n \)-qubit unitary \( U = \sum_{j=0}^{2^n-1} e^{i\tau_j |x_j \rangle \langle x_j|} \) and an \( n \)-qubit quantum state \( |\psi\rangle = \sum_{j=0}^{2^n-1} \alpha_j |x_j\rangle \), for any trigonometric polynomial \( F(x) = \sum_{j=-L}^L c_j e^{i j x} \) with \( \|c\|_1 \leq 1 \), there exist \( \omega \in \mathbb{R} \) and \( \theta, \phi \in \mathbb{R}^{2L+1} \) such that

\[
\langle 0 | \otimes I^{\otimes n} \rangle V^{2L}_{\omega, \theta, \phi}(U) |0, \psi\rangle = \sum_{j=0}^{2^n-1} \alpha_j F(\tau_j) |x_j\rangle.
\]

**Proof** By Corollary 2, there exists \( \omega \in \mathbb{R}, \theta \in \mathbb{R}^{2L+1} \) and \( \phi \in \mathbb{R}^{2L+1} \) such that \( \langle 0 | W^{2L}_{\omega, \theta, \phi}(x) |0\rangle = F(x) \). Then for such \( \omega, \theta \) and \( \phi \),

\[
\langle 0 | \otimes I^{\otimes n} \rangle V^{2L}_{\omega, \theta, \phi}(U) |0, \psi\rangle = \sum_{j=0}^{2^n-1} \alpha_j F(\tau_j) |x_j\rangle
\]

as required.

**Theorem 6 (Quantum phase evaluation)** Given an \( n \)-qubit unitary \( U = \sum_{j=0}^{2^n-1} e^{i\tau_j |x_j \rangle \langle x_j|} \) and an \( n \)-qubit quantum state \( \rho \), for any real-valued trigonometric polynomial \( F(x) = \sum_{j=-L}^L c_j e^{i j x} \) with \( \|c\|_1 \leq 1 \), there exist \( \omega \in \mathbb{R} \) and \( \theta, \phi \in \mathbb{R}^{L+1} \) such that \( \tilde{\rho} = V^{L}_{\omega, \theta, \phi}(U) (|0\rangle \langle 0| \otimes \rho) V^{L}_{\omega, \theta, \phi}(U)^\dagger \) satisfies

\[
f_V(U) := \text{tr} \left[ \left( Z^{(0)} \otimes I \right) \cdot \tilde{\rho} \right] = \sum_{j=0}^{2^n-1} p_j F(\tau_j),
\]

where \( p_j = \langle \chi_j | \rho | \chi_j \rangle \) and \( Z^{(0)} \) is a Pauli-Z observable acting on the first qubit.

**Proof** We begin the proof by decomposing the observable \( Z^{(0)} \otimes I \). Note that

\[
Z^{(0)} \otimes I = Z^{(0)} \otimes \bigoplus_{j=0}^{2^n-1} |x_j \rangle \langle x_j| = \bigoplus_{j=0}^{2^n-1} Z^{(0)} \mathbb{B}_j,
\]

where \( \mathbb{B}_j = \{|0, \chi_j\rangle, |1, \chi_j\rangle\} \). By Corollary 3, there exist \( \omega, \theta \) and \( \phi \) such that \( \langle 0 | W^{L}_{\omega, \theta, \phi}(x)^\dagger Z W^{L}_{\omega, \theta, \phi}(x) |0\rangle = F(x) \), we have

\[
\text{tr} \left[ \left( Z^{(0)} \otimes I \right) \cdot \tilde{\rho} \right] = \text{tr} \left[ \left( Z^{(0)} \otimes I \right) V^{L}_{\omega, \theta, \phi}(U) \left( \sum_{j,k=0}^{2^n-1} \langle \chi_j | \rho | \chi_k \rangle |0, \chi_j \rangle \langle 0, \chi_k| \right) V^{L}_{\omega, \theta, \phi}(U)^\dagger \right]
\]

\[
= \sum_{j=0}^{2^n-1} p_j \text{tr} \left[ |0, \chi_j \rangle \langle 0, \chi_j| \right] \text{tr} \left[ \left( Z^{(0)} \otimes I \right) V^{L}_{\omega, \theta, \phi}(U) \right]
\]

\[
= \sum_{j=0}^{2^n-1} p_j \langle 0 | W^{L}_{\omega, \theta, \phi}(\tau_j)^\dagger Z W^{L}_{\omega, \theta, \phi}(\tau_j) |0 \rangle \quad \text{(by Lemma 4)}
\]

\[
= \sum_{j=0}^{2^n-1} p_j F(\tau_j).
\]
Appendix B: Detailed Analysis of Quantum Phase Search

1. Proof of Lemma 7

First we show that there exists a trigonometric polynomial that approximates the square wave function \( \text{sqw}(x) := \text{sgn}(\sin x) \), following the results of approximating the sign function by polynomials [4].

**Lemma S3 (Trigonometric approximation of the square wave function)** For all \( \Delta \in (0, 1), \varepsilon \in (0, 1) \), there exists a trigonometric polynomial \( F \in \mathbb{C}[e^{-ix}, e^{ix}] \) of degree \( L = O\left(\frac{1}{\varepsilon} \log \frac{1}{\Delta}\right) \) such that

- for all \( x \in [-\pi, \pi] \), \( |F(x)| \leq 1 \), and
- for all \( x \in [-\pi + \Delta, -\Delta] \cup [\Delta, \pi - \Delta] \), \( |\text{sqw}(x) - F(x)| \leq \varepsilon \),

where \( \text{sqw}(x) := \text{sgn}(\sin x) \) is the square wave function.

**Proof** By Lemma 25 in [4], there exist a polynomial \( P \in \mathbb{R}[x] \) of degree \( L = O\left(\frac{1}{\varepsilon} \log \frac{1}{\Delta}\right) \) such that \( |P(x)| \leq 1 \) for all \( x \in [-1, 1] \) and \( |P(x) - \text{sgn}(x)| \leq \varepsilon \) for all \( x \in [-1, 1] \setminus (-\delta, \delta) \). Let \( \delta = \sin(\Delta) \), write the polynomial \( P \) in a Chebyshev form as \( P(x) = \sum_{j=0}^{L} a_j T_j(x) \) for some \( a_j \in \mathbb{C} \), then by a change of variable,

\[
P(\sin x) = \sum_{j=0}^{L} \frac{(-i)^j a_j}{2} \left[e^{ijx} + (-1)^j e^{-ijx}\right]
\]  

(B.1)

is a trigonometric polynomial of degree \( L = O\left(\frac{1}{\varepsilon} \log \frac{1}{\Delta}\right) = O\left(\frac{1}{\Delta} \log \frac{1}{\pi}\right) \). Simply let \( F(x) = P(\sin x) \), then we have \( |F(x)| \leq 1 \) for all \( x \in [-\pi, \pi] \) and \( |\text{sgn}(\sin x) - F(x)| \leq \varepsilon \) for all \( x \in [-\pi + \Delta, -\Delta] \cup [\Delta, \pi - \Delta] \).

Then we show that there exists a QPP that utilizes the approximated square wave function to classify phases on the interval

\( [-\pi + \Delta, -\Delta] \cup [\Delta, \pi - \Delta] \).

**Lemma 7 (Phase classification)** Given a unitary \( U = \sum_{j=0}^{2^n-1} e^{ij\tau_j} |\chi_j\rangle \langle \chi_j| \), then for any \( \Delta \in (0, \pi) \) and \( \varepsilon \in (0, 1) \), there exists a QPP circuit \( V(U) \) of \( L = O\left(\frac{1}{\varepsilon} \log \frac{1}{\Delta}\right) \) layers such that

\[
V(U) |0, \chi_k\rangle = \begin{cases} 
\sqrt{1 - \varepsilon_k} |0, \chi_k\rangle + \sqrt{\varepsilon_k} |1, \chi_k\rangle & \text{if } \tau_k \in [\Delta, \pi - \Delta], \\
\sqrt{\varepsilon_k} |0, \chi_k\rangle + \sqrt{1 - \varepsilon_k} |1, \chi_k\rangle & \text{if } \tau_k \in [-\pi + \Delta, -\Delta].
\end{cases}
\]  

(B.2)

for \( 0 \leq k < 2^n \), where \( \varepsilon_k \in (0, \varepsilon) \).

**Proof** By Lemma S3, there exists a trigonometric polynomial \( f(x) \) approximating the square wave function with order \( L = O\left(\frac{1}{\Delta} \log \frac{1}{\pi}\right) \), such that \( L \) is a multiple of 4 and \( |f(x) - \text{sqw}(x)| < \varepsilon \) for all \( x \in (-\pi + \Delta, -\Delta] \cup [\Delta, \pi - \Delta) \). It follows from Lemma S1 that there exist trigonometric polynomials \( P = \sqrt{1 + f(x)} \) and \( Q = \sqrt{1 - f(x)} \). By Theorem 5, there exist parameters \( \omega \in \mathbb{R}, \theta, \phi \in \mathbb{R}^{L+1} \) such that

\[
V(U) |0, \chi_k\rangle = \sqrt{\frac{1 + f(\tau_k)}{2}} |0, \chi_k\rangle + \sqrt{\frac{1 - f(\tau_k)}{2}} |1, \chi_k\rangle \ .
\]  

(B.3)

Denote \( \varepsilon_k := \frac{1}{2} |f(\tau_k) - \text{sqw}(\tau_k)| \). For \( \tau_k \in (-\pi + \Delta, -\Delta) \),

\[
V(U) |0, \chi_k\rangle = \sqrt{\varepsilon_k} |0, \chi_k\rangle + \sqrt{1 - \varepsilon_k} |1, \chi_k\rangle ;
\]  

(B.4)

and for \( \tau_k \in [\Delta, \pi - \Delta) \),

\[
V(U) |0, \chi_k\rangle = \sqrt{1 - \varepsilon_k} |0, \chi_k\rangle + \sqrt{\varepsilon_k} |1, \chi_k\rangle .
\]  

(B.5)

Since \( |f(x) - \text{sqw}(x)| < \varepsilon \) on the \( (-\pi + \Delta, -\Delta) \cup [\Delta, \pi - \Delta) \), we have \( \varepsilon_k < \varepsilon \) for each \( \tau_k \in (-\pi + \Delta, -\Delta) \cup [\Delta, \pi - \Delta) \).
2. Phase interval search

The phase interval is the region containing the eigenphase of the input state. According to Lemma 7, the main idea is to iteratively shrink the phase interval by the binary search method. At each iteration, we can decide the next subinterval, either \((-\pi + \Delta, -\Delta]\) or \([\Delta, \pi - \Delta]\), depending on the measurement result of the ancilla qubit. As \(\Delta\) is small, the length of the interval reduces by nearly half, and thus the size of which would exponentially converge to \(2\Delta\).

