Quantum Gaussian filter for exploring ground-state properties

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Filter methods realize a projection from a superposed quantum state onto a target state, which can be efficient if two states have a sufficient overlap. Here we propose a quantum Gaussian filter (QGF) with the filter operator being a Gaussian function of system Hamiltonian. A hybrid quantum-classical algorithm feasible on near-term quantum computers is developed, which implements the quantum Gaussian filter as a linear combination of Hamiltonian evolution at various times. Remarkably, the linear combination coefficients are determined classically and can be optimized in the post-processing procedure. We demonstrate the quantum Gaussian filter algorithm for the quantum Ising model with numeral simulations under noises. As a comparison, we also present a full-quantum realization of QSF with an ancillary continuous-variable. The comparison to the full-quantum algorithm suggests that the hybrid quantum-classical one can enjoy the flexibility of algorithmic design from the post-processing on classical computers.

I. INTRODUCTION

Solving the ground state problems plays a significant role in quantum simulation [1,2], which can be applied to many fields, such as quantum chemistry and condensed matter physics [3–6]. As classical algorithms would eventually meet the exponential wall issue when solving larger-size quantum systems, quantum computing offers a way forward that dramatically decreases the resource required. The quantum phase estimation (QPE), a milestone quantum algorithm for eigensolver, uses quantum Fourier transformation to extract eigenvalues and associated eigenstates from an initial state probabilistically [4,7,9]. However, QPE relies on long coherent evolution and can be resource-consuming for the era of Noisy Intermediate-Scale Quantum (NISQ) devices [10]. Unlike QPE, variational quantum eigensolvers (VQE) target the desired eigenstate with a parametrized quantum circuit [11–15], whose parameters can be optimized with a hybrid quantum-classical procedure. While the circuit depth can be much reduced, VQE strongly depends on the ansatz [16], and the optimizing process may be hindered by vanishing gradients known as the barren plateaus [17,18].

Rethinking the quantum phase estimation, it in principle treats all eigenstates as equal, and the distribution of results is determined by the overlapping between each eigenstate and the initial state. However, once focusing on eigenstates of physical interest, such as the ground state and low-lying excited states, a projection onto such an eigenstate may be much more efficient. The key point is to construct a filter operator on a quantum computer to single out the desired eigenstate from the initial state. As the unwanted components of eigenstates are filtered out and their information can be ignored, quantum filter methods do not require quantum Fourier transformation; thus, it may be realized with much fewer quantum resources.

Recently, there have been some proposals of quantum filters, including the cosine-filtering operator [19,20], the quantum inverse iteration algorithm [21], the quantum filter diagonalization [22], the powered Hamiltonian approximation [23,24]. Those methods construct the non-unitary filter operator as a linear combination of unitaries in a hybrid quantum-classical fashion, where the unitaries are performed on the quantum computer, and the linear combination coefficients are determined classically. The coefficients are given beforehand [19,21,23,24], enjoying a clear analysis of desired resources, but they may not be adjustable on noisy quantum devices or need to be obtained by optimization [22] in a high-dimension space. A compromise of two may make a quantum filter both theoretically promised and flexible for implementation on near-term quantum devices. It is required to design a proper quantum filter with some hyperparameters that can be fittingly optimized in classical post-processing.

In this work, we propose a quantum Gaussian filter for exploring the ground state properties of quantum systems. The QGF solves the approximate ground state by performing a Gaussian function of Hamiltonian on a given initial state which has a sufficient overlapping with the ground state. The Gaussian filter is parameterized with a shift-energy and a width, which can be adjusted for optimally singling out the ground state. We present a hybrid quantum-classical algorithm for implementing the QGF, optimizing the Gaussian filter operator in the classical post-processing. We demonstrate the algorithm by numeral simulating the quantum Ising
model under noises. In addition, we give a full-quantum version of QGF with an auxiliary continuous variable using only Gaussian states. A comparison between the two approaches suggests that the hybrid one allows optimizing the algorithm in classical post-processing procedures. This paper is organized as follows. We first introduce our algorithm’s principle and procedure in Sec. II and analyze its time complexity in Sec. III. Then, the numerical results of this algorithm are shown in Sec. IV. A continuous-variable assisted strategy is also presented in Sec. V. Lastly, the conclusion and discussion are given in Sec. VI.

