

Efficient quantum information-inspired ansatz for variational quantum eigensolver algorithm: Applications to atomic systems

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We present a quantum information-inspired ansatz for the variational quantum eigensolver and demonstrate its efficacy in calculating ground-state energies of atomic systems. Instead of adopting a heuristic approach, we start with an approximate multiqubit target state and utilize two quantum information-theoretic quantities, i.e., von Neumann entropy and quantum mutual information, to construct our ansatz. The quantum information encoded in the target state helps us design unique blocks and identify qubit pairs that exhibit maximal quantum correlations within the multi-qubit system, thereby enabling us to deterministically place two-qubit entanglers in the suitably constructed parametrized quantum circuit. We find that our approach offers the advantage of reduced circuit depth compared to the physics-inspired unitary coupled-cluster (UCC) ansatz, while yielding accurate results. To test the performance of our ansatz, we apply it to compute ground-state energies of atomic systems in the relativistic regime. Our results show that for up to 12-qubits (12-spinorbitals) noiseless calculations, our ansatz yields energies within chemical accuracy (~ 1.6 mhartree) relative to the complete active space configuration interaction values, while utilizing only a few blocks that contain in the best case 98% fewer two-qubit gates when compared with the UCC ansatz in the singles and doubles approximation.

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I. INTRODUCTION

Quantum computation promises a wide range of applications in both basic science and real-world problems. One of the important motivations underlying the development of quantum computers and algorithms is the simulation of quantum phenomena in atoms, molecules, and condensed-matter systems, to name a few [1–9], and studying various physical and chemical properties of these systems. An example of this is the computation of ground-state energies of atoms and molecules, which are of particular interest in quantum physics and chemistry. In recent years, considerable efforts have gone into developing and applying quantum algorithms to investigate this property. Among these algorithms, the ones based on variational quantum eigensolver (VQE) have been the most widely used [10–22]. VQE exploits both classical

and quantum resources, making it a hybrid quantum-classical algorithm. It has attracted much attention due to the feasibility of its implementation with a relatively few qubits on Noisy Intermediate-Scale Quantum (NISQ) devices [23–25]. Fault-tolerant-era quantum algorithms [26,27], aimed for the same purpose, lack the advantages provided by VQE, making them unsuitable for NISQ-era quantum computing. The starting point of VQE is the preparation of a trial wavefunction, which is based on an ansatz and is represented by the action of a parameter-dependent unitary operator on a reference state. This wavefunction is then used to evaluate the energy functional on a quantum computer, while the parameter update is performed on a classical computer. Broadly, there are two choices for the VQE ansatz; one of them is based on the unitary coupled-cluster (UCC) theory [28–31]—the UCC ansatz [adapted from the coupled-cluster (CC) method [32]]—and the other one is the Hardware-efficient ansatz (HEA) [16,24,33–35]. The UCC ansatz is physically motivated, but it quickly becomes impractical for large systems on current NISQ hardware due to its polynomial scaling in circuit depth. For instance, the UCC singles and doubles (UCCSD) ansatz exhibits a circuit depth scaling of $O(N^5)$, where N is the number of spin orbitals or qubits [13]. In contrast, HEA consists of layers of single-qubit rotation gates to create superposition and two-qubit gates to create entanglement, without any information of the chemical system [36]. HEAs, though shallow and compatible with current quantum hardware, suffer from limitations due to heuristic nature of their constructions. First,

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shallow circuits may fail to cover the relevant Hilbert space sufficiently, while deeper circuits with a larger number of qubits could encounter the barren plateau problem [37,38]. Second, the fixed pattern of entanglement in HEAs may not be universally suitable, leading to either lower or excessive entanglement in the system of interest [36]. In addition to the circuit depth of the ansatz, the number of measurements required on NISQ hardware also impacts performance. Since the atomic or molecular Hamiltonian H typically contains $\mathcal{O}(N^4)$ Pauli terms, an equivalent number of measurements may be needed. To reduce this overhead, several strategies have been explored, including qubit pairwise commutation [39] and employing joint Bell-basis measurements [40].

In this work, leveraging two quantum information-theoretic quantities—*von Neumann entropy* (S) [41] and *quantum mutual information* (I) [41], we construct a suitable HEA ansatz for VQE. Unlike traditional HEAs, which often rely on arbitrary arrangement of entangling gates between two qubits, our quantum information-inspired HEA (hereafter QIIA), inspired by the earlier work from Refs. [42–45], is systematically constructed based on the quantum information-theoretic quantities mentioned above and solves the arbitrary arrangement of entangling gates in the ansatz. Besides Refs. [42–44], there is another research work [45] that exploits mutual information for VQE, however, significantly differing from that of ours. In particular, the authors use mutual information but not von Neumann entropy for reducing the entangler pool size for adaptive ansätze in general.

To check the efficiency of our proposed ansatz, we apply it to relativistic atomic physics and evaluate ground-state energies of different atoms. We find that with only two blocks, the QIIA ansatz achieves 99.99% accuracy in the noiseless medium relative to the standard complete active space configuration interaction (CAS-CI) value. As a proof of principle, we executed the QIIA circuit on the IBM Sherbrooke quantum hardware, incorporating resource reduction techniques on both the Hamiltonian and the circuit. Albeit the QIIA ansatz is applied to the atomic Hamiltonian in this work, it can be easily extended to the molecular Hamiltonian, as well as calculating other properties of both atoms and molecules.

II. THEORY AND METHODOLOGY

A. Dirac-coulomb Hamiltonian

While the VQE algorithm has been widely applied to molecular systems, its application to atomic systems, particularly in the relativistic framework, remains comparatively underexplored. We therefore begin with the relativistic Dirac-Coulomb (DC) Hamiltonian for atomic systems (see Chap. 6 of Ref. [46]):

$$H_{\text{DC}} = \sum_i^{N_e} [c \vec{\alpha}_i \cdot \vec{p}_i + \beta_i c^2 + V_{\text{nuc}}(\vec{r}_i)] + \frac{1}{2} \sum_{i \neq j}^{N_e} \frac{1}{|\vec{r}_i - \vec{r}_j|}, \quad (1)$$

where c is the speed of light, $\vec{p}_i$ is the momentum of the i th electron, N_e is the number of electrons, and $\vec{r}_i$ is the coordinate vector of the i th electron. The quantities α_i and β_i are the Dirac spinors and $V_{\text{nuc}}(\vec{r}_i)$ is the electron-nucleus

potential of the i th electron (for this work, we considered the Fermi nuclear model). We have used the atomic units in Eq. (1). The initial ground state is obtained using the Dirac-Hartree-Fock (DF) method (see chap. 6 of Ref. [46]). By decomposing the Hamiltonian as $H_{\text{DC}} = H_0 + H'$, where H_0 is the one-body DF Hamiltonian and H' is the residual Hamiltonian (the difference between the exact two-body Coulomb and the DF Hamiltonians), the DF energy is given by $E_{\text{DF}} = \langle \Phi_0 | H_{\text{DC}} | \Phi_0 \rangle$, where $|\Phi_0\rangle$ is the DF state. The total energy includes the correlation correction to E_{DF} , i.e., $E_0 = E_{\text{DF}} + E_{\text{corr}}$. The second-quantized form of H_{DC} is given by $H = \sum_{pq} h_{pq} a_p^\dagger a_q + \frac{1}{2} \sum_{pqrs} g_{pqrs} a_p^\dagger a_q^\dagger a_s a_r$, where $a_p^\dagger$, for example is a fermionic creation operator whereas a_q is a fermionic annihilation operator. h_{pq} and g_{pqrs} are one- and two-electron integrals, respectively (pages 228–230 of Ref. [47]). To perform VQE, mapping to a qubit Hamiltonian yields $H_q = \sum_k w_k P_k$, where w_k are real coefficients and $P_k \in \{I, X, Y, Z\}^{\otimes N}$ are Pauli strings. We use the Jordan-Wigner transformation [48] for this mapping. Figure 1 schematically outlines the Hamiltonian construction and QIIA circuit preparation steps used for the VQE algorithm.