Formally, let \(U\) be a unitary, \(\Delta \in (0, \frac{\pi}{2})\) and \(\varepsilon \rightarrow 0\) (detailed analysis of success probability is discussed in section B 3). Suppose \(V(\cdot)\) is the quantum circuit stated in Lemma 7 with respect to \(\Delta\) and \(\varepsilon\). Denote \(G := [-\pi, -\pi + \Delta] \cup [-\Delta, \Delta] \cup [\pi - \Delta, \pi]\) as the area that produces garbage information. Then for any quantum state \(|\psi\rangle = \sum_{j=0}^{2^n-1} c_j |x_j\rangle\) and \(\zeta \in [-\pi, \pi]\), we have

\[
V(e^{-i\zeta}U) |0, \psi\rangle = |0\rangle \left( \sum_{j: \Delta < \tau_j < -\pi - \Delta} c_j |x_j\rangle + \sum_{j: \tau_j < \zeta \in G} g_j^{(0)} |x_j\rangle \right)
+ |1\rangle \left( \sum_{j: -\pi + \Delta < \tau_j < -\zeta < \Delta} c_j |x_j\rangle + \sum_{j: \tau_j < -\zeta \in G} g_j^{(1)} |x_j\rangle \right),
\]

where \(g_j^{(i)}\) are garbage coefficients corresponding to state \(|i\rangle\) of the ancilla qubit. Consequently, the measurement of the ancilla qubit can identify the interval containing the remaining eigenphases of measured state. Note that above approach is no longer applicable if the length of interval is close to \(2\Delta\), in which case \(\tau_j - \zeta\) will always fall into the garbage area \(G\). Such interval is referred to be “indistinguishable”. We could iteratively apply the binary search procedure to shrink the phase interval until it becomes indistinguishable. The following corollary guarantees that Algorithm 1 can reduce the length of input interval close to \(2\Delta\) with high probability.

**Lemma S4** Suppose \(\Delta, \varepsilon\) and \(Q\) are inputs of Algorithm 1, then the algorithm output an interval \([\zeta_l, \zeta_r]\) such that \(|\zeta_r - \zeta_l| = 2(\Delta + \frac{\pi}{2^Q})\) and \(\tau \in [\zeta_l, \zeta_r]\) with probability at least \((1 - \varepsilon)^Q\).

**Proof** Denote \([\zeta_l^{(j)}, \zeta_r^{(j)}]\) as the interval generated at the end of the \(j\)-th iteration and \(c_m^{(j)}\) as the middle point of this interval. Observe that for \(j > 0\), the interval generated at the end of the \(j + 1\)-th iteration is either \((\zeta_l^{(j)} - \Delta, \zeta_r^{(j)} + \Delta)\) or \((\zeta_r^{(j)} - \Delta, \zeta_l^{(j)} + \Delta)\). By induction we have

\[
|c_r^{(Q)} - c_l^{(Q)}| = \Delta + \frac{|c_r^{(Q-1)} - c_l^{(Q-1)}|}{2} = \Delta + \frac{1}{2} \left( \Delta + \frac{|c_r^{(Q-2)} - c_l^{(Q-2)}|}{2} \right)
\]

\[
= \Delta + \frac{\Delta}{2} + \frac{\Delta}{2^2} + \ldots + \frac{\Delta}{2^{Q-1}} + \frac{|c_r^{(0)} - c_l^{(0)}|}{2^Q}
\]

\[
= \Delta \left( 1 - 2^{-Q} \right) \frac{2^Q}{2} + \frac{2\Delta + \pi}{2^Q}
\]

\[
= 2\Delta + \frac{\pi}{2^Q}.
\]

as required. By Lemma 7, the probability of failing to decide the correct subinterval is at most \(\varepsilon\) in each iteration, thus the success probability of outputting an phase interval containing \(\tau\) is at least \((1 - \varepsilon)^Q\).

3. Phase search through interval amplification

Let \(\bar{\Delta} := \Delta + \frac{\pi}{2^Q}\), merely applying Algorithm 1 will not provide an estimate within expected precision, given that the error is at most the \(2\bar{\Delta}\). To address this issue, the main idea is to execute the phase interval search procedure on \((e^{i\zeta}U)^d\) for some appropriate integer \(d\) so that the binary search procedure can continue to locate the amplified phase \(d\tau \in [d\zeta_l, d\zeta_r]\), since the interval length is \(2d\bar{\Delta} \gg 2\bar{\Delta}\). Repeating the entire procedure can exponentially reduce estimation error.

Let us formally describe the entire procedure. In the first round of phase interval search, the initial phase interval is \([-\pi, \pi]\).

We iteratively apply QPP \(V(\cdot)\) on the target unitary \(U^{(0)} = U\) to obtain a phase interval \([\zeta_l^{(0)}, \zeta_r^{(0)}]\) of length \(2\bar{\Delta}\). We denote \(\zeta_m^{(0)} := (\zeta_l^{(0)} + \zeta_r^{(0)})/2\) the middle point of the interval. Let \(d := \lfloor 1/\bar{\Delta} \rfloor\), then we construct a unitary as \(U^{(1)} = (e^{-i\zeta_m^{(0)}}U^{(0)})^d\) so that the interval the amplified phase \(d\tau\) are rescaled to \([-1, 1]\). Therefore, we can run the phase interval search procedure on \(U^{(1)}\) to retrieve a new interval \([\zeta_l^{(1)}, \zeta_r^{(1)}]\) of length \(2\bar{\Delta}\). Repeating the entire procedure above gives an estimation of phase \(\tau\) up to required precision.
Now we analyze how above procedures improve the eigenphase estimation precision. For the target eigenphase $\tau$ of the input unitary $U$, the corresponding phase of unitary $U^{(1)}$ is $d(\tau - \zeta_m^{(0)}) \in [\zeta_m^{(1)}, \zeta_m^{(1)}]$. Let $\zeta_m^{(1)} = (\zeta_m^{(1)} + \zeta_m^{(1)})/2$ denote the middle point of the second interval $[\zeta_m^{(1)}, \zeta_m^{(1)}]$. Then we can readily give an inequality that characterizes the estimation error,

$$\left| \zeta_m^{(1)} - d(\tau - \zeta_m^{(0)}) \right| \leq \bar{\Delta}. \quad \text{(B.11)}$$

We further rewrite this inequality as below,

$$\left| \tau - \left( \zeta_m^{(0)} + \frac{\zeta_m^{(1)}}{d} \right) \right| \leq \frac{\bar{\Delta}}{d} \leq d^{-2}. \quad \text{(B.12)}$$

From this equation, we can see that this scheme gives an estimate of eigenphase with an error of $d^{-2}$. After repeating the procedure for sufficiently many times, we inductively obtain a sequence $(\zeta_m^{(0)}, \zeta_m^{(1)}, \cdots)$ that could be taken as an estimate of the eigenphase. Therefore, the estimation error will exponentially decay as iterating. For instance, assuming our scheme executes $T$ times, it will inductively give an estimate as follows.

$$\left| \tau - \left( \zeta_m^{(0)} + \frac{\zeta_m^{(1)}}{d} + \frac{\zeta_m^{(2)}}{d^2} + \cdots + \frac{\zeta_m^{(T-1)}}{d^{T-1}} \right) \right| \leq \frac{\bar{\Delta}}{d^{T-1}} \leq d^{-T}. \quad \text{(B.13)}$$

Note that $d = \lceil 1/\bar{\Delta} \rceil$ must be at least 2, otherwise we cannot find a sequence that converges to the eigenphase. Also, if the estimation precision is expected to be $\delta$, then $T$ should satisfy $d^{-T} \leq \delta$. Then it derives that

$$Q = \left\lceil \log \left( \frac{2\pi}{1 - 2\bar{\Delta}} \right) \right\rceil \quad \text{and} \quad T = \left\lceil \frac{\log(\frac{1}{\delta})}{\log(d)} \right\rceil. \quad \text{(B.14)}$$

The entire phase search procedure executes the phase interval search, i.e. Algorithm 1, for $T$ times. Then by Lemma S4, the success probability of the entire phase search procedure is $(1 - \eta)^{QT}$, where $\eta$ is the input threshold of Algorithm 1. For any $\varepsilon \in (0, 1)$, let $\eta = \frac{\varepsilon}{QT}$, then the total success probability is

$$Q^T > 1 - QT \eta = 1 - \varepsilon, \quad \text{(B.15)}$$

where the first strict inequality is the Bernoulli’s inequality for $\eta < 1$ and $QT \geq 2$. By Lemma 7, to ensure the success probability of the entire algorithm is at least $1 - \varepsilon$, the number of QPP layers $L$ should be

$$L = \mathcal{O} \left( \frac{1}{\Delta} \log \frac{QT}{\varepsilon} \right) = \mathcal{O} \left( \frac{1}{\Delta} \log \frac{1}{\varepsilon} + g(\Delta) \right). \quad \text{(B.16)}$$

Here $g(\Delta)$ is a function in terms of $\Delta$ only, and hence can be omitted in the complexity analysis of Theorem 8.

Overall, by running the scheme many times, we can find an estimate of eigenphase with precision $\delta$ and success probability at least $1 - \varepsilon$. Above results are summarized in Algorithm 2.