II. QUANTUM ALGORITHM

In this section, we present the principle and procedure of the QGF algorithm. The main idea of this algorithm is to perform a Gaussian filter operator $e^{-(\mu H - \mu I)^2/\sigma^2}$ on an arbitrary initial state $|\psi_i\rangle$ that has non-zero overlap with the exact ground state, where the expected value $\mu$ and variance $\sigma^2$ of the Gaussian function correspond to minus shift-energy and width of the Gaussian filter. By representing the initial state as a superposition of eigenstate of an $N$-qubit Hamiltonian $\hat{H}$, e.g. $|\psi_i\rangle = \sum_{j=0}^{2^{N-1}} a_j |\lambda_j\rangle$, a Gaussian filter operator $e^{-(\mu H - \mu I)^2/\sigma^2}$ converts it to

$$|\psi_f\rangle = \frac{1}{\sqrt{C}} \sum_{j=0}^{2^{N-1}} a_j e^{-(\lambda_j - \mu)^2/\sigma^2} |\lambda_j\rangle,$$

where $\frac{1}{\sqrt{C}} = (\sum_{j=0}^{2^{N-1}} |a_j|^2 e^{-(\lambda_j - \mu)^2/\sigma^2})^{-1/2}$ is the normalization factor, $|\lambda_j\rangle$ is the eigenstate of $\hat{H}$ corresponding to $j$-th smallest eigenvalue $\lambda_j$, and $a_j = \langle \lambda_j | \psi_i \rangle$ is the square root of overlap between initial state and eigenstate $|\lambda_j\rangle$. This Gaussian filter operator $e^{-(\mu H - \mu I)^2/\sigma^2}$ results in an additional weight $e^{-(\lambda_j - \mu)^2/\sigma^2}$ for each eigenstate, which monotonically decreases with the eigenvalue. In the case that all the eigenvalues are positive values, as the variance $\sigma^2$ or the expected value $\mu$ of the Gaussian function decreases, the resulting state converges to the ground state $|\lambda_0\rangle$.

Since the Gaussian filter operator $e^{-(\mu H - \mu I)^2/\sigma^2}$ is a non-unitary operator that cannot naturally be performed on quantum computers, it is approximated by a linear combination of unitary operators \cite{25,26} with the idea of Fourier approximation

$$e^{-(\mu H - \mu I)^2/\sigma^2} \approx \sum_{y=-M_y}^{M_y} b_{\mu,\sigma,y} e^{-i\mu H t_y} \Delta_y,$$

where $\Delta_y$ is slice size, $M_y$ is the cutoff number of terms of unitary operators, $t_y = y \Delta_y$ is evolution time of $y$-th term, $b_{\mu,\sigma,y} = \frac{\sigma}{2 \sqrt{\pi}} e^{-(\sigma^2\Delta_y^2)^2} e^{i\mu(y \Delta_y)}$ is the weight of $y$-th term, and the max evolution time is defined as $\phi_m = M_y \Delta_y$. Performing the above operator on an arbitrary initial state leads to an additional weight $g_{\lambda,\mu}(\lambda)$ for every eigenstate $|\lambda\rangle$ that is

$$g_{\lambda,\mu}(\lambda) = \sum_{y=-M_y}^{M_y} b_{\mu,\sigma,y} e^{-i\lambda t_y} \Delta_y. \quad (3)$$

It can well approximate $e^{-(\lambda - \mu)^2/\sigma^2}$ for $\lambda \in [\mu, \lambda_m + \mu]$ and oscillates around $e^{-(\lambda_m)^2/\sigma^2}$ for $\lambda > \lambda_m + \mu$ when $\phi_m = 2(\lambda_m + \mu)^2/\sigma^2$.

