Performance of quantum approximate optimization algorithm for preparing non-trivial quantum states: dependence of translational symmetry and improvement

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The variational preparation of complex quantum states using the quantum approximate optimization algorithm (QAOA) is of fundamental interest, and becomes a promising application of quantum computers. Here, we systematically study the performance of QAOA for preparing ground states of target Hamiltonians near the critical points of their quantum phase transitions, and generating Greenberger-Horne-Zeilinger (GHZ) states. We reveal that the performance of QAOA is related to the translational invariance of the target Hamiltonian: Without the translational symmetry, for instance due to the open boundary condition (OBC) or randomness in the system, the QAOA becomes less efficient. We then propose a generalized QAOA assisted by the parameterized resource Hamiltonian (PRH-QAOA), to achieve a better performance. In addition, based on the PRH-QAOA, we design a low-depth quantum circuit beyond one-dimensional geometry, to generate GHZ states with perfect fidelity. The experimental realization of the proposed scheme for generating GHZ states on Rydberg-dressing atoms is discussed. Our work paves the way for performing QAOA on programmable quantum processors without translational symmetry, especially for recently developed two-dimensional quantum processors with OBC.

I. INTRODUCTION

With recent experimental developments in the controllability of noisy intermediate scale quantum (NISQ) computers [1, 2], more and more attention has been paid to the variational quantum simulation (VQS) [3–8]. One primary task of the VQS is estimating the ground-state energy and preparing the ground state of many-body quantum systems, as target Hamiltonians, via hybrid quantum-classical variational algorithms, which is known as variational quantum eigensolvers (VQEs). A central ingredient of VQEs is the design of parametrized quantum circuits. For instance, a type of VQE, which is based on the hardware efficient ansatz comprised of layers of single-qubit rotation gates and blocks of non-parametrized entangling gates, has been applied to solve the ground-state energy of molecules [9–13] and condensed-matter systems [9, 14].

An alternative approach is the VQE inspired by the quantum approximate optimization algorithm (QAOA), which is originally employed to solve combinatorial optimization problems, such as the MaxCut problem [15–22], and the Maximum Independent Set problem [23].

More recently, numerical works show that the QAOA-inspired VQE can be used to efficiently prepare the ground states of quantum systems [24–30] as well. Experimentally, the ground states of both long-range and short-range Ising models have been generated using the QAOA on trapped-ion quantum simulators [31, 32]. Other important applications of the QAOA include the demonstration of quantum advantage [33, 34], and the generation of the Greenberger-Horne-Zeilinger (GHZ) state [24, 35].

Different from the VQE based on the hardware efficient ansatz, the quantum circuit of the QAOA-inspired VQE belongs to a family of problem-inspired ansatz [8]. More specifically, it is also called the Hamiltonian variational ansatz [25], because the design of the quantum circuit is closely related to the target Hamiltonian. Moreover, it is worthwhile emphasizing that while there exist barren plateaus on the optimization landscape of both VQEs based on the hardware efficient ansatz [36] and QAOA, the effect of barren plateaus is weaker for the latter [25].

The figure of merit for a VQE boils down to the distance of the VQE final state from the target state. Ingredients that affect the performance of the QAOA on ground-state preparation have been widely explored. It has been shown that essentially, the success of the QAOA depends on the depth of the quantum circuit. Specifically, the ground states of one-dimensional (1D) transverse field Ising model (TFIM) with periodic boundary conditions...
condition (PBC) and a system size $N$ can be prepared using the QAOA with a perfect fidelity $f = 1$, as long as the depth $p$ satisfies $p \geq N/2$ [24]. Moreover, it has been observed in Ref. [26], through numerically simulating the ground-state preparation for the non-integrable Ising models, that the perfect fidelity $f = 1$ with $p = N/2$ is only attainable for the scenario where the target ground state perturbs near closest free-fermion states.

In this work, we study the performance of QAOA for preparing the ground states of several target Hamiltonians, such as the 1D and two-dimensional (2D) TFIMs with both PBC and open boundary condition (OBC), the Ising model with random interactions and transverse-field strengths, and the 1D Heisenberg model with both PBC and OBC. In contrast to previous works which were mainly restricted to target Hamiltonians with PBC, i.e., translation-invariant systems, our results show that it is harder to perform QAOA without translation-invariant symmetry, for instance due to the OBC or strong randomness. To more efficiently prepare the those ground states, we propose a generalized QAOA-inspired VQE assisted by parametrized resource Hamiltonians (PRHs), and numerically demonstrate its advantage through several concrete examples.

In addition to the ground states preparation, we also pay attention to the generation of high-fidelity GHZ states via QAOA. We find that the PBC is necessary to achieve perfect fidelity of the $N$-qubit GHZ state by using the 1D quantum circuit of the conventional QAOA with a depth $N/2$, and the fidelity significantly drops for the 1D OBC quantum circuit with the same depth. Using the QAOA assisted by the PRH (PRH-QAOA), however, we can also obtain the perfect fidelity employing the 1D quantum circuit with a depth of $N/2$ even for OBC. Finally, enlightened by the PRH-QAOA, we propose a quantum circuit with a cross-shape geometry beyond 1D, which can generate the $N$-qubit GHZ state ($N$ is odd because of the geometry) with perfect fidelity, requiring a low circuit depth $p = (N - 1)/2$. We also discuss its experimental realization on Rydberg-dressing atoms.