4. Proof of Theorem 8

**Theorem 8 (Complexity of Quantum Phase Search)** Given an $n$-qubit unitary $U$ and an eigenstate $|\chi\rangle$ of $U$ with eigenvalue $e^{i\tau}$, Algorithm 2 can use one ancilla qubit and $\mathcal{O} \left( \frac{1}{\Delta} \log \left( \frac{\log \frac{1}{\epsilon}}{\log \frac{1}{\delta}} \right) \right)$ queries to controlled-$U$ and its inverse to obtain an estimation of $\tau$ up to $\delta$ precision with probability at least $1 - \varepsilon$.

**Proof** We analyze the number of queries to the controlled-$U$ oracle in Algorithm 2 to get an estimate within required precision $\delta > 0$, probability of failure $\varepsilon > 0$ and input $\Delta$. Note that $\Delta$ is a self-adjusted parameter and hence can be considered as a constant in complexity analysis.

Observe that Algorithm 2 executes the phase interval search procedure $T$ times, while the $t$-th phase interval search procedure requires $Q$ calls of circuit $V(U^{d^t})$ of $L$ layers. By Eq. (B.14) and Eq. (B.16), the total query complexity of the controlled-$U$ oracle is

$$\sum_{t=0}^{\tau-1} Q \times d^t \times L = \mathcal{O}(d^T L Q) = \mathcal{O} \left( \frac{1}{\Delta} \log \left( \frac{\log \frac{1}{\epsilon}}{\log \frac{1}{\delta}} \right) \log \left( \frac{2\pi}{1 - 2\bar{\Delta}} \right) \right) = \mathcal{O} \left( \frac{1}{\Delta} \log \left( \frac{1}{\epsilon} \log \frac{1}{\delta} \right) \right). \quad \text{(B.17)}$$
5. Application: period finding and factoring

In this section, we consider applying the quantum phase search algorithm to solve the period-finding problem. The goal of period-finding is to find the smallest integer \( r \) (namely the order) of a given element \( x \) in the rings of integers modulo \( N \in \mathbb{N} \) such that \( x^r \equiv 1 \pmod{N} \).

In the quantum setting, the problem of reversible quantum modular multiplier has been well-studied \([50, 51]\). It has been proved that the quantum operator

\[
U_x |y \mod N \rangle = |xy \mod N \rangle, \quad y \in \mathbb{Z}/N\mathbb{Z}
\]

(B.18)
can be constructed in cubic resources for every integer \( x \in \mathbb{Z}/N\mathbb{Z} \). A novel property of such modular multiplier is that there is no additional quantum cost to realize a power of \( U_x \) since \( U_x^r = U_x \). Moreover, an eigenvector of \( U_x \) is in form

\[
|u_s\rangle := \frac{1}{\sqrt{r}} \sum_{k=0}^{r-1} \exp \left( \frac{2\pi isk}{r} \right) |x^k \mod N\rangle
\]

(B.19)
corresponding to its eigenphase \( \frac{2\pi s}{r} \), and the uniform superposition of all eigenvectors is \( |1\rangle \), i.e. \( |1\rangle = \frac{1}{\sqrt{r}} \sum_{s=0}^{r-1} |u_s\rangle \).

The conventional quantum period-finding algorithm is to apply the quantum phase estimation algorithm to the modular multiplier with input state \( |1\rangle \), then use the continued fraction algorithm to extract the order from the estimated phases. Similarly, we use the quantum phase search algorithm to extract eigenphases of the modular operator. The details of the algorithm are shown below.

**Algorithm 4 Quantum Period Finding Algorithm**

**Require:** \( N \in \mathbb{Z}, x \in \mathbb{Z}/N\mathbb{Z}, \) constant \( \Delta \in (0, \frac{1}{2}) \) and error tolerance \( \varepsilon, \delta > 0 \).

**Ensure:** order \( r \) of \( x \) in \( \mathbb{Z}/N\mathbb{Z} \).
1. Construct the modular multiplier \( U_x \) by \( x \) and \( N \).
2. Retrieve an estimated eigenphase \( \tau \) of \( U_x \) by the QPS algorithm. That is, \( \tau \leftarrow \text{QPS}(U_x, |1\rangle, \Delta, \varepsilon, \delta) \).
3. Apply continued fractional algorithm on \( \tau \) to retrieve \( l \) and \( r \); return \( r \).

6. Application: amplitude estimation

The problem of quantum amplitude estimation (QAE) can be efficiently solved by the phase estimation algorithm \([27]\), providing a quadratic speedup over classical Monte Carlo methods. In recent years, several studies \([35, 52-54]\) can realize phase-estimation-free amplitude estimation with same quantum speedup. However, these works require large number of samplings i.e. measurements from quantum circuits. Here we show that our phase search algorithm can also apply to the amplitude estimation and inherit the computational advantage from conventional phase estimation.

Let \( \mathcal{A} \) denote a quantum circuit that acts on \( n \) qubits. Applying the circuit \( \mathcal{A} \) to \( |0^n\rangle \), the produced state is of the following form:

\[
\mathcal{A} |0^n\rangle = \cos(\tau) |0\rangle |\psi\rangle + \sin(\tau) |1\rangle |\phi\rangle.
\]

(B.20)
where \( |\psi\rangle \) and \( |\phi\rangle \) are \((n-1)\)-qubit states, and \( \tau \in (-\pi, \pi) \) is the phase. Here, \( \cos(\tau) \) and \( \sin(\tau) \) denote the amplitude of states \( |\psi\rangle \) and \( |\phi\rangle \), respectively. Our goal is to estimate \( |\sin(\tau)| \) up to a given precision with high probability.

Suppose we can repeatedly apply the circuit \( \mathcal{A} \) and its inverse \( \mathcal{A}^\dagger \). Then we can construct a circuit for the Grover operator

\[
G = \mathcal{A}(2|0^n\rangle \langle 0^n| - I^\otimes n) \mathcal{A}^\dagger \cdot (I - 2|1\rangle \langle 1|) \otimes I^\otimes (n-1).
\]

(B.21)
Note that, in the space spanned by \( \{|0\rangle \langle \psi|, |1\rangle \langle \phi|\} \), the Grover operator \( G \) has an eigenphase \( 2\tau \) or \(-2\tau \). Thus our amplitude estimation algorithm just applies the quantum phase search algorithm to Grover operator. Specifically, applying our quantum phase search algorithm can effectively extract eigenphases \( \pm 2\tau \). Moreover, post-processing can estimate the amplitude within the required precision. We show more details below.
Algorithm 5 Quantum Amplitude Estimation Algorithm

Require: circuit $A$, constant $\Delta \in (0, \frac{1}{4})$ and error tolerance $\epsilon, \delta > 0$.
Ensure: an amplitude $|\sin(\tau)|$.
1: Prepare the initial state $|\chi\rangle = A |0\rangle^\otimes n$ and construct the Grover operator $G$ in equation (B.21).
2: Retrieve an estimated eigenphase $\hat{\tau}$ of $G$ by the QPS algorithm. That is, $\hat{\tau} \leftarrow \text{QPS}(G, |\chi\rangle, \Delta, \epsilon, \delta)$.
3: Return $|\sin(\hat{\tau})|.$

Appendix C: Further Review for Block Encoding

1. Qubitization

In this section we review the technique of qubitization purposed by [7]. Such technique associates the spectrum of target block encoding $U_A$ with the block encoded matrix $A$. Assume $A$ is Hermitian with $||A|| \leq 1$, since our work only deal with Hamiltonians and density operators. Recent work has discussed an explicit construction scheme for building a block encoding sparse matrices [55]. To better understand qubitization, we analyze the spectral information of the circuit in Fig. S1.

![Circuit diagram](image)

Fig S1: Circuit realization for the qubitized unitary $\tilde{U}_A$. Here $U_A$ is a $(n + m)$-qubit block encoding of $n$-qubit matrix $A$, and the gate REFLECTOR is equivalent to $2(|0\rangle^\otimes (m+1))\langle 0| - I^\otimes (m+1)$. Note that it suffices to control the REFLECTOR and three X gates to realize controlled-$\tilde{U}_A$.

Let $\tilde{U}_A$ denotes the qubitization of block encoding unitary $U_A$ and $\tilde{U}_A$ denotes the unitary for dashed region in Fig. S1. Then Lemma 10 of [7] implies that $\tilde{U}_A$ satisfies

$$\langle 0^\otimes (m+1) I^\otimes n \rangle \tilde{U}_A$$

$$\langle 0^\otimes (m+1) I^\otimes n \rangle \tilde{U}_A^2$$

(C.1)

(C.2)

Let $|\psi_\lambda\rangle$ be an eigenstate of $A$ corresponding to its eigenvalue $\lambda$. Denote $|\tilde{\psi}_\lambda\rangle := |0^\otimes (m+1), \psi_\lambda\rangle$. After applying $\tilde{U}_A$ and $\tilde{U}_A^2$ to $|\psi_\lambda\rangle$ respectively, states are of the following form:

$$\tilde{U}_A |\psi_\lambda\rangle = \lambda |\tilde{\psi}_\lambda\rangle + \sqrt{1 - \lambda^2} |\perp_\lambda\rangle,$$

$$\tilde{U}_A^2 |\psi_\lambda\rangle = |\psi_\lambda\rangle,$$

(C.3)

(C.4)

where $|\perp_\lambda\rangle$ is an orthogonal state and satisfies $(|0^\otimes (m+1)\rangle|0^\otimes (m+1)\rangle \otimes I^\otimes n |\perp_\lambda\rangle = 0$. Above results also imply that all subspaces $\text{span}\{|\psi_\lambda\rangle, |\perp_\lambda\rangle\}$ are mutually perpendicular. Moreover, Eq. (C.4) implies

$$\tilde{U}_A |\perp_\lambda\rangle = \sqrt{1 - \lambda^2} |\tilde{\psi}_\lambda\rangle - \lambda |\perp_\lambda\rangle.$$

(C.5)

Note that it suffices to analyze $\tilde{U}_A$ under subspace

$$\mathcal{H}_A := \bigoplus_\lambda \text{span}\{|\psi_\lambda\rangle, |\perp_\lambda\rangle\},$$

