

Bridging quantum computing and nuclear structure: Atomic nuclei on a trapped-ion quantum computer

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We demonstrate quantum simulations of strongly correlated nuclear many-body systems on the RIKEN-Quantinuum Reimei trapped-ion quantum computer, targeting ground states of oxygen, calcium, and nickel isotopes. By combining a hard-core-boson representation of the nuclear shell model with a pair-unitary coupled-cluster doubles ansatz, we achieve subpercent relative error in the ground-state energies compared to noise-free state vector simulations. Our approach leverages symmetry-aware state preparation and particle-number postselection to efficiently capture pairing correlations characteristic of systems with same-species nucleons. These findings highlight the viability of high-fidelity trapped-ion platforms for nuclear physics applications and provide a foundation for scaling to more complex nuclear systems.

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I. INTRODUCTION

Quantum simulation of many-body systems is a leading application of quantum computing, with potential impact across quantum chemistry, condensed-matter physics, nuclear physics, and so on. While quantum algorithms and hardware have advanced rapidly, demonstrating clear advantage for interacting many-body problems remains an open challenge. For example, a recent study [1] identified scenarios in which quantum devices can outperform classical algorithms for certain spin models. Nonetheless, general claims of quantum advantage for many-body systems remain inconclusive and require careful, system-specific analysis.

On near-term devices, variational approaches such as the variational quantum eigensolver [2,3] rely crucially on the choice of an ansatz that balances implementability and expressivity. Common families of ansätze—including unitary coupled-cluster (UCC) variants—can be effective in some domains but often suffer from optimization difficulties, called barren plateaus [4], or unfavorable scaling of parameters and gate depth as system size grows. This situation has evoked a broader consideration of quantum algorithms beyond noisy intermediate-scale quantum (NISQ) toward fault-tolerant quantum computing (FTQC), leading to a term like early fault-tolerant quantum computing [5]. In such situations, it is essential to broadly examine each component of quantum computation—namely, state preparation (also simply called the ansatz), quantum algorithms, and measurement strategies for evaluating the observable of interest—for each specific problem.

The first part, the choice of the ansatz, is particularly crucial. This is because the success of most of quantum algorithms for quantum many-body problems largely depends on the quality of the prepared quantum state, i.e., the overlap between the prepared state and the target state. In spin

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systems or chemical systems, various ansätze have been proposed, such as UCC family, and ones based on matrix product states or tensor network states more generally [6–8]. Compared to other areas tackling quantum many-body problems, nuclear physics studies have seen relatively limited applications of quantum computing, despite several pioneering works [9–11], and recent reviews [12,13]. To date, only a few ansätze have been explored for nuclear systems, almost exclusively based on the UCC family [11,14,15] with some variations such as Adaptive Derivative-Assembled Pseudo-Trotter Variational Quantum Eigensolver (Adapt-VQE) [16]. A seminal work investigated the applicability of the UCC + Adapt-VQE to the nuclear shell model [11], where the number of cnot gates required to achieve a given accuracy for shell-model calculations of oxygen and calcium isotopes was estimated. Taking a look around existing literature, pioneering works have focused intensively on pairing Hamiltonians [10,17–22]. Building on these previous works on pairing Hamiltonians or pairing-like ansätze, this work aims to explore more expressive and scalable ansätze suitable for simplified representations of nuclear shell-model Hamiltonians, develop symmetry-aware postselection techniques, and evaluate their performance on quantum hardware across a range of nuclear systems.

Nuclear many-body systems are distinguished from other quantum many-body systems by exceptionally strong correlations arising from the nature of nuclear forces, posing a unique challenge for both classical and quantum computing. Even in the low-energy regime, where nucleons are the only explicit baryonic degrees of freedom, the problem is complicated by the fact that protons and neutrons—fermions of nearly equal mass—interact through multiple channels in an intricate manner. This results in a large number of non-negligible Hamiltonian terms and strong nonlocality. Furthermore, anisotropic components of the interaction, such as tensor forces [23] and three-body forces [24], play an essential role in describing the rich phenomena of nuclear systems. These features are generally difficult to capture with a simple wave-function ansatz. Another manifestation of the complexity is entanglement entropy, which in nuclear systems obeys a volume law rather than an area law [25], hindering straightforward application of tensor networks.