II. VARIATIONAL QUANTUM EIGENSOLVER BASED ON THE QUANTUM APPROXIMATE OPTIMIZATION ALGORITHM

A. Quantum circuit and algorithm

Here, we briefly introduce the quantum circuit and algorithm of the VQE inspired by the conventional QAOA. The VQE algorithm aims to generate the ground state of a target Hamiltonian $\hat{H}^{(T)}$, which can be often divided into $M \geq 2$ parts, i.e., $\hat{H}^{(T)} = \sum_{j=1}^{M} \hat{H}_{j}^{(T)}$ with $[\hat{H}_{j}^{(T)}, \hat{H}_{j+1}^{(T)}] \neq 0$ and any two terms inside each $\hat{H}_{j}^{(T)}$ commute with each other. We define the unitary matrix $U_{j}(x) = \exp(-ix\hat{H}^{(T)}_{j})$, and the quantum circuit of the QAOA-inspired VQE can be realized by repeatedly performing cycles of operations which consist of sequentially switching on the terms from $\hat{H}_{M}^{(T)}$ to $\hat{H}_{1}^{(T)}$ as

$$U(x) = \prod_{n=1}^{p} [U_{1}(x_{1}^{(n)})U_{2}(x_{2}^{(n)}) \ldots U_{M}(x_{M}^{(n)})]$$  \hspace{1cm} (1)

with $p$ being the depth of the quantum circuit, and $x = (x_{1}^{(1)}, x_{2}^{(1)}, \ldots, x_{M}^{(1)}, x_{1}^{(2)}, \ldots, x_{M}^{(2)})$. The parametrized final state of the quantum circuit is $|\psi(x)\rangle = U(x)|\psi_{0}\rangle$ with $|\psi_{0}\rangle$ being the initial state which can be chosen as the ground state of $\hat{H}_{j}^{(T)}$ ($j \neq M$). Then, the energy $E(x) = \langle \psi(x)|\hat{H}^{(T)}|\psi(x)\rangle$ and the fidelity $f(x) = \langle \psi_{\text{GS}}|\psi(x)\rangle^{2}$, where $|\psi_{\text{GS}}\rangle$ is the ground state of $\hat{H}^{(T)}$, can be directly obtained.

We can generate a final quantum state $|\psi(x)\rangle$, which is close to the ground state $|\psi_{\text{GS}}\rangle$ via a hybrid quantum-classical procedure, where the unitary evolution $U(x)$ are simulated and cost functions are measured on quantum computers, and the optimization of parameters $x$ is performed on classical computers. In this work, we adopt the BFGS method, a gradient-based approach, to optimize the cost functions.

B. Performance of the QAOA-inspired VQE

We first consider the 1D ferromagnetic TFIM with $N = 12$ as the target Hamiltonian, i.e., $\hat{H}^{(T)} = -\sum_{i=1}^{N} \hat{\sigma}_{x}^{i} \hat{\sigma}_{x}^{i+1} - \lambda \sum_{i=1}^{N} \hat{\sigma}_{z}^{i}$ for PBC ($i + N \equiv i$) and $\hat{H}^{(T)} = -\sum_{i=1}^{N-1} \hat{\sigma}_{z}^{i} \hat{\sigma}_{z}^{i+1} - \lambda \sum_{i=1}^{N} \hat{\sigma}_{z}^{i}$ for OBC. We choose $M = 2$. According to Eq. (1), the parametrized quantum circuit can be written as

$$U(x) = \prod_{n=1}^{p} [U_{1}(x_{1}^{(n)})U_{2}(x_{2}^{(n)})]$$  \hspace{1cm} (2)

with

$$U_{2}(x_{2}^{(n)}) = \exp(ix_{2}^{(n)} \sum_{i=1}^{N} \hat{\sigma}_{z}^{i} \hat{\sigma}_{z}^{i+1})$$  \hspace{1cm} (3)

and

$$U_{1}(x_{1}^{(n)}) = \exp(ix_{1}^{(n)} \sum_{i=1}^{N} \hat{\sigma}_{z}^{i})$$  \hspace{1cm} (4)

The initial state $|\psi_{0}\rangle = \bigotimes_{i=1}^{N} |+\rangle$, is the ground state of $\hat{H}^{(T)} = -\lambda \sum_{i=1}^{N} \hat{\sigma}_{z}^{i}$ ($\lambda > 0$), where $|+\rangle_{j}$ is the eigenstate of $\hat{\sigma}_{z}^{j}$ with the eigenvalue $+1$. Here, we focus on the critical point, i.e., $\lambda = 1$, separating the ferromagnetic and

\begin{itemize}
    \item \textbf{A. Quantum circuit and algorithm}
\end{itemize}
perfect fidelity is not achievable. This can be interpreted as the 1D and 2D models, the infidelities for PBC are larger than for OBC. The results for both OBC and PBC are displayed in Fig. 1(b). It is shown that for both the 1D and 2D models, the infidelities for PBC are larger than those for OBC when the circuit depth is shallow, whereas it is the opposite for deep circuits.

Moreover, for the 2D TFIM with both PBC and OBC, a perfect fidelity is not achievable. This can be interpreted by the fact that the 2D TFIM can not be mapped to free fermions via the Jordan-Wigner and Bogoloibov transformations [40], and this result generalizes the conjecture of Ref. [26] to 2D systems, suggesting that perfect fidelity of the QAOA-inspired VQE relies on the target Hamiltonian with a free-fermion-like ground state.

III. IMPROVEMENT OF THE VARIATIONAL QUANTUM EIGENSOLVER

A. Basic idea

For the QAOA-inspired VQE, the design of the quantum circuit is closely related to the target Hamiltonian \( \hat{H}^{(T)} \). Here, we explore whether the performance of the VQE can be improved if we adopt a resource Hamiltonian \( \hat{H}^{(R)} \), which is not identically to the target Hamiltonian. The resource Hamiltonian \( \hat{H}^{(R)} \) is then parametrized as \( \hat{H}^{(R)} = \hat{H}^{(R)}(y) \), where \( y = (y_1, y_2, \ldots, y_L) \). The quantum circuit based on the parametrized resource Hamiltonian (PRH) \( \hat{H}^{(R)} \) reads

\[
U(x, y) = \prod_{n=1}^{p} [U_1^{(R)}(x_1^{(n)}, y) \ldots U_M^{(R)}(x_M^{(n)}, y)],
\]

where \( U_j^{(R)}(x, y) = \exp[-i x \hat{H}_j^{(R)}(y)] \), and \( \hat{H}_j^{(R)}(y) = \sum_{j=1}^{M} \hat{H}_j^{(R)}(y) \) with \( \{ \hat{H}_j^{(R)}(y), \hat{H}_j^{(R)}(y) \} \neq 0 \). We note that the parameters \( y \) are fixed all the way through the evolution, i.e., \( n = 1, 2, \ldots, p \) in Eq. 5, and cannot be absorbed to the parameters \( x \). Next, by optimizing the cost functions, for example the energy and the fidelity, in the parameter space \( x \) and \( y \), it is possible to obtain a lower energy or higher fidelity than the conventional QAOA-inspired VQE with \( \hat{H}^{(R)}(y) \equiv \hat{H}^{(T)} \). In this paper, the generalized QAOA assisted by the PRH is labeled as PRH-QAOA for short.