(C.6)

since the input state of ancilla qubits is always $|0^\otimes (m+1)\rangle$. In this subspace, we can see that $\tilde{U}_A$ is essentially a rotation whose matrix is similar to $R_V$, i.e.

$$\tilde{U}_A = (\text{REFLECTOR} \otimes I^\otimes n) \cdot \tilde{U}_A = \bigoplus_\lambda \left[ \begin{array}{cc} \lambda & -\sqrt{1 - \lambda^2} \\ \sqrt{1 - \lambda^2} & \lambda \end{array} \right] |\psi_\lambda\rangle, |\perp_\lambda\rangle \bigoplus \cdots |\mathcal{H}_A\rangle.$$

(C.7)
The spectral details of \( \hat{U}_A \) in \( \mathcal{H} \) follow immediately:

\[
\begin{align*}
\text{eigenvector } & |\chi^+_\lambda\rangle = \frac{1}{\sqrt{2}}(|\tilde{\psi}_\lambda\rangle + i|\tilde{\Lambda}_\lambda\rangle), \quad \text{eigenvector } e^{+i\tau_\lambda}, \text{ where } \lambda = \cos(\tau_\lambda); \\
\text{eigenvector } & |\chi^-_\lambda\rangle = \frac{1}{\sqrt{2}}(|\tilde{\psi}_\lambda\rangle - i|\tilde{\Lambda}_\lambda\rangle), \quad \text{eigenvector } e^{-i\tau_\lambda}, \text{ where } \lambda = \cos(-\tau_\lambda).
\end{align*}
\]

(C.8)

Therefore, we can select \( \hat{U}_A \) as the input unitary in the QPP circuit, to access the cosine of eigenvalues of \( A \), allowing phase evolution and evaluation to be applied on block encoded matrices.

### 2. Block encoding construction for density matrices

The quantum purification model, which prepares a purification of a mixed state \( \rho \), is an extensively explored model for entropy in the literature. Consider quantum registers \( A \) and \( B \) storing \( n \) and \( n' \) qubits, respectively. Suppose we have accessed to a \((n + n')\)-qubit unitary oracle \( U_\rho \) acting on these two registers, such that

\[
|\Psi\rangle_{AB} := U_\rho |0^{\otimes n}\rangle_A |0^{\otimes n'}\rangle_B \quad \text{and} \quad \text{tr}_B(|\Psi\rangle_{AB} \langle \Psi|_{AB}) = \rho.
\]

(C.9)

Such oracle can be further employed to construct a block encoding \( \hat{U}_\rho \) of \( \rho \). We recall Lemma 7 in [7] and give the circuit construction for \( \hat{U}_\rho \) in Fig. S2, using \( U_\rho \) and \( U_\rho^\dagger \) once.

![Circuit realization for \( \hat{U}_\rho \). The input state for two ancilla registers is \( |0^{\otimes(n+n')}\rangle_{AB} \). Here SWAP is a 2n-qubit swap operator and REFLECTOR is equivalent to \( 2(|0^{\otimes(n+n')}\rangle \langle 0^{\otimes(n+n')}| - I^{\otimes(n+n')} \). Note that it suffices to control the SWAP and REFLECTOR gates to realize controlled-\( \hat{U}_\rho \).](attachment:Fig_S2.png)

Fig S2: Circuit realization for \( \hat{U}_\rho \). The input state for two ancilla registers is \( |0^{\otimes(n+n')}\rangle_{AB} \). Here SWAP is a 2n-qubit swap operator and REFLECTOR is equivalent to \( 2(|0^{\otimes(n+n')}\rangle \langle 0^{\otimes(n+n')}| - I^{\otimes(n+n')} \). Note that it suffices to control the SWAP and REFLECTOR gates to realize controlled-\( \hat{U}_\rho \).

Note that the unitary \( \tilde{U}_\rho \) for the dashed region in Fig. S2 satisfies

\[
\begin{align*}
(\langle 0^{\otimes(n+n')}|_{AB} \otimes I^{\otimes n}) \tilde{U}_\rho (\langle 0^{\otimes(n+n')}|_{AB} \otimes I^{\otimes n}) &= \rho, \quad \text{(C.10)} \\
(\langle 0^{\otimes(n+n')}|_{AB} \otimes I^{\otimes n}) \tilde{U}_\rho^2 (\langle 0^{\otimes(n+n')}|_{AB} \otimes I^{\otimes n}) &= I^{\otimes n}. \quad \text{(C.11)}
\end{align*}
\]

Denote \( \{p_j\}_{j=0}^{2^n-1} \) as the set of eigenvalues of \( \rho \), and \( \{\tau_j\}_{j=0}^{2^n-1} \) as the set of eigenphases of \( \hat{U}_\rho \) under subspace \( \mathcal{H}_\rho \) defined in Eq. (C.6). Through same reasoning in Appendix C 1, we have

\[
\{\tau_j\}_{j=0}^{2^n-1} = \{\arccos(p_j), -\arccos(p_j)\}_{j=0}^{2^n-1}. \quad \text{(C.12)}
\]

As shown above, the spectrum of \( \hat{U}_\rho \) is connected with that of \( \rho \) in subspace \( \mathcal{H}_\rho \).

### Appendix D: Further Discussion for Hamiltonian Problems

#### 1. Hamiltonian simulation

In this section, we explain the main idea of our method for Hamiltonian simulation and discuss how to find parameters for simulating the target function \( f(x) \). For convenience, let \( \hat{U}_H \) denote the qubitized block encoding of a Hamiltonian \( H \).

Prepare the initial state \( |0^{\otimes(m+2)}, \psi\rangle \), where the first one is the ancilla qubit of QPP, and the other \( m + 1 \) qubits are ancilla qubits of the qubitized block encoding \( \hat{U}_H \). Decompose the initial state \( |0^{\otimes(m+2)}, \psi\rangle \) by eigenvectors of the Hamiltonian.

\[
|0\rangle |0^{\otimes(m+1)}, \psi\rangle = \sum_{\lambda} \beta_\lambda |0\rangle |0^{\otimes(m+1)}, \psi_\lambda\rangle. \quad \text{(D.1)}
\]
where $\sum_\lambda |\beta_\lambda|^2 = 1$. As shown in Eq. (C.7), the qubitized block encoding $\hat{U}_H$ is a rotation in each subspace $\text{span}\{ |0^{\otimes (m+1)}\rangle, |\psi_\Lambda\rangle, |\Lambda_\lambda\rangle \}$. Then we construct the circuit of Hamiltonian simulation by incorporating $\hat{U}_H$ into the framework of QPP. Note that one eigenvalue of the Hamiltonian corresponds to two eigenvalues of $\hat{U}_H$, and then the action of the circuit can be described as the matrix below, with respect to the basis $\{ |0, \chi_\Lambda\rangle, |1, \chi_\Lambda\rangle \}$ for each eigenvalue $\lambda$.

$$
\bigoplus_\lambda \left( \begin{array}{cc}
P(\tau_\lambda) & -Q(\tau_\lambda) \\
 \lambda^* Q(\tau_\lambda) & P^*(\tau_\lambda)
\end{array} \right)_\lambda.
$$

(D.2)

On the other hand, note that each state $|0^{m+1}, \psi_\Lambda\rangle$ can be written as an equal-weighted sum of eigenvectors of $\hat{U}_H$, implying the following equation.

$$
\frac{1}{\sqrt{2}} \left[ \frac{1}{\sqrt{2}} |0\rangle \langle 0| + \frac{1}{\sqrt{2}} |0\rangle \langle 1| \right] \left( |0^{\otimes (m+1)}, \psi_\Lambda\rangle + i |1^{\otimes (m+1)}, \psi_\Lambda\rangle \right).
$$

(D.3)

Using Eq. (D.3), we thus rewrite the initial state as a superposition of eigenvectors of $\hat{U}_H$. With the decomposition in Eq. (D.2), applying QPP to the state $|0^{m+2}, \psi\rangle$ outputs a state of the following form

$$
\sum_\lambda \frac{\beta_\lambda}{\sqrt{2}} \left( |0\rangle + Q^*(\tau_\lambda)|1\rangle \right) |0^{\otimes (m+1)}, \psi_\Lambda\rangle + \frac{P(\tau_\lambda)}{\sqrt{2}} |0\rangle + Q^*(-\tau_\lambda)|1\rangle |0^{\otimes (m+1)}, \psi_\Lambda\rangle - i |1^{\otimes (m+1)}, \psi_\Lambda\rangle \right).
$$

(D.4)

The output state is near the target state as much as possible by suitably truncating the target function. In fact, the difference between the final output state and the target state is bounded by the quantity below.

$$
\text{error} \leq \left( \max_{x \in [-\pi, \pi]} \left| (P(x)|0\rangle + Q^*(x)|1\rangle) - e^{-i\cos(x)t}|0\rangle \right| \right) \leq \left( \frac{\pi}{\sqrt{2}} \right)^{m+2} \left( \max_{x \in [-\pi, \pi]} \sqrt{|P(x)|^2 + 1 - \frac{2\cos(x)t}{\sqrt{2}} |P(x)|^2} \right) \leq 2\epsilon.
$$

(D.5)

Let $a_x = P(x) - e^{-i\cos(x)t}$ denote the difference, and assume that $|a_x| \leq \epsilon$ for all $x \in [-\pi, \pi]$. Then we show how large $|P(x)|^2$ is.

$$
|a_x|^2 = (P(x) - e^{-i\cos(x)t})(P^*(x) - e^{i\cos(x)t}) \Rightarrow |P(x)|^2 = 2\text{Re}(e^{i\cos(x)t}P(x)) + |a_x|^2 \geq 1 - 2|a_x| + |a_x|^2 = (1 - |a_x|^2).
$$

(D.6)

The state approximation error is at most as large as

$$
\text{error} \leq \left( \frac{\max_{x \in [-\pi, \pi]} \sqrt{|a_x|^2 + 1 - (1 - |a_x|^2)}^2 \leq \sqrt{2}\epsilon. \right)
$$

(D.7)

Hence, Eq. (D.9) establishes the relation between the state approximation and the function approximation.