B. Input approximate state

The input approximate state, which we shall use to design our ansatz and which is *not* the same as the input state that the ansatz acts upon (which we will choose to be the DF state), is constructed using many-body perturbation theory (MBPT) with first-order correction to the wavefunction, i.e., second-order correction to the energy (Chap. 9 of Ref. [47]). The first-order wavefunction correction $|\Phi^{(1)}\rangle$ accounts for electron correlation and is given as

$$|\Phi^{(1)}\rangle = \sum_{I \neq 0} \frac{\langle \Phi_I | V(\vec{r}_1, \vec{r}_2) | \Phi_0 \rangle}{E_0 - E_I} |\Phi_I\rangle, \quad (2)$$

where $V(\vec{r}_1, \vec{r}_2)$ is the two-body Coulomb interaction, and E_0 and E_I are the DF ($|\Phi_0\rangle$) and excited determinant ($|\Phi_I\rangle$) energies, respectively. Because of the Slater-Condon rule, the wavefunction correction is dominated by double excitations, and thus

$$|\Phi^{(1)}\rangle = \sum_{\substack{i < j \\ a < b}} C_{ij}^{ab} |\Phi_{ij}^{ab}\rangle, \quad (3)$$

where $|\Phi_{ij}^{ab}\rangle$ denotes a doubly excited determinant formed by exciting two electrons from occupied orbitals i, j to virtual orbitals a, b . The amplitude is given by

$$C_{ij}^{ab} = \frac{\langle \Phi_{ij}^{ab} | V(\vec{r}_1, \vec{r}_2) | \Phi_0 \rangle}{\varepsilon_i + \varepsilon_j - \varepsilon_a - \varepsilon_b} = \frac{\int_0^\infty \int_0^\infty \phi_a^\dagger(\vec{r}_1) \phi_b^\dagger(\vec{r}_2) \frac{1}{r_{12}} \phi_i(\vec{r}_1) \phi_j(\vec{r}_2) d^3\vec{r}_2 d^3\vec{r}_1}{\varepsilon_i + \varepsilon_j - \varepsilon_a - \varepsilon_b}, \quad (4)$$

which depends on the interaction matrix elements and the orbital energy denominators, where ε_i and ε_j refer to the energies of the occupied orbitals involved in the excitation, while ε_a and ε_b are the energies of the virtual orbitals involved in the excitation. The resulting MBPT first-order corrected

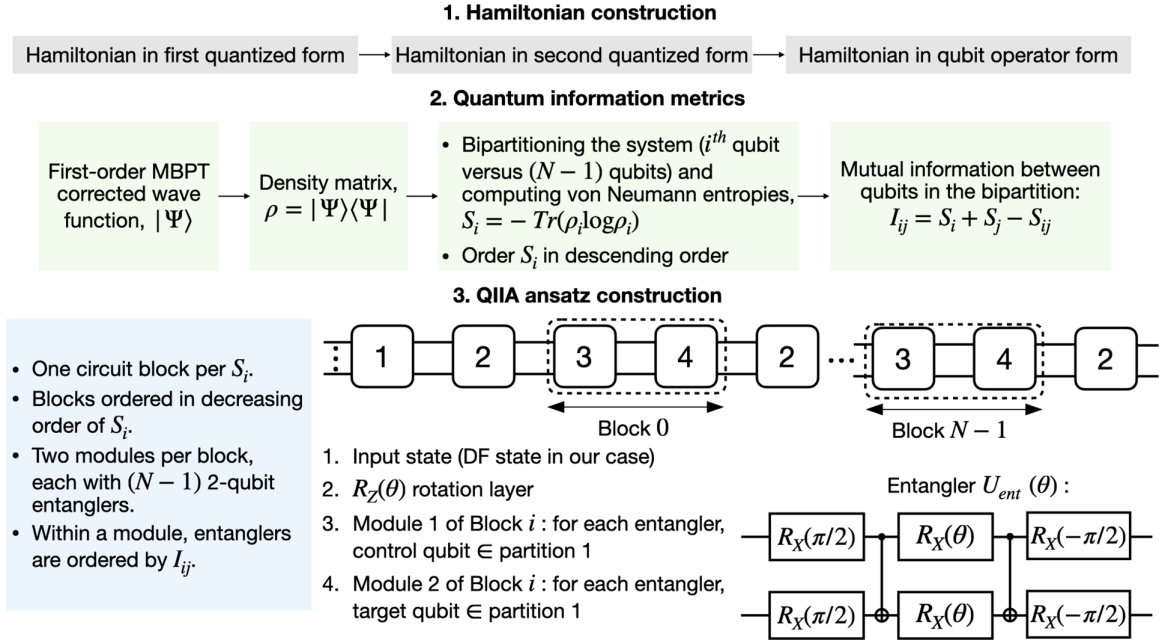


FIG. 1. Flowchart illustrating construction of the qubit Hamiltonian and QIIA ansatz, which will be fed into the standard VQE procedure. The relativistic DC Hamiltonian is mapped to a qubit Hamiltonian, and the MBPT first-order corrected wavefunction is used to compute the von Neumann entropy and mutual information between the qubit pairs. These quantum information metrics guide the placement of blocks and the entanglers inside the block. The two-qubit match-gate-type entangler used in QIIA is also shown in the flowchart.

wavefunction is normalized as

$$|\Psi\rangle = \frac{1}{\sqrt{\mathcal{N}}}(|\Phi_0\rangle + |\Phi^{(1)}\rangle), \quad (5)$$

where $\mathcal{N}$ is the normalization constant. $|\Phi_0\rangle$ and $|\Phi^{(1)}\rangle$ are built from single-particle orbitals characterized by the quantum numbers (n, l, s, j, m_j) , where n denotes the principal quantum number, l the orbital angular momentum quantum number, s the spin quantum number, j the total angular momentum quantum number, and m_j the magnetic quantum number. The computational basis states are expressed in the block-spin arrangement, where a basis state is divided into two equal length sets of qubits corresponding to orbitals with negative $(-m_j)$ and positive $(+m_j)$ magnetic quantum numbers. Each set (b_k) forms a multiqubit computational basis state, and the full state is obtained by taking the tensor product of these two sets. Accordingly, the many-body wavefunction can be written as $|\Psi\rangle = \sum_k c_k |b_k^{(-m_j)}\rangle \otimes |b_k^{(+m_j)}\rangle$. As an illustrative example, consider the normalized wavefunction for the B^+ ion ($2e^-$, eight qubits). In this system, the $1s$ orbital is frozen, the $2s$ orbital is occupied, and the $2p$ orbitals are unoccupied. The wavefunction can then be expressed in the computational basis as

$$|\Psi\rangle = 0.996\,389\,|00010001\rangle - 0.020\,173\,|00100010\rangle \\ - 0.024\,871\,|01000100\rangle + 0.078\,577\,|10001000\rangle. \quad (6)$$

Here, each qubit string follows the little-endian convention, where the zeroth qubit (q_0) corresponds to the least significant bit. As mentioned earlier, the qubits are ordered according to a block-spin arrangement, such that all orbitals with $-m_j$ appear first, followed by those with $+m_j$.