Actually, it has been numerically shown that employing the 1D Heisenberg model as the resource Hamiltonian, one can efficiently prepare the ground state of a modified Haldane-Shastry Hamiltonian, providing a revelation as to making the resource Hamiltonian different from the target one in designing QAOA-inspired VQEs [25]. We emphasize, however, that in Ref. [25], the Heisenberg model as the resource Hamiltonian \( \hat{H}^{(R)} \) is non-parametrized. Different from Ref. [25], here we consider a PRH \( \hat{H}^{(R)} = \hat{H}^{(R)}(y) \), and will later find out the most appropriate \( \hat{H}^{(R)} \) for preparing ground states of other \( \hat{H}^{(T)} \). More technical details of the QAOA-inspired VQE with 1D Heisenberg models being the resource Hamiltonian can be found in Appendix A.
inset of (e) shows the ratio of the depth obtained after optimization as a function of the depth with a depth.

FIG. 2. (a) The optimized parameter \( J_{i,i+1}^{\text{opt}} \) as a function of the spatial index \( i \) obtained from the quantum circuit Eq. (5) with a depth \( p = 6 \). (b) The optimized parameter \( h_i^{\text{opt}} \) as a function of the spatial index \( i \) obtained from the quantum circuit Eq. (5) with a depth \( p = 6 \). (c) is similar to (a) but for the quantum circuit with a depth \( p = 12 \). (d) is similar to (b) but for the quantum circuit with a depth \( p = 12 \). (e) The infidelities \( 1 - f \) obtained after optimization as a function of the depth \( p \). The inset of (e) shows the ratio \( R \) defined by Eq. (8) as a function of the depth \( p \).

B. Application 1: one-dimensional transverse-field Ising model with open boundary condition as the target Hamiltonian

In Fig. 1(a), we have seen the performance of conventional QAOA on 1D TFIM with OBC is less efficient. Here, we apply the PRH-QAOA to improve the performance of the VQE. The target Hamiltonian is still \( \hat{H}^{(T)} = -\sum_{i=1}^{N-1} \hat{\sigma}_i^z \hat{\sigma}_{i+1}^z - \sum_{i=1}^{N} \hat{\sigma}_i^x \) with \( N = 12 \), and we adopt a more generic Ising model as the resource Hamiltonian, which is divided into \( \hat{H}^{(R)}(y) = \hat{H}_1^{(R)}(h) + \hat{H}_2^{(R)}(J) \) with

\[
\hat{H}_1^{(R)}(h) = -\sum_{i=1}^{N} h_i \hat{\sigma}_i^z,
\]

and

\[
\hat{H}_2^{(R)}(J) = -\sum_{i=1}^{N-1} J_{i,i+1} \hat{\sigma}_i^z \hat{\sigma}_{i+1}^z.
\]

That is we generalize the \( \hat{H}^{(R)} \) to allow for parametrized site-dependent interactions and fields therein. It is obvious that the PRH covers the target Hamiltonian, being the \( \hat{H}^{(R)} \) in the conventional QAOA, as a subset with \( J_{i,i+1} = J \) and \( h_i = h, \forall j \). With the above resource Hamiltonian, the parameter space of the quantum circuit (5) is \( x \cup y \) with \( x \) being the same as the parameters in Eq. (2)-(4), and \( y = h \cup J = (h_1, h_2, \ldots, h_N) \cup (J_{1,2}, J_{2,3}, \ldots, J_{N-1,N}) \). With \( h_i \geq 0 \) for all \( i = 1, 2, \ldots, N \), the initial state is chosen as \( |\psi_0\rangle = \bigotimes_{i=1}^{N} |+\rangle_i \). Then, we can numerically obtain the final state \( |\psi(x, y)\rangle = U(x, y)|\psi_0\rangle \), and calculate the corresponding cost functions.

After optimizing the fidelity as the cost function, we demonstrate that for the 1D TFIM with OBC, the system with uniform interaction and magnetic field is not the optimal choice. We present two examples of the optimized \( h \) and \( J \) in Fig. 2(a)-(d). It is noted that there exists an inversion symmetry for the optimized parameters, i.e., \( J_{i,i+1}^{\text{opt}} = J_{N-i,N-i+1}^{\text{opt}} \) and \( h_i^{\text{opt}} = h_{N-i}^{\text{opt}} \).

In Fig. 2(e), we plot the infidelities \( 1 - f \) after optimization for the VQE based on the quantum circuit Eq. (1) and Eq. (5), known as the conventional QAOA and the PRH-QAOA, respectively. Moreover, to quantify the improvement of the PRH-QAOA-inspired VQE, we define a ratio

\[
R = \frac{(1 - f^C) - (1 - f^{\text{PRH}})}{1 - f^C} = \frac{f^{\text{PRH}} - f^C}{1 - f^C}
\]

with \( f^{\text{PRH}} \) and \( f^C \) being the fidelity after optimization of the VQE based on the PRH-QAOA and conventional QAOA, respectively, and plot the value of \( R \) as a function of the depth of quantum circuit \( p \) in the inset of Fig. 2(e).

C. Application 2: two-dimensional transverse-field Ising model as the target Hamiltonian

We now employ the PRH-QAOA-inspired VQE to generate the ground states of 2D ferromagnetic TFIM with \( N = 9 \) and \( \lambda = 3.05 \). Here, we focus on the model...
with OBC since the open-boundary system is experimentally more relevant for 2D superconducting circuits [41–43] and Rydberg quantum simulators [44–47]. We consider the resource Hamiltonian \( \hat{H}^{(R)}(y) = \hat{H}_1^{(R)}(h) + \hat{H}_2^{(R)}(J) \) with \( \hat{H}_1^{(R)}(h) \) being the same as Eq. (6) and
\[
\hat{H}_2^{(R)}(J) = \sum_{(i,j)} J_{i,j} \hat{\sigma}_i^z \hat{\sigma}_j^z, \tag{9}
\]
which describes ferromagnetic Ising interactions on a 2D square lattice.