The remaining is to show $P(x)$ can approximate $f(x) = e^{-i\cos(x)t}$ with arbitrary precision, which is true since $f(x)$ could be expanded into a trigonometric polynomial. We summarize the results in the following theorem and discuss how to truncate $f(x)$ in the proof.

**Theorem 9** Given a block encoding $U_H$ of $H/\Lambda$ for some $\Lambda \geq ||H||$, there exists an algorithm that simulates evolution under the Hamiltonian $H$ for time $t \in \mathbb{R}$ with precision $\delta > 0$, using two ancilla qubits and querying controlled-$U_H$ and controlled-$U_H^\dagger$ for a total number of times in

$$
\Theta \left( \Lambda |t| + \frac{\log(2/\delta^2)}{\log \left( \frac{1 + \log(2/\delta^2)}{\Lambda |t|} \right)} \right).
$$

Proof** By Theorem 5, QPP can simulate any trigonometric polynomial with an order $N$. Thus we just need to find such a polynomial that approximates the function $f(x) = e^{-i\cos(x)t}$ within the precision $\delta^2/2$. We recall the Jacobi-Anger expansion $e^{iz \cos(\theta)} = \sum_{k=-\infty}^{\infty} i^k J_k(z) e^{ik\theta}$ [56], where $J_k(z)$ is the $k$-th Bessel function of the first kind. The truncation error of the Jacobi-Anger expansion has been well-studied in the literature [4, 57]. Given the truncation error $\delta^2/2$, the order $N$ is given by

$$
N = \Theta \left( |z| + \frac{\log(2/\delta^2)}{|z|} \right).
$$

(D.10)

Then QPP circuit uses $N$ times controlled $U_H$ and $U_H^\dagger$. Recall that the evolution time is $t\Lambda$, thus we set the parameter $z = t\Lambda$. Clearly, the cost of the circuit is the same as claimed, and the proof is finished. ■
2. Hamiltonian eigensolver

A fundamental problem in physics is to calculate static properties of a quantum system. Of all the questions which one might ask about a quantum system, there is one most frequently asked: what are the energy and eigenstates of a Hamiltonian? After the development of quantum phase estimation, numerous quantum algorithms for computing the spectrum of a Hamiltonian have been developed. Clearly, we could just direct apply our phase search algorithm in a similar spirit to give quantum algorithms for extracting Hamiltonian eigen-information. To this end, we describe several quantum algorithms based on quantum phase estimation below.

The quantum algorithm proposed by Abrams and Lloyd [58] computes the eigenstates and eigenvalues of a Hamiltonian via applying quantum phase estimation to the simulated real-time evolution operator, resulting in exponential speedups over known classical methods. Under post-selection of the ancilla register, this approach can output the spectrum by reading an eigenvalue and obtaining the corresponding eigenvector. Despite being conceptually simple, the technical realization of the eigenvalue transformation of unitary matrices, which could be naturally generalized into the framework of QPP, implementation challenging.

In fact, the use of the time evolution operator is not necessary for phase estimation. Recent work by Poulin et al. [59] proposed a method that extracts the spectrum of a Hamiltonian \( H \) from a qubitized block encoding of \( H/\Lambda \). The idea is to estimate a phase of the qubitized block encoding \( \hat{U} \) then directly calculate the corresponding eigenvalue of \( H \) by the relationship between their spectrum, i.e. \( \lambda = \Lambda \cos(\tau_\lambda) \). To achieve the desired precision \( \delta \), one needs to apply the block encoding for \( \mathcal{O}(\Lambda/\delta) \) times.

Moreover, the eigenvector of the Hamiltonian can be extracted from the post-measurement state of quantum phase estimation. Specifically, suppose we obtain an eigenvector \( |\chi_\lambda^+\rangle = \frac{1}{\sqrt{2}}(|0\rangle \otimes (|\psi_\lambda\rangle + i|\downarrow_\lambda\rangle) \) by phase estimation. Since \( (|0\rangle \otimes (|m\rangle + |m+1\rangle) \otimes f^{n+1}) |\downarrow_\lambda\rangle = 0 \), we directly measure the ancilla register of the qubitized block encoding in the computational basis. Clearly, the probability of receiving all zeros from the measurement is exactly half, and the post-measurement state is the corresponding eigenvector. If the result is not as expected, we could re-apply the phase estimation and repeat the measurement, projecting the state into \( |\lambda^+_\rangle \) or \( |\lambda^-\rangle \). Repeating for \( k \) times makes the failure probability decay exponentially as \((1/2)^k\).

Another important Hamiltonian problem is to compute ground and excited state properties of many-body systems, which is quite a challenge in quantum physics and quantum chemistry. Recently, Dong et al. [17] proposed a method via quantum eigenvalue transformation of unitary matrices, which could be naturally generalized into the framework of QPP.

Appendix E: Theorems of Entropy Estimation

1. Proof of Theorem 10

**Theorem 10** Let \( |\Psi_\rho\rangle_{AB} \) be a purification of an \( n \)-qubit state \( \rho \) and \( \hat{U}_\sigma \) be a qubitized block encoding of an \( n \)-qubit state \( \sigma \) with \( m \) ancilla qubits. For any real-valued polynomial \( f(x) = \sum_{k=0}^L c_j x^k \) with \( ||c||_1 \leq 1 \), there exists a QPP circuit \( \mathcal{V}(\hat{U}_\sigma) \) of \( L \) layers such that

\[
\langle Z^{(0)} \rangle_{|\Phi\rangle} = \text{tr} \left( \rho f(\sigma) \right),
\]  

where \( |\Phi\rangle = (\mathcal{V}(\hat{U}_\sigma) \otimes I_B) |0\rangle \otimes |\Psi_\rho\rangle_{AB} \) and the polynomial on a quantum state is defined as \( f(\sigma) = \sum_{k=0}^L c_j \sigma^k \).

**Proof** We start with the spectral decomposition of \( \sigma \) and \( \hat{U}_\sigma \) under subspace \( \mathcal{H}_\sigma \) defined in Eq. (C.6). From equation Eq. (C.8) we have

\[
\sigma = \sum_{j=0}^{2^n-1} q_j |\psi_j\rangle \langle \psi_j|,
\]  

\[
\hat{U}_\sigma = \bigoplus_{j=0}^{2^n-1} \left[ \begin{array}{cc} e^{i\tau_j} & 0 \\ 0 & e^{-i\tau_j} \end{array} \right] \{|\chi_j^+\rangle, |\chi_j^-\rangle\} \oplus \cdots \otimes \mathcal{H}_\perp,
\]

where \( \tau_j = \arccos(q_j) \), and \( |\chi_j^\pm\rangle \) are eigenstates of \( \hat{U}_\sigma \) such that

\[
|\chi_j^+\rangle = \frac{1}{\sqrt{2}}(|\psi_j\rangle + i|\downarrow_j\rangle);
|\chi_j^-\rangle = \frac{1}{\sqrt{2}}(|\psi_j\rangle - i|\downarrow_j\rangle)
\]  

(E.4)
for some quantum state $|\hat{\rho}_j\rangle$ (defined in Appendix C 1) so that $(|0\rangle\langle0|^{\otimes m} \otimes I^{\otimes n}) |\hat{\rho}_j\rangle = 0$. Also, note that $|0\rangle\langle0|^{\otimes m} \otimes \rho$ is a density matrix in $\mathcal{H}_0$ and hence can be decomposed by the basis $\{|\chi_j^\pm\rangle\}_{j=0}^{2^n-1}$. Now we are ready to analyze the effect of QPP on the input state. Define the function $F(x) = \sum_{k=-L}^{L} d_k e^{ikx} := f(\cos(x))$. Note that $\|e\|_1 \leq 1$ implies $\|d\|_1 \leq 1$.

Suppose the input state is a purified state $|\Psi_\rho\rangle_{AB}$ so that $\tr_B(|\Psi_\rho\rangle_{AB}) = \rho$. Here, the register $A$ is the main register of the QPP circuit. By Schmidt decomposition, there exists an orthonormal set $\{|\phi_j\rangle\}_{j=0}^{2^n-1}$ of quantum states on register $B$ such that

$$|\Psi_\rho\rangle_{AB} = \sum_{j=0}^{2^n-1} \sqrt{p_j} |\psi_j\rangle_A |\phi_j\rangle_B.$$  \hspace{1cm} (E.5)

From Theorem 6, there exists a QPP circuit $V(\hat{U}_\sigma \otimes I_B)$ of $L$ layers such that

$$\langle Z^{(0)} \rangle_\psi = \tr \left[ (Z^{(0)} \otimes I^{\otimes(m+n)} \otimes I_B) \cdot |\Phi\rangle \langle \Phi | \right]$$

$$= \sum_{j=0}^{2^n-1} p_j^+ F(\tau_j) + \sum_{j=0}^{2^n-1} p_j^- F(-\tau_j) = \sum_{j=0}^{2^n-1} (p_j^+ + p_j^-) f(q_j),$$  \hspace{1cm} (E.6)

where $p_j^+ = \langle \chi_j^+ | (|0\rangle\langle0|^{\otimes m} \otimes \rho) | \chi_j^+ \rangle$. Further, Eq. (E.4) implies

$$p_j^+ + p_j^- = \langle \chi_j^+ | (|0\rangle\langle0|^{\otimes m} \otimes \rho) | \chi_j^- \rangle + \langle \chi_j^- | (|0\rangle\langle0|^{\otimes m} \otimes \rho) | \chi_j^+ \rangle$$

$$= \langle \psi_j | \rho | \psi_j \rangle.$$  \hspace{1cm} (E.7)

The statement holds as

$$\langle Z^{(0)} \rangle_\psi = \sum_{j=0}^{2^n-1} \langle \psi_j | \rho | \psi_j \rangle f(q_j) = \tr (\rho f(\sigma)).$$  \hspace{1cm} (E.10)

That is, for any entropic function that is well approximated by a polynomial, we can use QPP circuits to estimate such an entropy by Theorem 10. The following result guarantees that the number of circuit layers $L$ for polynomial approximation is $O(\log \frac{1}{\varepsilon})$ up to precision $\varepsilon$.