The approximate ground state energy is estimated as $\lambda_{\mu,\sigma} = \langle \hat{H} \rangle_{\mu,\sigma} / \langle \psi_{\mu,\sigma} \rangle_{\mu,\sigma}$. Considering the sequential energy estimation method \cite{21} that classically sums the overlap between the initial state and evolved state with corresponding weight, the estimated ground state energy is

$$\lambda_{\mu,\sigma} = \frac{\langle \hat{H} \rangle_{\mu,\sigma}}{\langle \psi_{\mu,\sigma} \rangle_{\mu,\sigma}} = \frac{\sum_{y,y'= -M_y}^{M_y} b_{\mu,\sigma,y} b^{*}_{\mu,\sigma,y'} \langle \psi \hat{H} e^{-i(t_y - t_{y'}) \hat{H}} | \psi \rangle}{\sum_{y,y'= -M_y}^{M_y} b_{\mu,\sigma,y} b^{*}_{\mu,\sigma,y'} \langle \psi | e^{-i(t_y - t_{y'}) \hat{H}} | \psi \rangle}. \quad (4)$$

As parameters of the Gaussian filter operator are determined by choice of classical weights $\{b_{\mu,\sigma,y}\}_{y=-M_y}^{M_y}$, the estimated energy can be optimized by classical post-processing without external quantum computation.

The procedure of the QGF algorithm to solve an approximate ground state energy is shown in Fig. 1, whose steps are as follows:

1. Set the approximation parameters $M_y$ and $\Delta_y$ according to the system size of Hamiltonian to be solved and the desired accuracy.
2. Prepare an initial state $|\psi_i\rangle$ that has non-zero overlap with the exact ground state.
3. Evaluate in Eq. (4) $\langle \psi | e^{-i(t_y - t_{y'}) H} | \psi \rangle$ and $\langle \psi | e^{-i(t_y - t_{y'}) H} | \psi \rangle$ for $y, y' \in [-M_y, M_y]$ by Hadamard test \cite{29} on a quantum processor.
4. Optimize the classical weights $\{b_{\mu,\sigma,y}\}_{y=-M_y}^{M_y}$ by minimizing the approximate ground state energy $\lambda_{\mu,\sigma}$ on a classical computer.

The above procedure can also be used as an iterative strategy. Starting from a certain level approximation parameter $M_y$ and $\Delta_y$ to obtain an estimated ground state energy. We may iteratively change the approximation parameters to increase the result accuracy until it meets the requirement. In each iteration, only additional overlaps in Eq. (4) are required to be measured. Moreover, once the best-performance parameters $\{b_{\mu,\sigma,y}\}_{y=-M_y}^{M_y}$ are obtained, any expectation value of the ground state can be solved by replacing $\hat{H}$ by an observable operator $\hat{A}$ in Eq. (4).
III. TIME COMPLEXITY ANALYSIS

We briefly discuss the time complexity of the QGF algorithm for estimating the ground state energy. As this hybrid quantum-classical algorithm consists of state evolution and measurement, we can analyze the required circuit depth and the number of measurements separately.

Consider a gapped quantum many-body model with a local Hamiltonian $\hat{H} = \sum_{i=1}^{L} c_i \hat{h}_i$, where $\hat{h}_i$ is a Pauli string performing on a subset of qudits and $L$ is the same order of the system size. Its energy spectrum lies in $[\lambda_0, \lambda_{2N-1}]$, and the energy gap is $\Delta$. It is necessary to start with a well-prepared initial state, which shall have a sufficient overlap to the ground state, e.g., $\langle \psi_i | \psi_f \rangle^2 = O(\text{poly}(1/N))$. In our analysis we assume the overlap is $O(1/N)$. This may be achieved by preparing an initial state with a prior-knowledge of the system or using a VQE to prepare an approximated ground state with a shallow quantum circuit. Otherwise, a random initial state may cause the overlap to exponentially decays, leading to an exponential time complexity for large size problems.