As shown in Fig. 3(a) and (c), a lower infidelity \( 1 - f \) can be obtained using the VQE based on the PRH-QAOA. We present an example of the optimized \( y \) for the resource Hamiltonian in Fig. 3(b). It is revealed that the optimized \( y \) satisfies both the inversion symmetry and rotation symmetry.

### D. Remarks

We also apply the PRH-QAOA-inspired VQE to the 2D TFIM with PBC and find out that \( \hat{H}^{(R)}(y) \equiv \hat{H}^{(T)} \) is the optimal choice, namely generalizing the QAOA to admit site-dependent parameter in the \( \hat{H}^{(R)} \) does not help for the target Hamiltonians with PBC.

Additionally, we also consider the Heisenberg model as the target Hamiltonian, and study the performance of both VQE inspired by the conventional QAOA and PRH-QAOA. The results and corresponding discussions are presented in Appendix A. The Heisenberg model is an integrable model exactly solved using the Bethe ansatz [48]. However, the Heisenberg model cannot be mapped to free fermions, and thus the perfect fidelity cannot be obtained via the VQE with a \( N/2 \) depth of quantum circuit. The dependence of the performance of the conventional QAOA-inspired VQE on the boundary condition is the same as that we have revealed in the TFIMs. For the Heisenberg model with OBC being the target Hamiltonian, the PRH-QAOA-inspired VQE can also obtain a higher fidelity of the ground state than the conventional QAOA.

Moreover, in Appendix B, we present the results of the energy as the cost function, the 2D TFIM with other values of \( \lambda \), as well as the 2D TFIM with triangular geometry, as the target Hamiltonians. The additional data displayed in Appendix A and B demonstrate that the improvement of the VQE based on the PRH-QAOA can be observed in all cases studied.

### IV. Generating Ground States of Ising Models with Random Interactions and Transverse-Field Strengths

After revealing the influence of boundary condition on the performance of QAOA, both for the conventional and the PRH-assisted scenarios, we now consider another source that can break the translational invariance, i.e., the randomness. We focus on the TFIM with PBC as the target Hamiltonian
\[
\hat{H}^{(T)} = -\sum_{i=1}^N J^{(T)}_{i,i+1} \hat{\sigma}_i^z \hat{\sigma}_{i+1}^z -\sum_{i=1}^N h_i^{(T)} \hat{\sigma}_i^z, \tag{10}
\]
where the Ising interactions \( J^{(T)}_{i,i+1} \) and the transverse-field strengths \( h_i^{(T)} \) are drawn from a uniform distribution \((2 - D)/2, (2 + D)/2\) with \( D \) being the disorder strength. If \( D \to 0 \), the Hamiltonian (10) becomes translation-invariant. With the increase of \( D \), one can explore how the breakdown of the translational invariance influences the performance of the VQE.

Here, for the conventional QAOA-inspired VQE, the quantum circuit can be written as Eq. (2) with \( U_2(x_2^{(n)}) = \exp(\mathrm{i} x_2^{(n)} \sum_{i=1}^N h_i^{(T)} \hat{\sigma}_i^z) \) and \( U_1(x_1^{(n)}) = \exp(\mathrm{i} x_1^{(n)} \sum_{i=1}^N J_{i,i+1}^{(T)} \hat{\sigma}_i^z \hat{\sigma}_{i+1}^z) \). For the PRH-QAOA-inspired VQE, the quantum circuit can be described by Eq. (5) with the resource Hamiltonian \( \hat{H}^{(R)} = \hat{H}_1^{(R)}(h) + \hat{H}_2^{(R)}(J) \), where \( \hat{H}_1^{(R)}(h) \) is the same as
Eq. (6), and \( \hat{H}_{2}^{(R)}(J) = - \sum_{i=1}^{N} J_{i,i+1} \hat{\sigma}_{+}^{i} \hat{\sigma}_{-}^{i+1} \) with \( J = (J_{1,2}, J_{2,3}, \ldots, J_{N,1}) \) for \( N = 12 \). We consider three disorder strengths \( D = 1, 0.1, \) and \( 0.01 \).

The results obtained from the VQE based on the conventional QAOA and PRH-QAOA are plotted in Fig. 4(a), where the infidelities are obtained by averaging 10 samples of \( J_{i,i+1} \) and \( h_{i}^{(T)} \) for each \( D \). It is shown that the performance of the VQEs is always better for smaller \( D \) regardless of the conventional QAOA or PRH-QAOA, and for each given \( D \), the VQE based on PRH-QAOA always outperforms the conventional one. Moreover, as shown in Fig. 4(b), when the depth \( p \geq 6 \), the improvement becomes significant. In Fig. 4(c) and (d), we also present an example of optimized parameters in the resource Hamiltonian \( \hat{H}^{(R)} \).

V. GENERATING THE GREENBERG-HORNE-ZEILINGER STATE VIA THE IMPROVED QUANTUM APPROXIMATE OPTIMIZATION ALGORITHM

The GHZ states, as a type of multipartite entangled states, are central for numerous quantum-based technologies, ranging from quantum teleportation [49], quantum metrology [50] to quantum error-correcting codes [51]. Experimental generation of high-fidelity GHZ states has been achieved on various quantum platforms, including superconducting circuits [52–55], trapped ions [56, 57] and Rydberg atoms [58, 59]. Nowadays, how to generate high-fidelity and large-scale GHZ states remains a central topic in quantum physics, and new schemes of preparing multi-qubit GHZ states are timely in need.