**Lemma S5 (Corollary 66 in [4])** Let $x_0 \in [-1, 1], r \in (0, 2], \delta \in (0, r]$, and let $f : [-x_0 - r + \delta, x_0 + r + \delta] \to \mathbb{C}$ and be such that $f(x_0 + x) = \sum_{k=0}^{\infty} c_k x^k$ for all $x \in [-r - \delta, r + \delta]$. Suppose $B > 0$ is such that $\sum_{k=0}^{\infty} (r + \delta)^k |c_k| \leq B$. Let $\varepsilon \in (0, \frac{1}{27}]$, then there is an efficiently computable polynomial $P \in \mathbb{C}[x]$ of degree $O(\frac{\log B}{\delta})$ such that

- for all $x \in [-1, 1], |P(x)| \leq \varepsilon + B$ and
- for all $x \in [x_0 - r, x_0 + r], |f(x) - P(x)| \leq \varepsilon$.

### 2. Proofs for von Neumann and relative entropy estimation

**Theorem 11 (von Neumann entropy estimation)** Given a purified quantum query oracle $U_\rho$ of a state $\rho$ whose non-zero eigenvalues are lower bounded by $\gamma > 0$, there exists an algorithm that estimates $S(\rho)$ up to precision $\varepsilon$ with high probability by measuring a single qubit, querying $U_\rho$ and $U_\rho^\dagger$ for $O\left(\frac{1}{\gamma^2} \log^2 \left(\frac{1}{\varepsilon} \log \frac{1}{\gamma} / \varepsilon\right)\right)$ times. Moreover, using amplitude estimation improves the query complexity to $O\left(\frac{1}{\gamma^2} \log \left(\frac{1}{\gamma^2} \log \frac{1}{\gamma} / \varepsilon\right)\right)$.

**Proof** Denote $f(x) = \frac{\ln(x)}{2\ln(\gamma)}$. We expect to find a polynomial $P(x) \in \mathbb{R}[x]$ such that for all $x \in [\gamma, 1]$, $|P(x) - f(x)| \leq \frac{\varepsilon}{4 \ln(1/\gamma)}$.  \hspace{1cm} (E.11)

By taking $x_0 = 1, r = 1 - \gamma, \delta = \frac{\gamma}{2}$, and $B = \frac{1}{\gamma}$ and $\eta = \frac{\varepsilon}{4 \ln(1/\gamma)}$ into Lemma S5, such polynomial $P$ exists with degree

$$L = O\left(\frac{1}{\delta} \log \frac{B}{\eta}\right) = O\left(\frac{1}{\delta} \log \frac{1}{\gamma} / \varepsilon\right).$$  \hspace{1cm} (E.12)
Note that Lemma 11 of previous work \cite{4} used the same setup for Lemma S5. Then Theorem 10 implies that there exists a QPP circuit $V(\tilde{U}_\rho)$ of $L$ layers to estimate $\text{tr}(\rho P(\rho))$. Up to precision $\frac{\varepsilon}{4\ln(1/\gamma)}$, the experimental estimation $E$ can be retrieved by measuring the first qubit of $V_{\omega, \theta, \phi}(\tilde{U}_\rho)$ with input state $|0^{\otimes (m+1)}\rangle (|0^{\otimes (m+1)}\rangle \otimes \rho$. We have

$$|E - \text{tr}(\rho f(\rho))| \leq |E - \text{tr}(\rho P(\rho))| + |\text{tr}(\rho P(\rho)) - \text{tr}(\rho f(\rho))| \leq \frac{\varepsilon}{4\ln(1/\gamma)} + \|P - f\|_{[\gamma, 1]} \leq \frac{\varepsilon}{2\ln(1/\gamma)} \tag{E.13}$$

and hence

$$|2\ln(\gamma)E - S(\rho)| \leq \varepsilon. \tag{E.15}$$

To receive the desired precision, by Chebyshev’s inequality, the total number of measurements is $O\left(\frac{\ln^2(1/\gamma)}{\varepsilon^2}\right)$, while each $\tilde{U}_\rho$ requires one call of $U_\rho$ and its inverse. Consequently, the total query complexity of $U_\rho$ and its inverse is

$$O\left(\frac{1}{\gamma^2} \log^2 \left(\frac{1}{\gamma}\right) \log \frac{\log(1/\gamma)}{\varepsilon}\right). \tag{E.16}$$

The statement for using amplitude estimation follows by switching Chebyshev’s inequality to the complexity of amplitude estimation \cite{27, 35}.

By replacing $\tilde{U}_\rho$ with $\tilde{U}_\sigma$, the proof of Theorem 13 is exactly the same as the proof of Theorem 11.

**Corollary 12** Given a purified quantum query oracle $U_\rho$ of a state $\rho$ whose rank is $\kappa \leq 2^n$, there exists an algorithm that estimates $S(\rho)$ up to precision $\varepsilon$ with high probability by measuring a single qubit, querying $U_\rho$ and $U_\rho^\dagger$ for $O\left(\frac{\kappa}{\gamma^2} \log^3 \left(\frac{1}{\gamma}\right) \log \left(\frac{1}{\varepsilon}\right)\right)$ times. Moreover, using amplitude estimation improves the query complexity to $O\left(\frac{\kappa}{\gamma^2} \log^2 \left(\frac{1}{\gamma}\right) \log \left(\frac{1}{\varepsilon}\right)\right)$.

**Proof** We follow the same proof in Theorem 11, with extra consideration on the threshold value $\gamma > 0$ and the error generated by this threshold value. We choose the same function $f$ and a polynomial $P$ of degree $O\left(\frac{\kappa}{\gamma^2} \log^3 \left(\frac{1}{\varepsilon}\right)\right)$ such that for all $x \in [\gamma, 1],$

$$|P(x) - f(x)| \leq \eta, \tag{E.17}$$

where $\eta > 0$ is decided later. Denote $E$ as the experiment estimation. Then

$$|E - \text{tr}(\rho f(\rho))| \leq |E - \text{tr}(\rho P(\rho))| + |\text{tr}(\rho P(\rho)) - \text{tr}(\rho f(\rho))| \leq |E - \text{tr}(\rho P(\rho))| + \kappa \|xP - xf\|_{[0, \gamma]} + \|P - f\|_{[\gamma, 1]} \tag{E.18}$$

$$\leq |E - \text{tr}(\rho P(\rho))| + 2\kappa\gamma + \eta. \tag{E.19}$$

Choose $|E - \text{tr}(\rho P(\rho))| \leq \frac{\varepsilon}{8\ln(1/\gamma)}$, $\gamma = \frac{\varepsilon}{8\ln(1/\gamma)}$ and $\eta = \frac{\varepsilon}{8\ln(1/\gamma)}$. We have

$$|2\ln(\gamma)E - S(\rho)| \leq \frac{\varepsilon}{4} + \frac{\varepsilon}{4} + \frac{\varepsilon}{4} = \varepsilon. \tag{E.21}$$

Then the total complexity is

$$O\left(\frac{1}{\varepsilon^2} \log^2 \left(\frac{1}{\gamma}\right)\right) \cdot O\left(\frac{\kappa}{\varepsilon} \log \left(\frac{1}{\varepsilon}\right) \log \left(\frac{1}{\gamma}\right)\right) = O\left(\frac{\kappa}{\varepsilon^3} \log^3 \left(\frac{1}{\varepsilon}\right) \log \left(\frac{1}{\gamma}\right)\right), \tag{E.22}$$

as required. The statement for using amplitude estimation follows by switching Chebyshev’s inequality to the complexity of amplitude estimation \cite{27, 35}.

3. Proofs for quantum Rényi entropy estimation

An extra lemma is required for proceeding to the main content. Note that this lemma is the result of Lemma S5.

**Lemma S6 (Corollary 67 in \cite{4})** Suppose $\gamma, \varepsilon \in (0, 1)$ and $c \in (0, 1)$. Then there exists a polynomial $P \in \mathbb{R}[x]$ of degree $O\left(\frac{1}{\gamma^2} \log \frac{1}{\varepsilon}\right)$ such that
• for all $x \in [-1, 1]$, $|P(x)| \leq 1$ and

• for all $x \in [\gamma, 1]$, $\left| P(x) - \frac{\gamma^x}{2}x^{-\alpha} \right| \leq \varepsilon$.

**Theorem 14 (Quantum Rényi entropy estimation for real $\alpha$)** Given a purified quantum query oracle $U_\rho$ of a state $\rho$ whose non-zero eigenvalues are lower bounded by $\gamma > 0$, there exists an algorithm that estimates $S_\alpha(\rho)$ up to precision $\varepsilon$ with high probability by measuring a single qubit, querying $U_\rho$ and $U_\rho^\dagger$ for a total number of times in

\[
\mathcal{O}\left( \frac{\text{tr}(\rho^\alpha)^{-2}}{|1 - \alpha|^2 \gamma^{1 - 2\alpha} \varepsilon^2} \log \left( \frac{\text{tr}(\rho^\alpha)}{\gamma^{1 - \alpha} \varepsilon} \right) \right), \quad \text{if } \alpha \in (0, 1); \\
\mathcal{O}\left( \frac{\text{tr}(\rho^\alpha)^{-2} \log^2(1/\gamma)}{|1 - \alpha|^2 \gamma^2 \varepsilon^2} \left[ \alpha \gamma + \log \left( \frac{\text{tr}(\rho^\alpha) \log(1/\gamma)}{\varepsilon} \right) \right] \right), \quad \text{if } \alpha \in (1, \infty); \\
\mathcal{O}\left( \frac{\text{tr}(\rho^\alpha)^{-1} \log(1/\gamma)}{|1 - \alpha| \gamma \varepsilon} \left[ \alpha \gamma + \log \left( \frac{\text{tr}(\rho^\alpha) \log(1/\gamma)}{\varepsilon} \right) \right] \right), \quad \text{if } \alpha \in (1, \infty).
\]

(E.23)

where $\eta = \frac{\text{tr}(\rho^\alpha)^{-1}}{|1 - \alpha|}$. Moreover, using amplitude estimation improves the query complexity to

\[
\mathcal{O}\left( \frac{\text{tr}(\rho^\alpha)^{-1}}{|1 - \alpha| \gamma^2 \alpha^2} \log \left( \frac{\text{tr}(\rho^\alpha)}{\gamma^{1 - \alpha} \varepsilon} \right) \right), \quad \text{if } \alpha \in (0, 1).
\]

(E.24)

**Proof** Previous work [60] states that it is able to obtain an estimation of $S_\alpha(\rho)$ up to precision $\varepsilon$, by an estimation of $\text{tr}(\rho^\alpha)$ within error $\varepsilon' = \frac{|1 - \alpha| \text{tr}(\rho^\alpha)}{2} \varepsilon$. Then we turn to demonstrate how to obtain $\text{tr}(\rho^\alpha)$ with error bounded by $\varepsilon'$.