The magnitude of the coefficients corresponding to the configurations in the first-order perturbed wavefunction $\langle\Phi_I|V(\vec{r}_1, \vec{r}_2)|\Phi_0\rangle/(E_0 - E_I)$ given in Eq. (6) reflects the relative importance of different excited configurations, and it depends on the electronic structure. In particular, orbital pairs are more strongly correlated when the overlap between the occupied and virtual orbitals is large, and/or when the energy difference between occupied and virtual orbitals is small (Chap. 10 of Ref. [47]). These factors are responsible for increasing the correlation in the wavefunction.

With this information, one could pick important determinants and thus important amplitudes for a VQE-UCC calculation, and design, for example, an adaptive ansatz. However, we depart from this approach in our work, since although the presence of multiple significant contributions implies that the state in Eq. (6) is no longer separable but exhibits multipartite entanglement, the perturbative amplitudes alone do not reveal how this entanglement is distributed across qubits, i.e., which qubits are strongly correlated and how correlations are shared pairwise. We instead use the state obtained from the relatively (computationally) cheap MBPT protocol only as an input approximate state, and leverage quantum information theoretic quantities calculated using this state, namely, von Neumann entropy and quantum mutual information, for ansatz design. All input approximate states used for computing these metrics are provided in Appendix A of the Supplemental Material [49]. It is also worth adding that one could have used some other many-body theories, for example, linearized coupled cluster method, to obtain the initial trial state. In the following paragraphs, we discuss the two quantum information theoretic metrics followed by how we leverage them to design our ansatz.

C. Quantum information-theoretic metrics

The von Neumann entropy of a two-level quantum system is defined as

$$S(\rho) = -\text{Tr}(\rho \log_2 \rho), \quad (7)$$

where ρ is the density matrix representing the state of the system and “Tr” denotes the usual trace operation on matrices. For a pure state, $S(\rho) = 0$, whereas it is nonzero for mixed states. For multipartite pure states, the von Neumann entropy of any subsystem quantifies the bipartite entanglement between that subsystem and the rest of the system [50]. For example, consider the two-qubit states $|00\rangle$ and $\frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$. As both states are pure, their global entropy is zero. However, when we compute the entropy of a single qubit (subsystem), the first state gives zero (separable state), while the second gives unity, indicating maximal entanglement. The second state is a Bell state, which contains one *ebit* of entanglement.

In particular, for an N -qubit system, we consider bipartitions of the form $q_i|\text{rest}$ [and, in particular, we pick 1 qubit $(N - 1)$ qubits], where q_i denotes the i th qubit and “rest” denotes the remaining part of the qubit system. The reduced state ρ_i of the i th qubit can be found by taking partial trace [50] of the N -qubit state with respect to the rest of the system, i.e., $\rho_i = \text{Tr}_{\text{rest}}(\rho)$, where ρ is the N -qubit state. Using Eq. (7), we can find the von Neumann entropy of this qubit,

$$S_i \equiv S(\rho_i). \quad (8)$$

This entropy measures how strongly qubit q_i is entangled with the remaining $N - 1$ qubits. $S_i = 0$ indicates that qubit q_i is unentangled (separable), while a nonzero value indicates that it is entangled with the rest of the system.

To further characterize correlations between pairs of qubits, we employ the measure of quantum mutual information. For qubits i and j , it is defined as

$$I_{ij} = S_i + S_j - S_{ij}, \quad (9)$$

where $S_{ij} = S(\rho_{ij})$ is the entropy of the joint state of the qubits ρ_{ij} , which can be derived from the N -qubit state ρ using partial trace operation.

D. QIIA ansatz

The construction of the QIIA ansatz follows the workflow illustrated in Fig. 1. For clarity, we first define the key components of the ansatz. As stated in the earlier paragraphs, we restrict ourselves to bipartitions of the form $q_i|\text{rest}$, where subsystem A consists of a single qubit q_i and subsystem B contains the remaining $(N - 1)$ qubits. A *block* is a circuit unit associated with a given bipartition (each block represents a unique bipartition), designed to incorporate the correlations between the selected qubit q_i and the rest of the system. The ordering of the blocks is determined by the von Neumann entropy S_i of each bipartition. Each block is built out of two *modules*, with each module comprising $(N - 1)$ parametrized two-qubit gates (which we term as *entanglers*, $U_{\text{ent}}(\theta)$) connecting the qubit in one partition with all other qubits in the other. In module 1, the qubit q_i acts as the control qubit, while in module 2, the direction is reversed, and q_i acts as the target. Within a module, the mutual information between

each pair of qubits decides the ordering of those entanglers within the module. In this work, we employ a variational matchgate-style entangler [51], whose structure is shown in Fig. 1. This entangler preserves particle number and can be implemented using only two cnot gates. Further details are provided in Appendix B of the Supplemental Material [49].

Starting from the first-order MBPT-corrected wavefunction $|\Psi\rangle$, which we recall was termed the input approximate state and stated as being distinct from the initial state that the ansatz acts upon, we construct the corresponding density matrix $\rho = |\Psi\rangle\langle\Psi|$, which serves as the approximate state for extracting the quantum correlation structure of the system. We then perform bipartitioning of the N -qubit system by separating one qubit from the remaining $(N - 1)$ qubits, i.e., partitions of the form $q_i|\text{rest}$. For each such partition, we compute the von Neumann entropy S_i , where ρ_i is the reduced density matrix of qubit q_i . These entropies quantify how strongly each qubit is entangled with the rest of the system. The qubits are subsequently ordered in descending order of S_i , thereby identifying the most relevant qubits for correlation. In the language of particle-hole excitations, a large value for S_i indicates that the i th spin orbital is involved in a large number of particle-hole excitations. In the next step, we compute the quantum mutual information I_{ij} between all pairs of qubits. This provides an entanglement map that captures the distribution of correlations across qubit pairs. The circuit begins with preparation of the DF state as the initial state upon which our ansatz is to act on, followed by a layer of single-qubit R_z rotations. This is succeeded by a sequence of circuit blocks, with additional R_z rotation layers inserted between consecutive blocks.

To illustrate the construction, we consider the B^+ ion in a $(2e^-, 8q)$ active space and the first-order MBPT-corrected wavefunction given in Eq. (6). In the first step, we compute the von Neumann entropies S_i for all bipartitions of the form $q_i|\text{rest}$. For this system, the two largest entropies are found to be S_0 and S_4 , indicating that qubits q_0 and q_4 are the most strongly entangled with the rest of the system. Next, we compute the quantum mutual information I_{ij} between all qubit pairs to determine how correlations are distributed. Figure 2 presents the resulting entanglement structure through a connectivity graph and a heat map, highlighting both the dominant qubits and the strength of pairwise correlations. The construction of the first circuit block, corresponding to the highest entropy S_0 , is shown in Fig. 3. The circuit begins with preparation of the DF state, followed by a layer of R_z rotations. Since q_0 has the highest entropy, it defines the bipartition $q_0|\text{rest}$. Accordingly, in module 1 of the block, q_0 acts as the control qubit and is entangled with all other qubits as targets, while in module 2, the roles are reversed. The ordering of the entangling gates within each module is determined by the mutual information values. In this case, the entangling gates are applied to qubit pairs in the order of $(0, 4)$, $(0, 3)$, $(0, 7)$, and $(0, 1)$, $(0, 5)$, $(0, 2)$, and $(0, 6)$, where (i, j) denotes the qubit pair indices.