A. One-dimensional quantum circuit

Using the 1D quantum circuit Eq. (2-4), adopting the PBC, with the initial state \( |\psi_{0}\rangle = \bigotimes_{i=1}^{N} |\uparrow\rangle_{i} \) and a cost function

\[
\begin{align*}
    f & \equiv |\langle \text{GHZ} | \psi(x) \rangle|^{2}, \\
    \text{where} |\text{GHZ}\rangle & \text{refers to a \( N \)-qubit GHZ state defined as} \\
    |\text{GHZ}\rangle & \equiv \bigotimes_{i=1}^{N} |\uparrow\rangle_{i} + \bigotimes_{i=1}^{N} |\downarrow\rangle_{i} \sqrt{2}
\end{align*}
\]

(11)

(12)

with \( |\uparrow (\downarrow)\rangle_{i} \) being the eigenstate of \( \hat{\sigma}_{z}^{i} \) with the eigenvalue \(+1(-1)\), it has been numerically shown that a \( N \)-qubit GHZ state with a perfect fidelity \( f \approx 1 \) can be generated via the QAOA with a depth \( p = N/2 \) [24] [also see the results in Fig. 5(a)].

It has been pointed out that the performance of the QAOA-inspired VQE depends on the boundary condition of the quantum circuit (see Fig. 1). Here, we demonstrate that a perfect fidelity cannot be achieved when employing the OBC in Eq. (2). As shown in Fig. 5(a), with the OBC, a 12-qubit GHZ state with a perfect fidelity can be generated if the depth of the QAOA is \( p = 12 \), much deeper than the required depth \( p = N/2 = 6 \) when the PBC is adopted. Next, in order to generate a GHZ state with a perfect fidelity using a shallower depth of the OBC quantum circuit, we consider the PRH-QAOA with the circuit Eq. (5) and the resource Hamiltonian Eq. (6) and (7). The results of infidelity \( 1 - f \) is plotted in Fig. 5(a), and the optimized parameters in the resource Hamiltonian are dis-
FIG. 5. (a) The infidelities $1 - f$ with $f$ being the GHZ state fidelity, obtained after optimization, as a function of the depth $p$. The resource Hamiltonian is chosen as the 1D transverse-field Ising model with OBC or PBC. The inset of (a) plots the $1 - f$ as a function of the depth $p$ in a linear y-axis. (b) The optimized parameter $J_{i,i+1}^\text{opt}$ as a function of the spatial index $i$ obtained from the PRH-QAOA with a depth $p = 6$. (c) is similar to (b) but for the optimized parameter $h_i^\text{opt}$.

It is seen that a 12-qubit GHZ state with $f \approx 1$ can be generated via the PRH-QAOA with a depth $p \geq 6$ of the OBC quantum circuit.

B. Quantum circuit beyond one-dimensional geometry

We also study the performance of QAOA for generating GHZ states using a 2D quantum circuit with a size $N = 3 \times 3$, i.e., the TFIM on 2D square lattice as the resource Hamiltonian [see the inset of Fig. 1(b)]. We first focus on the conventional QAOA for 2D quantum circuits with both OBC and PBC, in comparison with the results of 1D quantum circuit with PBC. The results of the GHZ state fidelity are shown in Fig. 6(a). For a 1D PBC quantum circuit with $N = 9$, the fidelity reaches a value $1 - f \approx 10^{-11}$ when $p = 4$, and a perfect fidelity $1 - f \approx 10^{-15}$ can be achieved when $p \geq 5$. For a 2D PBC quantum circuit, a perfect fidelity is attainable when $p \geq 4$. However, with a depth $p \geq 5$ the obtained GHZ state fidelities are much smaller for the 2D OBC quantum circuit than those for the PBC quantum circuit.

Here, we consider the PRH-QAOA with a 2D OBC quantum circuit. The resource Hamiltonian is the summation of Eq. (6) and Eq. (9). As shown in Fig. 6(a), a 9-qubit GHZ state with perfect fidelity can be generated by the algorithm with a quite shallow depth $p = 2$ of the quantum circuit. The optimized parameters are presented in Fig. 6(b). It is revealed that there are four ferromagnetic Ising interactions whose strength is 0, marked by the dashed lines in Fig. 6(b), in the resource Hamiltonian Eq. (9). Moreover, for the resource Hamiltonian Eq. (6), the strength of transverse field of the central qubit is 0.

The resource Hamiltonian with the parameters obtained after optimization leads to a Ising model with a cross-shape geometry of the interactions, as plotted in Fig. 6(c). The size of the quantum circuit with the cross-shape geometry is scalable, i.e., $N = 5 + 4m$ ($m = 0, 1, \ldots$) [see Fig. 7 (b) and (c)]. Furthermore, the transverse-field strength of the central spin of the resource Hamiltonian is fixed as 0. As shown in Fig. 7(a), 13-qubit and 17-qubit GHZ state with perfect fidelity can be generated by the algorithm with the 3-depth and 4-depth quantum circuit, respectively, indicating that employing the Ising model with the special geometry
FIG. 7. (a) The infidelities 1 − f with f being the GHZ state fidelity, obtained after optimization, as a function of the depth p, with the system size N = 13 and N = 17. (b) The geometry of the Ising interactions (presented as the solid lines) of the resource Hamiltonian with N = 13. (c) is similar to (b) but for the system size N = 17.

and parameters as the resource Hamiltonian, the QAOA quantum circuit with a depth m can generate (5 + 4m)-qubit GHZ state with perfect fidelity.

We note that the shallow depth of the quantum circuit with the ability of generating perfect-fidelity GHZ states benefits from the special geometry of the resource Ising Hamiltonian plotted in Figs. 6(c), 7(b), and 7(c). In Appendix C, it is seen that using the square-lattice Ising model with N = 16, both the conventional QAOA and PRH-QAOA can not generate the perfect-fidelity GHZ state with a 4-depth quantum circuit.

C. Rydberg dressing scheme of realizing the improved QAOA for generating the Greenberg-Horne-Zeilinger state

In neutral-atom quantum processors, GHZ states with a fidelity f > 0.5 have been prepared via the optimal control of the adiabatic dynamics [58, 60], and digital-gate-model quantum circuits with CNOT gates implemented on local pairs of atoms [59]. Here, we discuss the experimental realization of generating the GHZ state via the PRH-QAOA with the special geometry in Fig. 6(c), 7(b) and (c), in Rydberg-dressing neutral atoms [61–63], accompanied with recent developed mixed-species atom arrays [64, 65].