Suppose $\alpha \in (0, 1)$. By Lemma S6, there exists a polynomial $P \in \mathbb{R}[x]$ of degree $O(\frac{1}{\gamma} \log \frac{1}{\gamma^{1 - \alpha} \varepsilon})$ such that

• for all $x \in [-1, 1]$, $|P(x)| \leq 1$,

• for all $x \in [\gamma, 1]$, $\left| P(x) - \frac{x^{1-\alpha}}{2}x^{-\alpha-1} \right| \leq \frac{x^{1-\alpha}}{4} \varepsilon'$.

Similar to the proof of Theorem 11, Theorem 10 implies that there exists a QPP circuit $V(\tilde{U}_\rho)$ of $L$ layers to estimate $\text{tr}(\rho P(\rho))$. Up to precision $\frac{x^{1-\alpha}}{4} \varepsilon'$, the experimental estimation $E$ can be retrieved by measuring the first qubit of $V(\tilde{U}_\rho)$ with input state $|0\otimes(m+1)\rangle |0\otimes(m+1)\rangle \otimes \rho$. We have

\[
|E - \frac{\gamma^{1-\alpha}}{2} \text{tr}(\rho^\alpha)| \leq \frac{\gamma^{1-\alpha}}{2} \varepsilon'
\]

(E.25)

and hence

\[
|2\gamma^{1-\alpha}E - \text{tr}(\rho^\alpha)| \leq \varepsilon'.
\]

(E.26)

By considering Chebyshev’s inequality, the total query complexity of $U_\rho$ and $U_\rho^\dagger$ is $O(\frac{1}{\gamma^{1 - 2\alpha} \varepsilon^2} \log \frac{1}{\gamma^{1 - \alpha} \varepsilon})$. Now substitute $\varepsilon'$ back to $\varepsilon$. The query complexity turns to

\[
\mathcal{O}\left( \frac{\text{tr}(\rho^\alpha)^{-2}}{|1 - \alpha|^2 \gamma^{3 - 2\alpha} \varepsilon^2} \log \left( \frac{\text{tr}(\rho^\alpha)}{\gamma^{1 - \alpha} \varepsilon} \right) \right).
\]

(E.27)

Now suppose $\alpha > 1$. Define $f(x) := \frac{1}{2 \text{ln}(2e/\gamma)} x^{\alpha - [\alpha]}$ which is bounded by $\frac{1}{2 \text{ln}(2e/\gamma)}$ for $x \in [0, 1]$. Using the same setup in the proof of Theorem 11, we would have $B = \frac{1}{2}$. See deductions below.

\[
\sum_{l=0}^{\infty} \left| \binom{\alpha - [\alpha]}{l} (1 - \gamma/2)^l \right| (1 - \gamma/2)^l \leq \sum_{l=0}^{\infty} \binom{\alpha - [\alpha]}{l} (1 + \gamma/2)^l
\]

(E.28)

\[
= 1 - (\alpha - [\alpha]) \sum_{l=1}^{\infty} \frac{(-1)^{l-1}}{l} (1 + \gamma/2)^l
\]

(E.29)
implies the query complexity is simply

\[ \frac{\varepsilon'}{4 \ln(2e/\gamma)}. \]

(R31)

Redefine \( P(x) := x^{[\alpha]} \tilde{P}(x) \) of degree \( O(\alpha + \frac{1}{\gamma} \log \frac{\log(1/\varepsilon)}{\varepsilon}) \). By the same procedure in the case of \( \alpha \in (0, 1) \), we can find a QPP circuit estimating \( \text{tr}(\rho P(\rho)) \), so that the experimental estimation \( \tilde{E} \) satisfies

\[ |2 \ln(2e/\gamma) E - \text{tr}(\rho^\alpha)| \leq \varepsilon'. \]

(R32)

As a result, the total query complexity in terms of \( \varepsilon \) is

\[ O\left( \frac{\text{tr}(\rho^\alpha)^{-2} \log^2(1/\gamma)}{|1 - \alpha|^2 \gamma \varepsilon^2} \left( \alpha \gamma + \log \frac{\text{tr}(\rho^\alpha) \log(1/\gamma)}{\varepsilon} \right) \right). \]

(R33)

The statement for using amplitude estimation follows by switching Chebyshev's inequality to the complexity of amplitude estimation.



As for the proof of Theorem 15, Theorem 10 implies the query complexity is simply \( O(\frac{1}{\gamma}) \) when \( \alpha \) is an integer. Then the statement of Theorem 15 follows by replacing \( \varepsilon' \) with \( \varepsilon \). Note that in this case \( |1 - \alpha| \in O(\alpha) \). In the following corollary, we present a method to estimate \( S_\alpha(\rho) \) when \( \gamma \) is unknown.

**Corollary S7** Assume a rank \( \kappa \leq 2^n \) for an \( n \)-qubit state \( \rho \) and a purified quantum oracle \( U_\rho \). There exists a QPP circuit that estimates \( S_\alpha(\rho) \) within precision \( \varepsilon \) by measuring a single qubit, at an expense of querying \( U_\rho \) and \( U_\rho^\dagger \) for a number of

\[
\begin{aligned}
&O\left( \frac{2^{212/\alpha} \text{tr}(\rho^\alpha)^{-3/\alpha} \kappa^{3/\alpha - 2}}{\alpha |1 - \alpha|^3 \alpha \varepsilon^{3/\alpha}} \left[ 3 + \log \left( \frac{\text{tr}(\rho^\alpha) \kappa}{|1 - \alpha| \varepsilon} \right) \right] \right), & \text{if } \alpha \in (0, 1),
\end{aligned}
\]

(R34)

\[
\begin{aligned}
&O\left( \frac{\text{tr}(\rho^\alpha)^{-3} \kappa}{|1 - \alpha|^3 \varepsilon ^3} \log^2 \left( \frac{\text{tr}(\rho^\alpha)^{-1} \kappa}{|1 - \alpha| \varepsilon} \right) \left[ \alpha^2 \varepsilon^2 + \log \left( \frac{\text{tr}(\rho^\alpha)^{-1} \kappa}{|1 - \alpha| \varepsilon} \right) \log \left( \frac{\text{tr}(\rho^\alpha)^{-1}}{|1 - \alpha| \varepsilon} \right) \right] \right), & \text{if } \alpha \in (1, \infty),
\end{aligned}
\]

Moreover, using amplitude estimation improves query complexity to

\[
\begin{aligned}
&O\left( \frac{2^{8/\alpha} \text{tr}(\rho^\alpha)^{-2} \kappa^{2/\alpha - 1}}{|1 - \alpha|^{2/\alpha} \varepsilon^{2/\alpha}} \left[ 3 + \log \left( \frac{\text{tr}(\rho^\alpha) \kappa}{|1 - \alpha| \varepsilon} \right) \right] \right), & \text{if } \alpha \in (0, 1).
\end{aligned}
\]

(R35)

\[
\begin{aligned}
&O\left( \frac{\text{tr}(\rho^\alpha)^{-2} \kappa}{|1 - \alpha|^2 \varepsilon ^2} \log \left( \frac{\text{tr}(\rho^\alpha)^{-1} \kappa}{|1 - \alpha| \varepsilon} \right) \left[ \alpha^2 \varepsilon^2 + \log \left( \frac{\text{tr}(\rho^\alpha)^{-1} \kappa}{|1 - \alpha| \varepsilon} \right) \log \left( \frac{\text{tr}(\rho^\alpha)^{-1}}{|1 - \alpha| \varepsilon} \right) \right] \right), & \text{if } \alpha \in (1, \infty).
\end{aligned}
\]

**Proof** As shown in the proof of Theorem 14, we could find a polynomial \( P(x) \) such that

\[ |P(x) - f_\alpha(x)| \leq \eta, \forall x \in [\gamma, 1]. \]

(R36)

where

\[ f_\alpha(x) = \begin{cases} 
\frac{\gamma - \alpha}{2} x^{\alpha - 1}, & \text{if } \alpha \in (0, 1), \\
\frac{2}{2 \ln(2e/\gamma)} x^{\alpha}, & \text{if } \alpha > 1.
\end{cases} \]

(R37)

Denote \( E \) as the experiment estimation. Then

\[ |E - \text{tr}(\rho f(\rho))| \leq |E - \text{tr}(\rho P(\rho))| + |\text{tr}(\rho P(\rho)) - \text{tr}(\rho f(\rho))| \]

(R38)

\[ \leq |E - \text{tr}(\rho P(\rho))| + \kappa \|xP - xf\|_{[0,\gamma]} + \|P - f\|_{[\gamma, 1]} \]

(R39)
Then the total complexity is
\[
|2 \ln(2e/\gamma) E - \text{tr}(\rho^\alpha)| \leq \frac{\epsilon'}{4} + \frac{\epsilon'}{2} + \frac{\epsilon'}{4} = \epsilon'.
\]

Then the total complexity is
\[
\mathcal{O}\left(\frac{1}{\epsilon'}^2 \log^2 \left(\frac{K}{\epsilon'}\right)\right) \cdot \mathcal{O}\left(\alpha + \frac{K}{\epsilon'} \log \left(\frac{K}{\epsilon'}\right) \log \left(\frac{1}{\epsilon'}\right)\right)
= \mathcal{O}\left(\frac{K}{\epsilon'}^3 \log^2 \left(\frac{K}{\epsilon'}\right) \left[\frac{\alpha \epsilon'}{\kappa} + \log \left(\frac{K}{\epsilon'}\right) \log \left(\frac{1}{\epsilon'}\right)\right]\right)
= \mathcal{O}\left(\frac{\text{tr}(\rho^\alpha)^{-3} \kappa}{|1 - \alpha|^3 \epsilon^3} \log^2 \left(\frac{\text{tr}(\rho^\alpha)^{-1} \kappa}{|1 - \alpha| \epsilon}\right) \left[\alpha |1 - \alpha| \text{tr}(\rho^\alpha) \epsilon + \log \left(\frac{\text{tr}(\rho^\alpha)^{-1} \kappa}{|1 - \alpha| \epsilon}\right) \log \left(\frac{\text{tr}(\rho^\alpha)^{-1} \kappa}{|1 - \alpha| \epsilon}\right)\right]\right).
\]

The result follows by the fact that \(\alpha|1 - \alpha| = \mathcal{O}(\alpha^2)\) and \(\text{tr}(\rho^\alpha) \leq 1\).