Let us firstly consider the maximum circuit depth, which is determined by the maximum evolution time. The initial state can be written as a superposition of the target ground state and its orthogonal state, $|\psi_i\rangle \sim O\left(\sqrt{\frac{1}{N}}\right)|\lambda_0\rangle + O\left(\sqrt{\frac{N-1}{N}}\right)|\lambda_\perp\rangle$. For a Gaussian filter $e^{-\frac{(\hat{H}-\mu)^2}{\sigma^2}}$ constructed in Eq. (2), the Gaussian function $e^{-\frac{(\hat{H}-\mu)^2}{\sigma^2}}$ can be approximated for the spectrum $\lambda \in [\mu, \mu + \lambda_m]$, where $\mu = \lambda_0 + \Delta - \lambda_m$. By performing the constructed Gaussian filter on the initial state, the final state turns to be $|\psi_f\rangle \sim O\left(\sqrt{\frac{1}{N}} e^{-\frac{(\lambda_m - \Delta)^2}{\sigma^2}}|\lambda_0\rangle + O\left(\sqrt{\frac{N-1}{N}} e^{-\frac{\lambda^2_m}{\sigma^2}}|\lambda_\perp\rangle\right)\right)$. The estimated energy then is $E_e = E_g + O(N e^{(2\Delta^2 - 4\lambda_m)/\sigma^2})$. As the energy gap is independent to the system size, the requirement of $\lambda_m$ for a fixed accuracy $\epsilon$ is $O(\sigma^2 \log(N/\epsilon))$, corresponding to a maximum evolution time $\phi_m = O(\log(N/\epsilon))$. The evolution of Hamiltonian $e^{-\hat{H}t}$ can be decomposed by the Trotterization [30]:

$$e^{-\hat{H}t} \approx (\prod_{j=1}^{M} e^{-ic_j \hat{h}_j t/n})^n. \quad (5)$$

The circuit depth is $O(N^3 t^2 / \epsilon')$ for a state error $\epsilon'$ (we have used $L \approx O(N)$). Note that the state error $\epsilon'$ is related to the energy error $\epsilon$ as $\epsilon \sim \epsilon'^2$. Then, the maximum circuit depth is $O(N^3 \log^2(N/\epsilon)/\sqrt{\epsilon})$.

We continue to discuss the total measurement times of this algorithm, which includes the number of terms and measurement times required for each term in Eq. (4). To approximate $e^{-(\lambda - \mu)^2/\sigma^2}$ for $\lambda \in [\mu, \mu + \lambda_m]$, the slice fineness of the Fourier approximation $\Delta_y$ should be at least equal to $4\sigma^2 / \lambda_m$. Then, there should be $9\lambda^2_m / 2\sigma^2$ terms of overlapping for evaluation. As both the numerator and denominator in Eq. (4) are in the order of $O(e^{-2\lambda^2_m / \sigma^2})$, the statistical error of measurements should be $O(\epsilon e^{-2\lambda^2_m / \sigma^2})$. The total number of measurement times is $O(\lambda^3_m e^{-2\lambda^2_m / \sigma^2})$, which becomes $O(1/\epsilon)$ by setting $\sigma = O(1/\log(N/\epsilon))$. It is noted that such a choice of $\sigma$ will not increase the maximum circuit depth.

In total, the time complexity of the quantum Gaussian filter is $O[N^3 e^{-3/2 \log^2(N/\epsilon)}]$ for solving an approximate ground state energy with the desired accuracy $\epsilon$, which is a polynomial of system size and accuracy.

IV. DEMONSTRATION

In this section, we simulate the QGF algorithm to solve the approximate ground state energy of a transverse-field Ising model, whose Hamiltonian is

$$\hat{H} = -J \sum_{n=1}^{N} \hat{\sigma}_n^x \hat{\sigma}_{n+1}^x + g \sum_{n=1}^{N} \hat{\sigma}_n^z. \quad (6)$$

where $J$ is the interaction strength of nearby sites and $g$ is the scale of the external transverse field. The whole simulation was done in QuTip [31].

We firstly consider solving the transverse-field Ising model with $J = 1$, $g = 2$, and $N = 8$ under a fixed discrete parameter that is $\Delta_y = 0.16$ and $M_y = 50$. A shift-energy 15 is applied to shift all the eigenvalues, and a random initial state is used. As shown in Fig. 2 result error firstly decreases and then increases as $\mu (\sigma^2)$.
decreases for a fixed $\sigma^2 (\mu)$. It results from that Gaussian filter with a smaller width and minus shift-energy has a better performance but is more difficult to be well approximated. The result also shows that even starting from a random initial state that has a low overlap to the ground state, a high accuracy result can be reached by this QGF algorithm with max phase $\phi_{max} = 8$.