We first consider the generation of the 9-qubit GHZ state. The realization of this protocol requires an Ising interaction −∑_{(i,j)} J_{i,j} \hat{\sigma}_i^z \hat{\sigma}_j^z with \langle i, j \rangle meaning the nearest-neighbor sites i and j on the lattice in Fig. 6(c) [also see Fig. 8(a)]. For Rydberg-dressing quantum processors, qubits are encoded in two hyperfine ground states \ket{\downarrow} and \ket{\uparrow}, with one of the ground state \ket{\uparrow} coupled to a Rydberg state \ket{R} via a laser field of detuning δ and Rabi frequency Ω [61–63]. When Ω/δ ≪ 1, the Rydberg-dressing state can induce a pairwise energy shift dependent on the distance between two atoms, which can be described by the Hamiltonian

\[ \hat{H}_D = \sum_{(i,j)} V_{i,j} \hat{n}_i \hat{n}_j, \]  

(13)

where \hat{n}_i = \ket{\uparrow}_i \bra{\uparrow}_i, \hat{n} = (\hat{\sigma}_z^i + 1)/2 with 1 being the two-dimensional identity matrix, and the strength of Rydberg-dressing interaction reads

\[ V_{i,j} = V_0 \frac{R_0^6}{|r_i - r_j|^6 + R_0^6}, \]  

(14)

with the positions of atoms \( r_{i,j} \), \( V_0 = \hbar \Omega^2/8\delta^3 \), \( R_C = |C_0/2\hbar \delta|^{1/6} \), and \( C_0 \) being the van der Waals coefficient of the Rydberg state. We define the unitary dynamics of \( \hat{H}_D \) as \( U_{NN}(t) = \exp(-it\hat{H}_D) \). By using a spin echo shown in Fig. 8(c), one can realize the Ising dynamics [see Fig. 8(b)]

\[ U_{ZZ}(\gamma) = \exp[-i\gamma \sum_{(i,j)} (V_{i,j}/4) \hat{\sigma}_i^z \hat{\sigma}_j^z]. \]  

(15)

According to Eq. (14), non-local interactions should be considered. Here, we take into account the additional
interactions presented as \( J_0 \) in Fig. 8(a). The nearest-neighbor interactions includes \( J_1 \) and \( J_2 \) in Fig. 8(a). Both the interactions \( J_1 \) and \( J_2 \) can be adjusted by changing the corresponding intra-atom distance. In addition to the distance, the interaction \( J_1 \) can also be adjusted by choosing different species type-2 [see Fig. 8(a)] and different Rydberg states, which essentially results in different coefficient \( C_0 \). In short, the interactions \( J_0 \), \( J_1 \), and \( J_2 \) can be separately adjusted. Moreover, the Rydberg-dressing quantum processor with mixed-species atoms allows the single-qubit gate performed on the central qubit [the type-1 atom in Fig. 8(a)] except for the central one.

Enlightened by the results shown in Fig. 6(b), for the QAOA, the resource Hamiltonian is chosen as

\[
\hat{H}_1^{(R)} = - \sum_{i \in \text{type-1}} \hat{\sigma}_i^x,
\]

and

\[
\hat{H}_2^{(R)}(J_0, J_1, J_2) = - \sum_{\langle i,j \rangle} J_{i,j} \hat{\sigma}_i^z \hat{\sigma}_j^z,
\]

with \( J_{i,j} \in \{ J_0, J_1, J_2 \} \). Based on Eq. (5), the quantum circuit with a depth \( p = 2 \) can be written as

\[
U(x, y) = U_1^{(R)}(x_1) U_2^{(R)}(x_2, y)
\]

\[
\times U_1^{(R)}(x_1) U_2^{(R)}(x_2, y)
\]

with \( x = (x_1, x_2, x_2', x_2') \) and \( y = (J_0, J_1, J_2) \). The initial state is \( |\psi_0 \rangle = \otimes_{i=1}^N |\uparrow \rangle \). The preparation of the initial state \( |\psi_0 \rangle \) and the unitary evolution \( U_1^{(R)}(x) \) can be experimentally realized by imposing the microwave pulse on the qubits encoded by the hyperfine ground state \( | \uparrow \rangle \) and \( | \downarrow \rangle \) of neutral atoms [61, 62]. The unitary evolution \( U_2^{(R)}(x, y) \) is the same as Eq. (15), which can be realized by the dressing pulse and the spin echo [see Fig. 8(b) and (c)]. The optimization parameters for generating the GHZ state with perfect fidelity are \( y^{opt} = (4/3, 1, 1/3) \) and \( x^{opt} = (\pi/4, 3\pi/4, 3\pi/4, 3\pi/4) \).

Finally, we generalize the results of \( N = 9 \) to larger size \( N = 13 \) and 17 [see Fig. 9 for the geometry of the lattice with \( N = 17 \)]. Generating the perfect-fidelity GHZ with \( N = 13 \) and 17 requires the depth of the quantum circuit \( p = 3 \), and \( p = 4 \), respectively. For \( N = 13 \) and \( p = 3 \), the optimization parameters are \( y^{opt} = (4/3, 1, 1/3) \) and \( x^{opt} = (x_1, x_2, x_1, x_2, x_2, x_2') = (\pi/4, \pi/4, 3\pi/4, 3\pi/4, 3\pi/4, 3\pi/4) \). For \( N = 17 \) and \( p = 4 \), \( y^{opt} = (4/3, 1, 1/3) \) and \( x^{opt} = (x_1, x_2, x_2, x_1, x_2, x_2') = (\pi/4, \pi/4, \pi/4, 3\pi/4, 3\pi/4, 3\pi/4, 3\pi/4, 3\pi/4) \).