Now, if we adopt the random-permutation approach to place the entanglers in the correct positions, the number of possible unique circuits increases rapidly with system size. For example, if we have taken $\mathcal{L}$ blocks and each block is arranged in $\mathcal{P}$ possible ways, then the total number of circuit permutations will be $\mathcal{P}^{\mathcal{L}}$. Instead, to determine the

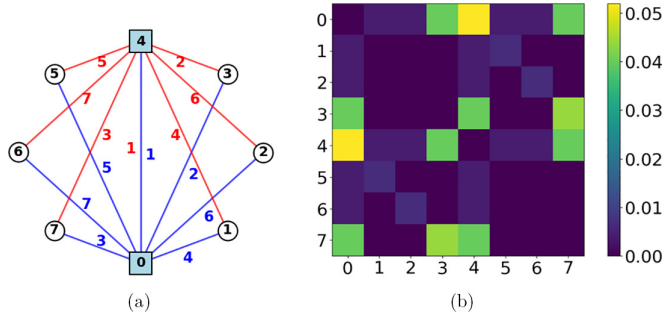


FIG. 2. Entanglement structure used for constructing our proposed ansatz. (a) Graph representation of the QIIA circuit, where nodes denote qubits and edges indicate entangling gates. Only the two bipartitions with the largest von Neumann entropies are selected, yielding two circuit blocks in the ansatz. The nodes marked inside a square represent those whose entropies are the largest, with the rest of them marked in a circle. The edge weights on the blue colored edges indicate the order of occurrence of the entanglers in the zeroth block, whereas those for the red colored ones denote the order of occurrence in the first block. The order of occurrence is decided by mutual information, as subfigure (b) shows. The mutual information between two qubits (shown along the x and y axes) is color-coded in the subfigure.

optimal configuration of the entangling gates between the qubits within a block, we utilize the mutual information data. This ensures insertion of entangling gates between the highly correlated qubit pairs first, followed by the other pairs in the descending order of mutual information value. Thus, our proposed ansatz not only captures most of the quantum correlations present in the many-body system, but it also excludes the qubit pairs having a negligible amount of entanglement between them, thereby significantly reducing the number of two-qubit gates. Notably, the same entangler ordering was obtained using the more accurate and rigorous linearized

coupled-cluster method, consistent with that derived from the first-order MBPT-corrected wavefunction.

Previous studies have also utilized mutual information for designing ansätze [43,45]; however, the optimal circuit configuration is found using repeated permutations. In QIIA, due to the prior analysis of quantum correlations, mainly entanglement, between the i th qubit and each of the remaining qubits, random gate permutations become unnecessary, resulting in a significant reduction in the complexity of the parametrized circuit. The entire construction becomes fully deterministic, requiring no stochastic sampling. Due to practical computational limitations, we have employed the QIIA up to four blocks in our numerical simulation.

III. RESULTS AND DISCUSSIONS

A. Simulation results

In this work, we have calculated the ground-state energies of four Be-like systems with the chosen active spaces: $2s^2 2p^0$ (0 represents the unoccupied orbitals) corresponding to two electrons and eight qubits ($2e^-$, 8q), and $1s^2 2s^2 2p^0$ for four electrons and ten qubits ($4e^-$, 10q). Similarly, for four Mg-like systems, the active spaces are $3s^2 3p^0$ for ($2e^-$, 8q), $2p_{1/2}^2 3s^2 3p^0$ for ($4e^-$, 10q), and $2p_{3/2}^4 3s^2 3p^0$ for ($6e^-$, 12q). In the DF calculations, we employ Gaussian-type orbitals (GTOs) as the single-particle basis functions. Specifically, we use a universal basis [52] set, where the i th function (or basis) is defined as $g_i(r) := N_i r^{l_i} e^{-\alpha_i r^2}$, l_i being the angular momentum quantum number and α_i the exponent of the Gaussian. The distance from the center of the Gaussian to the origin is given by r . Further, α_i is expressed as $\alpha_i = \alpha_0 \beta^{i-1}$, for some suitable values of α_0 and β . Since we truncate our Hilbert space, we carefully choose the values of α_0 and β that still give the optimal single-particle energies as well as the total energy ($\alpha_0 = 0.0009$ and $\beta = 2.15$). Within a given basis set,

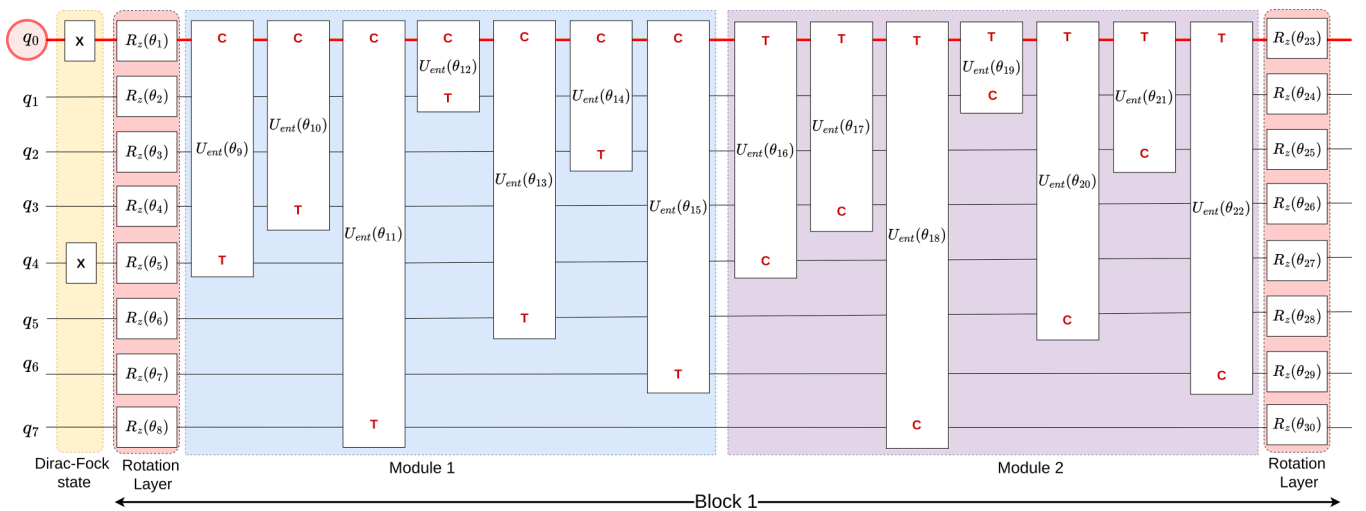


FIG. 3. A single block consists of two modules: in module 1, the highest-entropy qubit acts as the control and connects to all other qubits, while in module 2, the direction is reversed, and the same qubit acts as the target of the parametrized circuit corresponding to the proposed ansatz for B^+ ion ($2e^-$, 8q) system. The block is dedicated to q_0 as it has the highest von Neumann entropy (marked as a red circle), and the red line in q_0 indicates that the bipartition is between q_0 and the remaining qubits. So, the entanglers connect q_0 and the remaining qubits. The letters ‘C’ and ‘T’ indicate the qubits that are set as control and target, respectively. The circuit for $U_{\text{ent}}(\theta_i)$ is given in Fig. 1.