We also demonstrate the process of solving the above problem with $N = 6, 8$ and $10$ by an iterative approach, where $\Delta_y = 0.08$ and $M_y$ gradually increases from $30$ to $130$ corresponding to $\phi_{max} \in [2.4, 10.4]$. In each iteration, new quantum values are computed, and minimum energy is obtained by searching $1/\sigma^2 \in [0.1, 3]$ and $\mu \in [\lambda_0, \lambda_0 - 1]$. The result is shown in Fig. 3 where the energy difference between the exact ground state and approximate one solved by this iterative method decreases as the max evolution time increases for all three models.

While universal fault-tolerant quantum computers have not been developed yet, noises on near-term quantum processors should be considered. We demonstrate the quantum Gaussian filter algorithm by solving the above problem with $N = 4$ under noises. Here, Trotter decomposition [30] is applied for decomposing the Hamiltonian evolution into a sequence of one-qubit and two-qubit gates. We consider two noises models, the bit-flip and the phase-flip channels, which are applied for all qubits after each gate with a probability of $p = 0.0001$. The Trotter step is chosen as $20$ for single discrete time evolution $\Delta_y = 0.08$. As the long evolution term suffers a larger noise effect but has a smaller weight, this quantum algorithm may naturally resist some noise influence. As shown in Fig. 4, the result is affected by the noise since the scale of noise is large. However, this still can be mitigated to a certain lower level by error mitigation using the zero limit extrapolation method [32], which is well suitable for short-depth quantum circuits.

**V. CONTINUOUS VARIABLE ASSISTED STRATEGY**

In this section, we introduce an alternative iterative quantum algorithm with the assistance of continuous-variable quantum mode (qumode) [33, 34]. In this strategy, the Gaussian function of Hamiltonian is constructed by integration of unitary operators, which is completed by entangling qubit and qumode since the infinity integration naturally exists in qumode state [35, 36]. Qumode state can be presented as a Fock state $\sum_{n=0}^{\infty} c_n |n\rangle$ or a pair of conjugate quadrature states $\int_{-\infty}^{\infty} f_p(p) |p\rangle dp$ and $\int_{-\infty}^{\infty} f_q(q) |q\rangle dq$, such as momentum $\hat{q}$ and position $\hat{p}$ of photons. Consider a finite squeezed state $|\phi\rangle = s^{-1/2} e^{-q^2/2\sigma^2} |p\rangle dp$, where $s$ is the squeezing factor, and this qumode is finitely squeezed on momentum space and extended on position space.

The Gaussian filter operator can be constructed by firstly performing a unitary operator $e^{-i\hat{H}_B}$ on the hybrid qubit-qumode initial state $|\psi_i\rangle |\phi\rangle$ then projecting the ancillary qumode on $|\phi\rangle$ by homodyne measurement [37].

**FIG. 2. Demonstration of the ground state energy estimation by QGF algorithm for a $N = 8$ qubits transverse-field Ising model.** The discrete parameters are set as $\Delta_y = 0.16$ and $M_y = 50$. (a) Energy between exact ground state energy and the estimated one for different minus shift-energy $\mu$. Red, green, and blue lines correspond the cases $1/\sigma^2 = 1, 1.5$, and $2$. (b) Energy difference as a function of $1/\sigma^2$. Red, green, and blue lines correspond the cases $\mu = -2, -3$, and $-4$.

**FIG. 3. Energy difference between estimated ground state energy and the exact ground state energy as a function of max evolution time.** The red, green, and blue lines correspond to the case of $N = 6, 8$, and $10$. 