**VI. DISCUSSION**

We have studied the performance of the QAOA-inspired VQE for target Hamiltonians with and without translation-invariant symmetry. For systems without the symmetry, including the models with OBC or strong randomness, the performance of the VQE is less efficient, in comparison with the case of translation-invariant target Hamiltonians. In general, QAOA steers a controllable quantum system, which we call the resource Hamiltonian in this paper. Previous studies in the literature mainly focused on the QAOA-inspired VQE, restricted to the scenario that the resource Hamiltonian is exactly identical to the target Hamiltonian. We generalize the QAOA to allow the PRH to be possibly different from the target Hamiltonian. If the translation-invariant symmetry in the target Hamiltonian is broken, one can use the PRH-QAOA-inspired VQE to achieve higher fidelity of the target ground state or lower energy corresponding to the target Hamiltonian.

In the NISQ era, quantum computers are not perfectly translation-invariant, due to their OBC [18, 41–47, 66–69], and randomness induced by experimental imperfections. At the same time, for lack of efficient error correction technique for NISQ computers, the affordable circuit depth is also limited. Consequently, the improved QAOA-inspired VQE proposed in our work opens up an avenue for the VQE experimentally generating states closer to the target ground state than using the conventional protocol. Moreover, it is also shown that the perfect fidelity GHZ state can be generated by the PRH-QAOA with shallow-depth quantum circuit. Taking the non-local interactions in Rydberg-dressing quantum simulators [62] into consideration, we believe our work pro-

![FIG. 9. An array of mixed-species atoms with N = 17.](image-url)
vides an alternative way of generating high-fidelity GHZ states in neutral atoms.

Our work points to several further directions: (i) exploring how the translation-invariant symmetry of target Hamiltonians or quantum circuits can influence the performance of VQEs based on other ansatz, such as the hardware efficient ansatzes [9–14], (ii) exploring the performance of QAOA-inspired VQEs for other complex target Hamiltonians, such as trapped-ion systems with long-range interactions satisfying a power-law decay [4, 31, 32, 70], and (iii) finding more efficient ansatzes, taking the PRH into consideration, to design quantum circuits of VQEs, in combination with other QAOA-like subsequence, for example, the counterdiabatic QAOA [30, 71, 72] and the QAOA assisted by the quantum annealing [73, 74].

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Appendix A: Results for 1D Heisenberg models

The Hamiltonian of the 1D Heisenberg model with PBC is given by

\[ \hat{H} = \sum_{i=1}^{N} [\hat{\sigma}_i^x \hat{\sigma}_{i+1}^x + \hat{\sigma}_i^y \hat{\sigma}_{i+1}^y + \hat{\sigma}_i^z \hat{\sigma}_{i+1}^z]. \] (A1)

For the model with OBC, the superscript of the summation in Eq. (A1) is replaced by \(N - 1\). To prepare the ground states of the 1D Heisenberg model with both OBC and PBC, we design the quantum circuit of the QAOA-inspired QVE by employing Eq. (A1) with corresponding boundary condition being the resource Hamiltonian. The resource Hamiltonian (A1) is divided into four parts, i.e., \(H_{\text{even}}^{XY} + H_{\text{even}}^{Z} + H_{\text{odd}}^{XY} + H_{\text{odd}}^{Z}\), where \(H_{\text{even}}^{XY} = \sum_{i=1}^{N/2} [\hat{\sigma}_{2i-1}^{x} \hat{\sigma}_{2i}^{x} + \hat{\sigma}_{2i-1}^{y} \hat{\sigma}_{2i}^{y}], \ H_{\text{odd}}^{XY} = \sum_{i=1}^{N/2} [\hat{\sigma}_{2i-1}^{x} \hat{\sigma}_{2i}^{x} + \hat{\sigma}_{2i-1}^{y} \hat{\sigma}_{2i}^{y}], \ H_{\text{even}}^{Z} = \sum_{i=1}^{N/2} \hat{\sigma}_{2i-1}^{z} \hat{\sigma}_{2i}^{z} \) and \(H_{\text{odd}}^{Z} = \sum_{i=1}^{N/2} \hat{\sigma}_{2i-1}^{z} \hat{\sigma}_{2i}^{z} \). According to Eq. (1), the quantum circuit can be written as

\[ U(x) = \prod_{n=1}^{p} [U_1(x_1^{(n)}), U_2(x_2^{(n)}) U_3(x_3^{(n)}) U_4(x_4^{(n)})] \] (A2)

with \(U_1(x_1^{(n)}) = \exp(-ix_1^{(n)} \hat{H}_{\text{even}}^{Z}), \ U_2(x_2^{(n)}) = \exp(-ix_2^{(n)} \hat{H}_{\text{even}}^{XY}), \ U_3(x_3^{(n)}) = \exp(-ix_3^{(n)} \hat{H}_{\text{odd}}^{Z}), \) and \(U_4(x_4^{(n)}) = \exp(-ix_4^{(n)} \hat{H}_{\text{odd}}^{XY})\). The initial state of the VQE is chosen as the ground state of both \(\hat{H}_{\text{even}}^{Z}\) and
\[ H^{\text{even}}, \text{i.e., } |\psi_0\rangle = \bigotimes_{i=1}^{N/2} (|0\rangle_{2i-1}|1\rangle_{2i} - |1\rangle_{2i-1}|0\rangle_{2i}) / \sqrt{2}. \]

In Ref. [25], the quantum circuit (A3) has been employed to prepare the ground state of the modified Haldane-Shastry Hamiltonian
\[ H^{(T)} = \sum_{n,m} a_{nm} \left[ \hat{\sigma}_n^z \hat{\sigma}_m^z - \hat{\sigma}_n^x \hat{\sigma}_m^x - \hat{\sigma}_n^y \hat{\sigma}_m^y \right] \]
with a complex long-range interactions \(a_{nm} = \frac{N}{|n-m|}\). Here, the target Hamiltonian \( H^{(T)} \) is different from the resource Hamiltonian \( (A1) \) where the interactions are nearest-neighbor.