TABLE I. Calculated total energies (in Hartree) for different atomic systems. E_{DF} refers to the DF energy, while $E_{\text{MBPT}}^{(2)}$ is the energy obtained using many-body perturbation theory to first-order correction in wavefunction, i.e., the second-order correction in energy (also referred to as MP2 in the literature). $E_{\text{CAS-CI}}$, E_{UCCSD} , and E_{QIIA} are energies calculated using CAS-CI (benchmark value), UCCSD-VQE, and the QIIA-VQE approaches, respectively. $2e^-$, $8q$ refers to a two-electron, eight-qubit computation.

System	E_{DF}	$E_{\text{MBPT}}^{(2)}$	$E_{\text{CAS-CI}}$	E_{UCCSD}	E_{QIIA}
$2e^-$, $8q$					
B^+	-4.971 28	-4.991 41	-4.994 29	-4.994 29	-4.994 29
C^{2+}	-7.591 41	-7.622 404	-7.643 57	-7.643 57	-7.643 57
N^{3+}	-10.706 16	-10.745 33	-10.787 70	-10.787 70	-10.787 70
O^{4+}	-14.319 62	-14.366 00	-14.430 26	-14.430 26	-14.430 26
$4e^-$, $10q$					
B^+	-24.245 16	-24.265 51	-24.284 48	-24.284 48	-24.284 41
C^{2+}	-36.425 14	-36.456 68	-36.486 98	-36.486 98	-36.486 90
N^{3+}	-51.114 48	-51.154 51	-51.192 77	-51.192 77	-51.192 71
O^{4+}	-68.314 39	-68.361 90	-68.406 96	-68.406 96	-68.406 84

atomic orbitals are expressed as linear combinations of basis functions [53]. We perform DF calculations using 40 $s_{1/2}$, 39 $p_{1/2}$, 39 $p_{3/2}$, 38 $d_{3/2}$, and 38 $d_{5/2}$ GTOs [54].

The input state to the ansatz is set to be the DF state. All noiseless simulations are carried out using the state-vector backend of Qiskit 1.4.2 [55]. For our work, we use the Sequential Least Squares Programming [56,57] optimizer, with the threshold for convergence set to 10^{-6} throughout. The initial parameters in the optimization are randomly chosen. Table I presents the total ground-state energies (in Hartree) for Be-like ions, computed using various methods across the two active spaces. The results show that the QIIA ansatz, informed by the MBPT first-order wavefunction correction, achieves excellent agreement with CAS-CI reference energies, validating the accuracy of the method and its ability to capture electron correlation effects accurately.

Figure 4 shows the absolute energy deviations (ΔE) of the QIIA and UCCSD methods with respect to the CAS-CI benchmark for different atomic systems and active spaces. The deviation is defined as $\Delta E = |E_{\text{method}} - E_{\text{CAS-CI}}|$, and is reported in mhartree. The dashed horizontal line indicates the chemical accuracy threshold (~ 1.6 mhartree). The results are organized into three panels corresponding to the $(2e^-, 8q)$, $(4e^-, 10q)$, and $(6e^-, 12q)$ active spaces. For the QIIA ansatz, we employ two entangling blocks in the $(2e^-, 8q)$ and $(4e^-, 10q)$ cases, and four blocks for the $(6e^-, 12q)$ case. From the figure, it is evident that both QIIA and UCCSD yield very small deviations from the CAS-CI reference across all systems. In particular, QIIA consistently remains well below the chemical accuracy threshold in all cases. Even for the larger $(6e^-, 12q)$ systems, the deviations remain within sub-mhartree accuracy. Another metric called percentage fractional difference with respect to the CAS-CI energy (percentage fractional difference (PFD)) = $\frac{E_{\text{CAS-CI}} - E_{\text{method}}}{E_{\text{CAS-CI}}} \times 100$ is also defined, which indicates the percentage of the total energy lost compared to CAS-CI energy using different methods. QIIA consistently achieves high accuracy, with deviations under 0.0009%, closely matching the CAS-CI result. Detailed simulation results for all the atomic systems are provided in Appendix C of the Supplemental Material (see Tables II, III, and IV) [49].

The resources taken up in the systems considered for numerical simulations can be found in Fig. 5. To achieve chemical accuracy comparable to the UCCSD method, our approach uses significantly fewer one-qubit ($\sim 93\%$) and two-qubit gates ($\sim 98\%$), and lower circuit depth ($\sim 96\%$). Both the QIIA and UCCSD ansätze conserve particle number by construction. For a fair comparison, we also benchmark against a standard excitation-preserving ansatz with full entanglement connectivity available in Qiskit [55]. We find that QIIA maintains particle-number conservation while requiring significantly fewer variational parameters, fewer single- and two-qubit gates, and lower circuit depth.

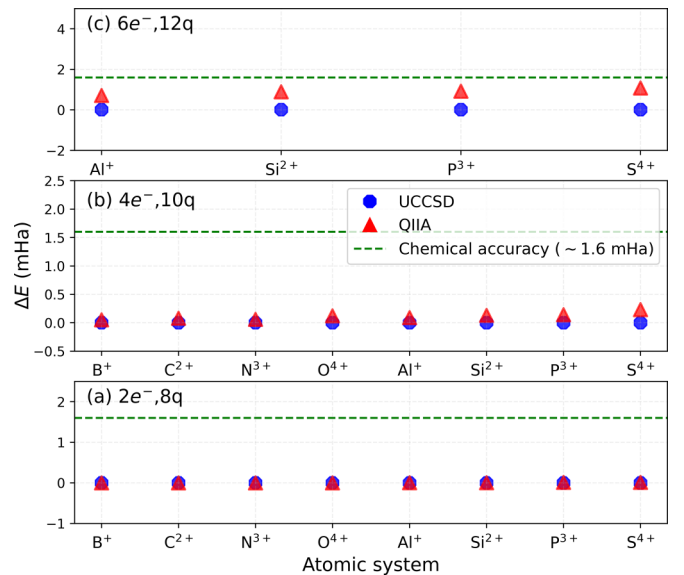


FIG. 4. Plots showing a comparison between the ground-state energies computed using UCCSD and QIIA ansatz for various atomic systems. ΔE (mhartree) refers to the absolute energy difference from the CAS-CI energy in the mhartree scale, and the green line shows the chemical accuracy. For the $(6e^-, 12q)$ case, the results were obtained using four blocks in the QIIA ansatz, and for the $(2e^-, 8q)$ and $(4e^-, 10q)$ cases, the results were obtained with just two blocks in the QIIA ansatz.