**FIG. 4.**
The result state is shown as

\[ \langle \phi | e^{-iHt} \hat{\phi} | \psi_i \rangle = \frac{1}{\sqrt{s}} \int_{-\infty}^{\infty} e^{-p^2/s^2} e^{-ipft} \langle \psi_i | dp \]

\[ = \frac{1}{\sqrt{C}} \sum_j b_j e^{-s\lambda_j^2/2} | \psi_i \rangle, \]

where \( \frac{1}{\sqrt{C}} = \frac{1}{\sqrt{\sum_j b_j^2 e^{-s\lambda_j^2}}} \) is the normalization factor and determines the successful projection rate of qumode. The projection process is accomplished by squeezing the ancillary qumode then measuring the vacuum state, which is a post-selection process. The above equation indicates that both larger squeezing factor and scale of eigenvalues lead to higher accuracy but lower successful projection rate. Moreover, squeezing factor \( s/2 \) represents the inverse of the variance of the Gaussian filter \( 1/\sigma^2 \), and shift-energy is encoded into Hamiltonian.

Our strategy is iteratively increasing the shift-energy applied with a fixed squeezing factor \( s \) to estimate the ground state \( |\lambda_0\rangle \) and its corresponding eigenvalue \( \lambda_0 \) until the desired accuracy is reached. Compared to the hybrid quantum-classical approach, this one does not need to measure many discrete terms but cannot adjust the parameters of Gaussian filter classically.

We demonstrate this continuous-variable assisted QGF algorithm by solving the approximate ground state and its corresponding energy of a transverse-field Ising model with \( J = 1 \), \( g = 2 \), and \( N = 4 \). The squeezing factor and max Fock state of qumode are set as \( s = 1 \) and \( cut = 50 \), and a random initial state is applied. As the exact ground state energy is \(-8.543\) without applying external shift-energy, it starts from shifting exact ground state energy to zero, and then it is gradually increased. Fig. 5 shows that result error exponentially decays, but required measurement times exponentially grow as shift-energy rises. In practice, this procedure can stop when a result with the desired accuracy is obtained.

Lastly, we briefly analyze the time complexity of this continuous-variable assisted quantum algorithm. Consider the case of solving a gapped model with a well-prepared initial state under the same assumption as mentioned in Sec. 111. The result state after the Gaussian filter is performed approximated as \( |\psi_f\rangle \sim O(\frac{1}{\sqrt{N}}) e^{-s\lambda_0^2} |\lambda_0\rangle + O(\frac{\sqrt{\lambda_0}}{\sqrt{N}}) e^{-s(\lambda_0+\Delta)^2} |\lambda_{\perp}\rangle \). The requirement of the ground state energy scale is \( \lambda_0 = O(s^{-1}\log(N/\epsilon')) \) for solving approximate ground state with the desired accuracy \( \epsilon' \). The repetition times should be \( O(e^{\log^2(N/\epsilon')/2s}) \), and the circuit depth is \( O(N^3/\epsilon') \) while considering the first order Trotter decomposition. The time complexity in total is \( O(N^3 e^{\log^2(N/\epsilon')/2s}/\epsilon') \). For a squeezing factor \( O(\log^2(N/\epsilon')) \), a polynomial time complexity \( O(N^3/\epsilon') \) can be reached.
VI. CONCLUSION

We have proposed a hybrid quantum-classical algorithm for solving the approximate ground state energy well suited on NISQ computers. By approximately constructing a Gaussian filter as a linear combination of unitary operators and expressing the estimated energy as a weighted summation of state overlap, the best-performance coefficient can be obtained with the help of post-processing to exploit the quantum resources efficiently. This strategy solves an approximate ground state energy with a time complexity that is a polynomial of system size and the desired accuracy, showing quantum advantages. After solving the ground state energy, any other expectation values of observable for the ground state can be estimated by replacing $H$ with an observable operator $A$.

We have shown the performance of our algorithm by solving the ground state energy of a transverse-field Ising model with numeral simulations. In practice, this algorithm can be used iteratively by extending the evolution time series to obtain a higher accuracy result. Moreover, we have also simulated our algorithm under a noisy environment, which still performs well with the help of error mitigation without using any ancilla. A continuous-variable assisted iterative quantum algorithm has also been presented, which constructs the Gaussian filter by qubit-qumode entanglement and solves the approximate ground state by iteratively increasing the applied shift-energy. Its time complexity can be a quasi-polynomial of system size and the desired accuracy if a well-prepared initial state can be offered. This alternative method is well suited for hybrid qubit-qumode quantum processors, and the numerical demonstration shows its good performance.

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