As shown in Fig. 10(a), the boundary condition of the 1D Heisenberg model still influences the performance of the conventional QAOA-inspired VQE, similar to the results in Fig. 1. To more efficiently prepare the ground state of the 1D Heisenberg model with OBC, we also briefly introduce the quantum circuit of the PRH-QAOA-inspired VQE according to Eq. (5). The PRH is
\[
\hat{H}^{(R)}(y) = \sum_{i=1}^{N-1} \left[ g_{i,i+1} \hat{\sigma}_i^x \hat{\sigma}_{i+1}^x + \hat{\sigma}_i^y \hat{\sigma}_{i+1}^y \right] \quad (A3)
+ \Delta_{i,i+1} \hat{\sigma}_i^z \hat{\sigma}_{i+1}^z,
\]
which is decomposed into four parts, i.e., \( \hat{H}^{(R)}(y) = \hat{H}_1^{(R)}(y_1) + \hat{H}_2^{(R)}(y_2) + \hat{H}_3^{(R)}(y_3) + \hat{H}_4^{(R)}(y_4) \) with
\[
\hat{H}_1^{(R)}(y_1) = \sum_{i=1}^{N/2} g_{2i-1,2i} \left[ \hat{\sigma}_{2i-1}^z \hat{\sigma}_{2i}^z + \hat{\sigma}_{2i-1}^x \hat{\sigma}_{2i}^x \right],
\hat{H}_2^{(R)}(y_2) = \sum_{i=1}^{N/2} \Delta_{2i-1,2i} \hat{\sigma}_{2i-1}^z \hat{\sigma}_{2i}^z,
\hat{H}_3^{(R)}(y_3) = \sum_{i=1}^{N/2} g_{2i,2i+1} \left[ \hat{\sigma}_{2i-1}^z \hat{\sigma}_{2i+1}^z + \hat{\sigma}_{2i-1}^x \hat{\sigma}_{2i+1}^x \right],
\hat{H}_4^{(R)}(y_4) = \sum_{i=1}^{N/2} \Delta_{2i,2i+1} \hat{\sigma}_{2i}^z \hat{\sigma}_{2i+1}^z.
\]
In comparison with the conventional QAOA-inspired VQE, the additional parameters in the resource Hamiltonian are \( y = y_1 \cup y_2 \cup y_3 \cup y_4 \), with \( y_1 = (g_{1,2}, g_{3,4}, \ldots, g_{11,12}), y_2 = (\Delta_{1,2}, \Delta_{3,4}, \ldots, \Delta_{11,12}), y_3 = (g_{2,3}, g_{4,5}, \ldots, g_{10,11}), \) and \( y_4 = (\Delta_{2,3}, \Delta_{4,5}, \ldots, \Delta_{10,11}) \). The results of the PRH-QAOA-inspired VQE are plotted in Fig. 10(b)-(d). Similar to the results in Fig. 2(a)-(d), the parameters of the resource Hamiltonian \( y \) obtained from optimization still satisfy an inversion symmetry [see Fig. 10(c) and (d)].

**Appendix B: Additional numerics of Ising models**

In this section, we present several additional numerical results. First, above studies mainly focus on the fidelity as the cost function. We now employ the energy as the cost function. The target Hamiltonian \( H^{(T)} \) is chosen as the critical 1D TFIM (\( \lambda = 1 \)) with both PBC and OBC. The system size is \( N = 12 \). For the conventional QAOA-inspired VQE, the quantum circuit is Eq. (2), and the energy is \( E(x) = \langle \psi(x) | H^{(T)} | \psi(x) \rangle \). For the PRH-QAOA-inspired VQE, the quantum circuit is Eq. (5), and the energy is \( E(x, y) = \langle \psi(x, y) | H^{(T)} | \psi(x, y) \rangle \) with the additional parameters \( y \) in Eq. (6) and (7). In Fig. 11, we...
with such triangular geometry has been experimentally realized in Ref. [45]. The results are plotted in Fig. 13. It is seen that the PRH-QAOA can improve the performance of the VQE for 2D target Hamiltonians with triangular geometry, which may enlightens further works aiming to improve the performance of the VQE for frustrated quantum systems [75–77].

Appendix C: Additional numerics of generating the Greenberg-Horne-Zeilinger state with square lattice geometry

As shown in Fig. 7(a), one can generate the 17-qubit GHZ state with perfect fidelity using the 4-depth quantum circuit of the QAOA with the special geometry shown in Fig. 7(c). We now consider the Ising model on 2D square lattice with larger system size $N = 4 \times 4$ as the resource Hamiltonian, and to generate 16-qubit GHZ state, both the conventional QAOA and PRH-QAOA are studied. The results are plotted in Fig. 14. It is seen that for the depth of quantum circuit $p \leq 4$, all of the conventional QAOA with the OBC or PBC quantum circuit, and the PRH-QAOA cannot achieve the perfect fidelity of the 16-qubit GHZ state. When $p > 4$, the PRH-QAOA can generate higher fidelity GHZ states than that generated by the convention QAOA. Nevertheless, employing the Ising model on 2D square lattice as the resource Hamiltonian, for generating GHZ states, the performance of QAOA is less efficient than that employing the the special geometry shown in Fig. 7(b) and (c).

![Graph showing the infidelities $1 - f$ obtained after optimization for different quantum circuits](image)

FIG. 13. (a) The infidelities $1 - f$ obtained after optimization as a function of the depth $p$ for the 2D ferromagnetic TFIM with the triangular geometry. (b) The values of optimized parameters $J_{i,j}^{opt}$ (represented by dashed lines, dotted lines, and solid lines with different colors) and $H_{i,j}^{opt}$ (inside the circles) with the depth $p = 6$. (c) The ratio $R$ defined by Eq. (8) as a function of $p$. The inset of (a) shows a schematic of a triangular 2D lattice with $N = 10$ spins (represented by circles), and the ferromagnetic Ising interactions between spins (represented by solid lines).

![Graph showing the ratios $R$ obtained after optimization](image)

FIG. 14. The infidelities $1 - f$ with $f$ being the GHZ state fidelity, obtained after optimization, as a function of the depth $p$. The inset shows a schematic of a regular 2D lattice with $N = 16$ spins (represented by circles). For the OBC case, only the interactions represented by solid lines are considered. For the PBC case, both the interactions represented by solid and dashed lines are considered.
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