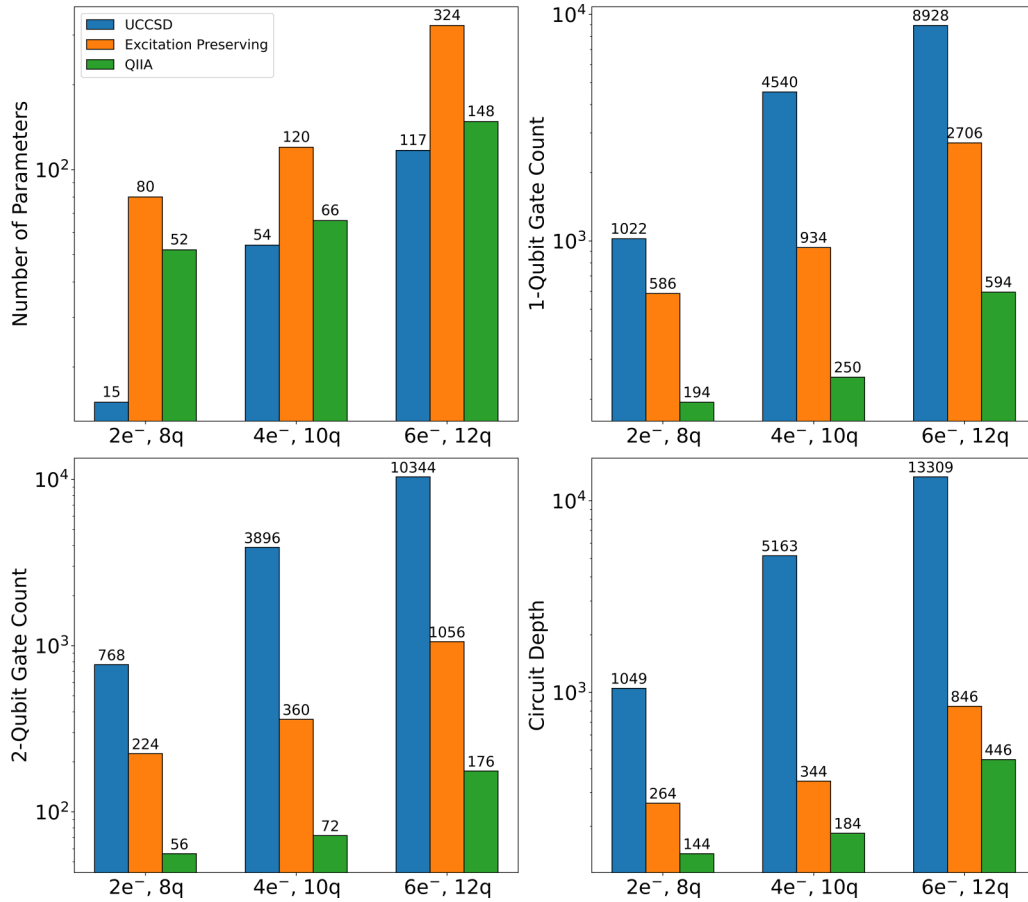


FIG. 5. Comparison of the quantum resource requirements for UCCSD (blue), excitation-preserving ansatz with full entanglement (orange), and QIIA ansatz (green) across the three different active spaces: $(2e^-, 8q)$, $(4e^-, 10q)$, and $(6e^-, 12q)$ to reach the chemical accuracy. The panels show (top left) the number of variational parameters, (top right) one-qubit gate count, (bottom left) two-qubit gate count, and (bottom right) total circuit depth. In the $(2e^-, 8q)$ and $(4e^-, 10q)$ cases, two blocks, and in the $(6e^-, 12q)$ case, four blocks are used in the QIIA ansatz.

In terms of scaling, the number of parameters scales as $\sim \mathcal{O}(N^4)$ for UCCSD; however, QIIA requires only $\sim \mathcal{O}(N^3)$ parameters. Furthermore, the two-qubit gate count reduces from UCCSD's $\sim \mathcal{O}(N^5)$ to $\sim \mathcal{O}(N^2)$ for our QIIA ansatz. One interesting aspect would be to check the performance of the proposed ansatz when only a single module is used per block (Numerical details are provided in Appendix C of the Supplemental Material [49]). Our findings show that having two modules per block plays an important role in the circuit design. In the QIIA design, each block consists of entanglers constructed from cx gates. In module 1, the highest-entropy qubit acts as the control and connects to all other qubits, while in module 2, the direction is reversed, and the same qubit acts as the target. Since cx gates are intrinsically unidirectional, the addition of module 2 enables bidirectional information flow between qubits. This facilitates a more uniform spread of quantum correlations.

Finding the optimal ordering of operators while preparing the quantum circuit is, in general, a nontrivial problem, as also highlighted in Ref. [56], where global optimization over operator sequences is considered. In this work, we employ a combination of ordering based on entropy and mutual

information that provides an efficient strategy for circuit construction. To address the efficacy of our strategy, we perform a comparative numerical assessment between the performance of the ansätze constructed using the strategy and random orderings for three systems of different sizes: eight qubits [C^{2+} ($2e^-, 8q$)], ten qubits [O^{4+} ($4e^-, 10q$)], and ten qubits [Al^{1+} ($4e^-, 10q$)]. For all of these cases, we first generate two blocks using the bipartitions having maximal entanglement entropy and then generate 20 different random orderings of the same set of entanglers within the two blocks of the QIIA ansatz. We shuffle the position of the entanglers inside each module of the block; however, analyzing the effect of shuffling across two modules of a block is outside the scope of our work. We find that for all the systems under consideration, the ansatz constructed using mutual-information-based ordering of gates yields the lowest energy. Moreover, the obtained values of energy are found to be below the chemical accuracy threshold in each case. The results are shown in Fig. 6. We find that while several random orderings can capture a significant fraction of the correlation energy, and in most cases, they can capture energy in the chemical accuracy range; however, mutual-information-based ordering always yields an energy

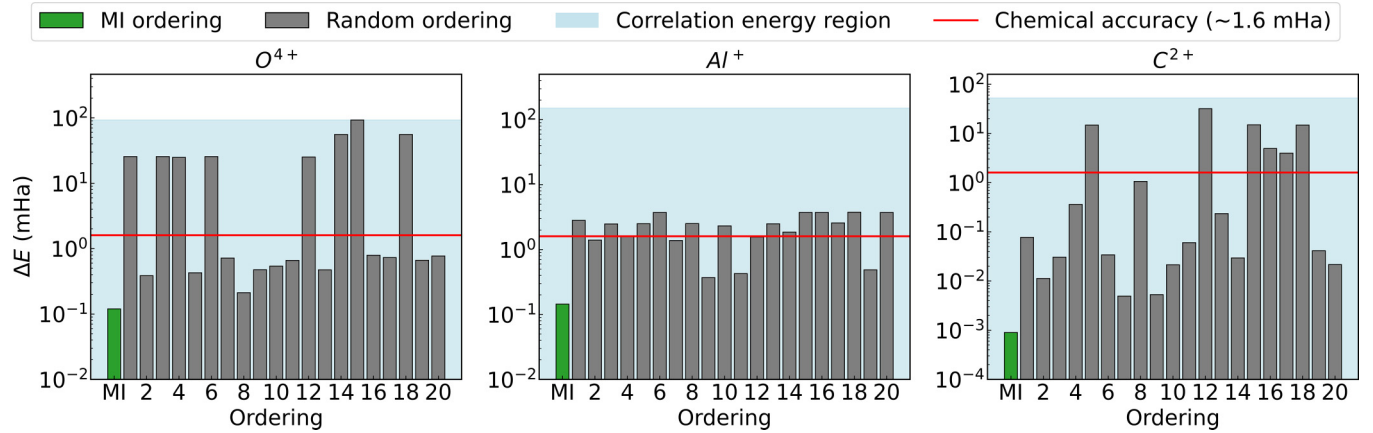


FIG. 6. Comparison of absolute energy errors relative to CASCI for different entangler orderings within the QIIA ansatz. Results are shown for O^{4+} ($4e^-$, 10q) (left), Al^+ ($4e^-$, 10q) (middle), and C^{2+} ($2e^-$, 8q) (right). The green bar corresponds to the mutual-information-based ordering, while the gray bars represent 20 random orderings of the same set of entanglers. The dashed red line indicates the chemical accuracy threshold (1.6 mhartree). The mutual-information-based ordering consistently achieves the lowest energy error and remains within chemical accuracy across all systems.

within chemical accuracy (1.6 mhartree) of the reference CASCI result, and always yields the lowest energy compared to the random orderings.