For \(\alpha \in (0, 1)\), choose \(|E - \text{tr}(\rho P(\rho))| \leq \frac{1-\alpha'}{8}, \gamma = 8^{-1/\alpha}, \left(\frac{\epsilon'}{\kappa}\right)^{1/\alpha}\) and \(\eta = \frac{1-\alpha'}{8}\). We have
\[
|2\gamma^{\alpha-1} E - \text{tr}(\rho^\alpha)| \leq \frac{\epsilon'}{4} + \frac{\epsilon'}{2} + \frac{\epsilon'}{4} = \epsilon'.
\]

Then the total complexity is
\[
\mathcal{O}\left(\frac{\gamma^{2(\alpha-1)}}{\epsilon'!^2}\right) \cdot \mathcal{O}\left(\frac{1}{\gamma} \log \left(\frac{\gamma^{\alpha-1}}{\epsilon'}\right)\right)
= \mathcal{O}\left(\frac{\alpha^{6/\alpha} K^{2/\alpha - 2}}{\epsilon'!^{2/\alpha}}\right) \cdot \mathcal{O}\left(\frac{\alpha^{3/\alpha} K^{1/\alpha}}{\epsilon'!^{1/\alpha}} \log \left(\frac{8^{1/\alpha - 1} K^{1/\alpha - 1}}{\epsilon'!^{1/\alpha}}\right)\right)
= \mathcal{O}\left(\frac{\alpha^{9/\alpha} K^{3/\alpha - 2}}{\epsilon'!^{3/\alpha}} \left[3 + \log \left(\frac{K}{\epsilon'}\right)\right]\right)
= \mathcal{O}\left(\frac{\alpha^{12/\alpha} \text{tr}(\rho^\alpha)^{-3} \kappa^{3/\alpha - 2}}{\alpha |1 - \alpha|^3 \epsilon^3} \left[3 + \log \left(\frac{\text{tr}(\rho^\alpha) \kappa}{|1 - \alpha| \epsilon}\right)\right]\right),
\]
as required. The statement for using amplitude estimation follows by switching Chebyshev’s inequality to the complexity of amplitude estimation.

4. Comparison on entropies estimation algorithms

We present further comparison on different entropies estimation algorithms in this section. In Table S1, we add the von Neumann entropy estimation algorithm proposed by Wang et al. [48]. When assuming rank \(\kappa\), the QPP-based algorithm improves the result in [48] by a factor of \(\kappa\). In Table S2, we add Rényi entropy estimation algorithms proposed by Wang et al. [48].
| Methods for $S(\rho)$ estimation | Total queries to $U_\rho$ and $U_\rho^\dagger$ | Queries per use of circuit |
|----------------------------------|--------------------------------------------|----------------------------|
| QSVT-based with QAE ([11])      | $\tilde{O}(\frac{d^2}{\kappa^2 \epsilon})$ | $\tilde{O}(\frac{d^2}{\kappa^2 \epsilon})$ |
| QSVT-based with QAE (assumes rank, [48]) | $\tilde{O}(\frac{\rho^2}{\epsilon^2})$ | $\tilde{O}(\frac{\rho^2}{\epsilon^2})$ |
| QPP-based (assumes rank, in Corollary 12) | $\tilde{O}(\frac{\rho}{\epsilon})$ | $\tilde{O}(\frac{\rho}{\epsilon})$ |
| QPP-based with QAE (assumes rank, in Corollary 12) | $\tilde{O}(\frac{\rho}{\epsilon})$ | $\tilde{O}(\frac{\rho}{\epsilon})$ |
| QPP-based (in Theorem 11)       | $\tilde{O}(\frac{\rho}{\epsilon})$ | $\tilde{O}(\frac{\rho}{\epsilon})$ |
| QPP-based with QAE (in Theorem 11) | $\tilde{O}(\frac{\rho}{\epsilon})$ | $\tilde{O}(\frac{\rho}{\epsilon})$ |

TABLE S1: Comparison of algorithms on estimating von Neumann entropy within additive error. Here the $\tilde{O}$ notation omits log factors, $\gamma > 0$ is the lower bound of eigenvalues, $\kappa > 0$ is the rank of the state $\rho \in \mathbb{C}^{d \times d}$, and $\epsilon$ is the additive error of estimating $S(\rho)$. QAE is short for quantum amplitude estimation.

| Methods for $S_\alpha(\rho)$ estimation | Total queries to $U_\rho$ and $U_\rho^\dagger$ | $\alpha \in (0, 1)$ | $\alpha \in (1, \infty)$ | $\alpha \in \mathbb{N}_+$ |
|----------------------------------|--------------------------------------------|-----------------|-----------------|-----------------|
| QSVT-based with DQC1 ([12])      | $\tilde{O}(\frac{d^3}{\kappa^2 \epsilon^{\alpha+2}} \cdot \eta^{3/\alpha})$ | $\tilde{O}(\frac{d^2}{\kappa^2 \epsilon^{\alpha+2}} \cdot \eta^2)$ | $\tilde{O}(\frac{d^3}{\kappa^2 \epsilon^{\alpha+2}})$ (only for odd $\alpha$) | $\tilde{O}(\frac{d^3}{\kappa^2 \epsilon^{\alpha+2}})$ (only for odd $\alpha$) |
| QSVT-based with QAE (assume rank, [48]) | $\tilde{O}(\frac{\rho^2}{\epsilon^2})$ | $\tilde{O}(\frac{\rho^2}{\epsilon^2})$ | $\tilde{O}(\frac{\rho^2}{\epsilon^2})$ | $\tilde{O}(\frac{\rho^2}{\epsilon^2})$ |
| QPP-based (assume rank, in Corollary S7) | $\tilde{O}(\frac{\rho^{\alpha-1}}{\epsilon^{\alpha-2}} \cdot \eta^{\alpha^2/\alpha})$ | $\tilde{O}(\frac{\rho^{\alpha-1}}{\epsilon^{\alpha-2}} \cdot \eta^{\alpha^2/\alpha})$ | $\tilde{O}(\frac{\rho^{\alpha-1}}{\epsilon^{\alpha-2}} \cdot \eta^{\alpha^2/\alpha})$ | $\tilde{O}(\frac{\rho^{\alpha-1}}{\epsilon^{\alpha-2}} \cdot \eta^{\alpha^2/\alpha})$ |
| QPP-based with QAE (assume rank, in Corollary S7) | $\tilde{O}(\frac{\rho^{\alpha-1}}{\epsilon^{\alpha-2}} \cdot \eta^{\alpha^2/\alpha})$ | $\tilde{O}(\frac{\rho^{\alpha-1}}{\epsilon^{\alpha-2}} \cdot \eta^{\alpha^2/\alpha})$ | $\tilde{O}(\frac{\rho^{\alpha-1}}{\epsilon^{\alpha-2}} \cdot \eta^{\alpha^2/\alpha})$ | $\tilde{O}(\frac{\rho^{\alpha-1}}{\epsilon^{\alpha-2}} \cdot \eta^{\alpha^2/\alpha})$ |
| QPP-based (in Theorem 14 and 15) | $\tilde{O}(\frac{\rho^{\alpha-1}}{\epsilon^{\alpha-2}} \cdot \eta^{\alpha^2/\alpha})$ | $\tilde{O}(\frac{\rho^{\alpha-1}}{\epsilon^{\alpha-2}} \cdot \eta^{\alpha^2/\alpha})$ | $\tilde{O}(\frac{\rho^{\alpha-1}}{\epsilon^{\alpha-2}} \cdot \eta^{\alpha^2/\alpha})$ | $\tilde{O}(\frac{\rho^{\alpha-1}}{\epsilon^{\alpha-2}} \cdot \eta^{\alpha^2/\alpha})$ |
| QPP-based with QAE (in Theorem 14 and 15) | $\tilde{O}(\frac{\rho^{\alpha-1}}{\epsilon^{\alpha-2}} \cdot \eta^{\alpha^2/\alpha})$ | $\tilde{O}(\frac{\rho^{\alpha-1}}{\epsilon^{\alpha-2}} \cdot \eta^{\alpha^2/\alpha})$ | $\tilde{O}(\frac{\rho^{\alpha-1}}{\epsilon^{\alpha-2}} \cdot \eta^{\alpha^2/\alpha})$ | $\tilde{O}(\frac{\rho^{\alpha-1}}{\epsilon^{\alpha-2}} \cdot \eta^{\alpha^2/\alpha})$ |

TABLE S2: Comparison of algorithms on estimating quantum $\alpha$-Rényi entropies for different $\alpha$, in terms of the query complexity of $U_\rho$ and $U_\rho^\dagger$. Here the $\tilde{O}$ notation omits the log and $\alpha$ factors. $\gamma > 0$ is the lower bound of eigenvalues and $\kappa > 0$ is the rank of a mixed state $\rho \in \mathbb{C}^{d \times d}$, and $\epsilon$ is the additive error of estimating $S_\alpha(\rho)$. QAE is short for quantum amplitude estimation.