Introducing our algorithm and applying it to find numerical results for a number of atomic systems, we now compare QIIA with other ansätze such as QCC [58] and Rycascade ansatz [59]. We begin with the QCC method, which is an adaptive circuit construction, and the entangler pool consists of unitary operators of the form $\{e^{-i\hat{P}_k\tau_k}\}$, where $\hat{P}_k$ runs over all the Pauli words and τ_k are the adjustable parameters. To select the best $\hat{P}_k$'s, this method uses a screening procedure that is based on calculating energy derivatives with respect to $\hat{P}_k$'s, with $\hat{P}_k$'s growing exponentially with the number of qubits. Similarly, the Rycascade ansatz is a HEA, which shares a staircaselike structure with the UCC-type ansatz, and is constructed such that when applied to the initial Hartree-Fock (HF) state at $\vec{\theta} = \vec{0}$, it yields the identity, which means that the optimization will always be initialized from the HF state. We note that our ansatz too leaves the HF state invariant when all the parameters are initialized to zero. To compare with both these methods, we performed the nonrelativistic calculation on H_2 , LiH, and H_2O with QIIA and found that QIIA achieves chemical accuracy more efficiently than these two methods, which we have explained in Appendix D of the Supplemental Material [49].

Additionally, we extend our analysis to the H_4 molecular system, which provides an interesting test for the QIIA ansatz due to its strongly correlated nature. In this regime, the first-order MBPT wavefunction is expected to be a less accurate starting point in determining the input approximate state and therefore yielding less accurate entropies and mutual information values, making it particularly insightful to assess the performance of QIIA. We find that even under a strongly correlated regime, the QIIA ansatz with four entangling blocks achieves chemical accuracy. This is not too surprising, given that our ansatz design requires not predicting the values themselves of entropies and mutual information values but rather their ordering. Further details of this analysis are provided in Appendix E of the Supplemental Material [49].

B. Hardware results

Furthermore, we perform the quantum hardware computations of the two atoms, P^{3+} and S^{4+} , with an active space of $2p_{1/2}^2 3s^2 3p^0$ for four electrons and ten qubits ($4e^-$, 10q). For hardware calculation, we first perform the VQE on a classical computer with our QIIA ansatz to obtain the converged amplitudes, which we then use to construct the circuit and measure the Hamiltonian on a quantum computer to obtain the ground-state energy. The computations were performed on IBM's Sherbrooke machine having an Eagle R3 processor, which employs a native gate set comprising {ecr, id, rz, sx, x}. The quantum device exhibited median error rates of 6.184×10^{-3} (ecr), 2.305×10^{-4} (sx), and 2.051×10^{-2} (readout), with coherence times of $T_1 = 267.74 \mu s$ and $T_2 = 208.12 \mu s$. The qubit layout follows a heavy-hexagonal lattice topology with a CLOPS (Circuit layer operations per second score of 150 K. Obtaining good results on the current noisy hardware requires a workflow with several resource-reduction steps, both in the Hamiltonian and in the wavefunction as shown in Fig. 7. The number of terms in the Hamiltonian scales as N^4 , where N is the number of spin orbitals, which means that many circuits have to be measured per iteration. This will be difficult to implement on hardware due to error accumulation. To reduce the number of terms in the Hamiltonian, we apply a qubit pairwise commuting grouping called cliques [14] that allows simultaneous measurement of commuting Pauli terms. For the ten-qubit Hamiltonian of P^{3+} and S^{4+} , the 464 terms in the qubit Hamiltonian are grouped into 209 cliques. Every term is analyzed qubitwise, and suitable gates are applied to each qubit to rotate the state to the shared eigenbasis of qubitwise commuting terms [18]. Thus, only one term from each clique has to be measured in hardware. Further, if two cliques have the same energy contribution, we term them supercliques [18]; 209 cliques are grouped into 18 supercliques (S) for P^{3+} and 14 for S^{4+} , out of which we measured only the two dominant supercliques (S_0 having clique 0 and S_1 having cliques 1 and 2) in the hardware for both cases.

Once the ansatz is constructed using the converged parameters from the classical simulation, it undergoes resource

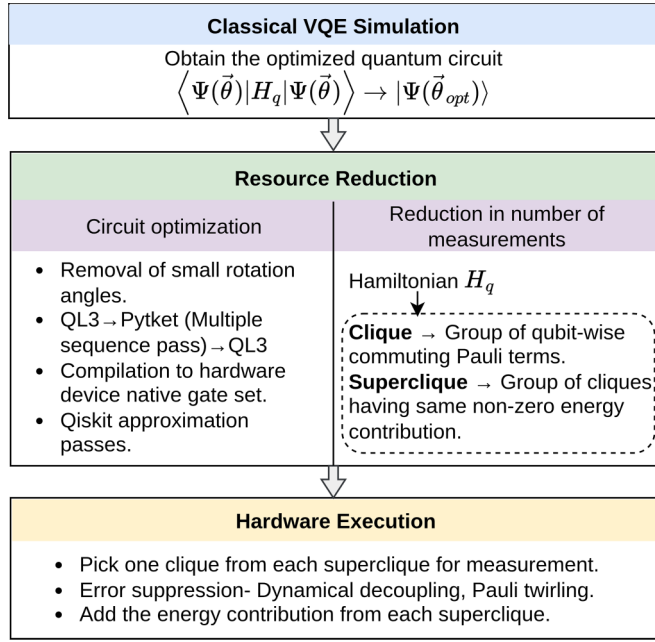


FIG. 7. Workflow for executing calculations on quantum hardware. First, a classical VQE simulation is performed to obtain the optimized wavefunction $|\Psi(\vec{\theta}_{opt})\rangle$. Next, the circuit is optimized by removing small rotation angles (order of 10^{-3}), applying Qiskit level-3 (QL3) and Pytket optimization passes, and compiling to the native hardware gate set. To reduce the number of measurements, the Hamiltonian is divided into qubitwise commuting groups (cliques), which are further grouped into supercliques. Finally, the optimized circuit is executed on quantum hardware with error suppression techniques (dynamical decoupling and Pauli twirling), and the total energy is obtained by combining the contributions from the selected supercliques.

reduction strategies to reduce gate counts (especially the number of two-qubit gates) in the circuit. Starting from the entanglers of QIIA ansatz, if the value of θ in R_X and R_Z gates is small (at the level of 10^{-3}), we remove them. Then, the circuit is passed to the Qiskit L3 [55] $\Rightarrow$ Pytket [60] $\Rightarrow$ Qiskit L3 routines. After all these steps, the cx gate count

reduces from 72 to 48, and the circuit depth reduces from 184 to 80. To execute this reduced QIIA ansatz on IBM hardware, we translate it to the instruction set architecture [55] circuit, which heavily depends on the quantum computer architecture beneath. To reduce the two-qubit gate on hardware, we use the approximation degree function provided by Qiskit to add another layer to our quantum circuit optimization [55]. During the computation, we employed error suppression techniques, including dynamical decoupling [61] to suppress the effects of decoherence on the data qubits, and Pauli twirling [62] to suppress the coherent noise. The QASM (quantum assembly language) simulation and quantum hardware results from the resource-reduced circuits, where we consider only the supercliques S_0 and S_1 , are shown in Tables II and III. The QASM simulation emulates the behavior of a noiseless quantum device on a classical computer by executing the quantum circuits and returning measurement counts based on a finite number of shots. For the same set of supercliques, we have compared the hardware results with both state-vector and QASM simulations.

The experiments were performed for P^{3+} and S^{4+} having configuration of $(4e^-, 10q)$. The resource reduction strategy includes compressing the Hamiltonian into cliques and supercliques (S). For example, P^{3+} , the full Hamiltonian had 464 Pauli terms, grouped into 209 cliques and further into 18 supercliques. Only two dominant supercliques were selected for hardware measurements, reducing the number of distinct measurement settings to 2. Further circuit resource reduction is applied to the QIIA ansatz. Small-angle single-qubit gates (e.g., R_X , R_Z with $\theta \sim 10^{-3}$) and the corresponding cnots were pruned. The circuit was transpiled via Qiskit L3 $\rightarrow$ Pytket $\rightarrow$ Qiskit L3 flow, which reduced the cx gate counts from 72 to 48 and the circuit depth from 184 to 80. The circuit was then compiled to the device's native gate set, accounting for the heavy-hexagonal lattice connectivity of the hardware. This mapping introduced additional SWAP operations, increasing the two-qubit ecr gate count to 114 and the depth to 770. Applying Qiskit's approximation passes subsequently reduced the ecr gate count to 17, while maintaining the overall depth at 184. For handling the hardware noise, Error suppression techniques such as dynamical decoupling (XX-type) and

TABLE II. For the P^{3+} and S^{4+} systems with active space of $(4e^-, 10q)$, the Hamiltonian is decomposed into supercliques (S), which are further divided into cliques containing specific Pauli terms. For each superclique, we list the expectation values from state-vector simulation, QASM simulation, and IBM quantum hardware runs. The total energy is calculated from the contributions of the two supercliques.

P^{3+}					
Superclique (S)	Cliques in S_i	Terms	$E_{\text{State-vector}}$	E_{QASM}	E_{Hardware}
S_0	Clique 0	IIIIIIII, IIIIIZII, ..., ZZIIIIII	-64.977 21	-64.977 19	-64.943 49
S_1	Clique 1	IIZYIIII, IIIIIZYZ, ..., IIIIIZYYII	-0.410 85	-0.410 84	-0.054 91
	Clique 2	IIXZXIIII, IIIIIXZX, ..., IIIIIZXXII	-0.410 85	-0.410 84	-0.054 91
		Total Energy =	-65.798 91	-65.798 87	-64.998 40
S^{4+}					
S_0	Clique 0	IIIIIIII, IIIIIZII, ..., ZZIIIIII	-75.693 58	-75.693 18	-75.692 71
S_1	Clique 1	IIZYIIII, IIIIIZYZ, ..., IIIIIZYYII	-0.516 10	-0.516 02	-0.056 01
	Clique 2	IIXZXIIII, IIIIIXZX, ..., IIIIIZXXII	-0.516 10	-0.516 02	-0.056 01
		Total Energy =	-76.725 78	-76.725 22	-75.804 73

TABLE III. Computed ground-state energies (E) and percent-age fractional differences (PFD) with respect to CAS-CI for P^{3+} and S^{4+} atomic systems using methods such as Dirac-Fock (E_{DF}), MBPT first-order wavefunction correction, and second-order energy correction ($E_{MBPT(1)}$), CAS-CI (E_{CAS-CI}), UCCSD (E_{UCCSD}), and QIIA with two blocks (E_{QIIA}). $E_{QIIA(Reduced)}$ denotes the QASM simulation results using the reduced QIIA circuit after applying resource reduction on it, and $E_{QIIA(Reduced)^*}$ denotes the hardware results from IBM Sherbrooke with a reduced circuit using only two dominant supercliques. PFD calculation is done with respect to the CAS-CI energy.

System	Method	Energy E (a.u.)	PFD
P^{3+} ($4e^-$, 10q)	E_{DF}	-65.369 36	0.630 51
	$E_{MBPT}^{(2)}$	-65.392 04	0.596 04
	E_{CAS-CI}	-65.784 14	–
	E_{UCCSD}	-65.784 14	0.000 00
	E_{QIIA}	-65.784 00	0.000 21
	$E_{QIIA(Reduced)}$	-65.774 33	0.014 91
	$E_{QIIA(Reduced)^*}$	-64.998 40	1.194 42
S^{4+} ($4e^-$, 10q)	E_{DF}	-76.188 99	0.685 04
	$E_{MBPT}^{(2)}$	-76.215 58	0.650 39
	E_{CAS-CI}	-76.714 52	–
	E_{UCCSD}	-76.714 52	0.000 00
	E_{QIIA}	-76.714 09	0.000 56
	$E_{QIIA(Reduced)}$	-76.704 33	0.013 28
	$E_{QIIA(Reduced)^*}$	-75.804 73	1.185 94

Pauli twirling were used. Measurements from supercliques $\mathcal{S}_0$ and $\mathcal{S}_1$ are shown in Table II. Table III compares total energy (from two dominant supercliques) with DF, MBPT⁽²⁾, CAS-CI, UCCSD, and QIIA energies.

We observe that, in the noiseless calculations, the energies of the supercliques from the state-vector and QASM simulations are in close agreement. $\mathcal{S}_0$ consists of Pauli terms with I and Z operators, allowing it direct computational basis measurement and particle-number postselection, due to which we obtain an accuracy of 99.95% for P^{3+} and 99.99% for S^{4+} on hardware with respect to the state-vector energy. However, not only is the energy contribution from $\mathcal{S}_1$ much smaller, but it also consists of Pauli terms with X , Y , and Z operators, which requires basis rotations for measurement (thus not accommo-

dating our postselection scheme). Therefore, we only obtain an accuracy of 13.37% for P^{3+} and 10.85% for S^{4+} relative to the state-vector energy. This in turn adversely impacts our energy estimates, as seen in Table III. We anticipate that in the foreseeable future, quantum hardware advances will alleviate this issue.

IV. CONCLUSION

In summary, we have introduced a shallow-depth quantum information-inspired ansatz for the VQE algorithm. Rather than taking recourse to a heuristic approach to design the parametrized circuits as reported in many previous works [13], we employ quantum information-theoretic quantities, i.e., von Neumann entropy and quantum mutual information, to build unique blocks and determine the exact positions of the two-qubit entangling gates in the circuit. This results in very accurate ground-state energies of the systems of interest. Our proposed ansatz is therefore more efficient compared to UCC-VQE. The match gate-type particle-conserving entangler keeps the number of particles fixed during the computation, thereby ensuring that the results remain physically correct. QIIA is versatile and can be applied to other quantum many-electron systems. It only relies on a reasonable guess of the target state to arrive at an efficient parametrized circuit using the von Neumann entropy and mutual information data corresponding to the state.

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DATA AVAILABILITY

The data that support the findings of this article are not publicly available. The data are available from the authors upon reasonable request.

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