Consequently, most quantum-computing studies of nuclear structure have focused on small systems or relied on classical simulators. Reported errors in ground-state energy estimates on quantum hardware range from 4% to 13% for ${}^6\text{Li}$ [14] and 3% to 13% for oxygen isotopes [15]. In our previous work [26], we achieved relative errors below 0.1% for ${}^6\text{He}$ and ${}^{18}\text{O}$, and about 1% for ${}^{42}\text{Ca}$ on an IBM superconducting quantum device. However, the target systems were limited to valence two-neutron configurations, and our method is not straightforwardly extendable to more general nuclear systems. This motivates the present work to develop more general and scalable approaches.

In this work, we introduce a hard-core-boson (HCB) mapping of the nuclear shell model combined with the pair-unitary coupled-cluster doubles (pUCCD) ansatz, which efficiently captures strong pairing correlations between nucleons of the same species. While pUCCD ansätze have been shown to be effective for chemical systems [27–29], applications of such

TABLE I. Target nuclei, interactions, and model spaces.

Nuclide	Interaction	Model space
${}^{18-26}\text{O}$	USDB [33]	sd ($1s_{1/2}, 0d_{3/2}, 0d_{5/2}$)
${}^{42-58}\text{Ca}$	GXPFI1A [34]	pf ($1p_{1/2}, 1p_{3/2}, 0f_{5/2}, 0f_{7/2}$)
${}^{58-76}\text{Ni}$	JUN45 [35]	$j j45$ ($1p_{1/2}, 1p_{3/2}, 0f_{5/2}, 0g_{9/2}$)

pair-based ansätze to nuclear systems have been limited to a few pioneering studies [19,22,30]. This work extends these previous studies to shell-model Hamiltonians and reports the first hardware implementation of HCB and pUCCD for nuclear systems. Implemented on the high-fidelity trapped-ion processor RIKEN-Quantinuum Reimei, and augmented by symmetry-aware ansätze and postselection techniques, our approach yields ground-state energies for oxygen, calcium, and nickel isotopes that agree with noise-free state vector simulations within subpercent relative error. These results establish an experimental benchmark for quantum simulations of strongly correlated nuclear systems and demonstrate the near-term potential of trapped-ion platforms for nuclear-structure calculations.

This paper is organized as follows. In Sec. II, we describe the methods used in this work, including the Hamiltonian mapping, the adopted ansatz, and the measurement strategies. In Sec. III, we present the results for oxygen, calcium, and nickel isotopes, noise-free simulations, and hardware experiments. Finally, we summarize our findings and discuss future outlooks in Sec. IV.

II. METHODS

A. Target systems and Hamiltonian mapping

General shell-model Hamiltonians with up to two-body interactions can be expressed as

$$\hat{H} = \sum_i h_{ij} a_i^\dagger a_j + \frac{1}{4} \sum_{ijkl} V_{ijkl} a_i^\dagger a_j^\dagger a_l a_k, \quad (1)$$

where i denotes the single-particle state characterized by the quantum numbers $\{n, l, j, j_z, t_z\}$. Here, n is the principal quantum number, l is the orbital angular momentum, j is the total angular momentum, j_z its projection onto the z axis, and t_z is the isospin projection.

For systems within single major shell, as in this work, the one-body term reduces to the diagonal form $\varepsilon_i \equiv h_{ii}$, called the single-particle energies (SPEs). The fermionic creation and annihilation operators, $a_i^\dagger$ and a_i , act on these single-particle states, while V_{ijkl} denotes the two-body matrix elements (TBMEs).

These SPEs and TBMEs can be either derived from the realistic nucleon-nucleon interactions or from the phenomenological adjustments to reproduce experimental data for binding energies, excitation energies, and so on. The target nuclei, model space, and adopted interactions in this work are summarized in Table I. The methods in this work can be applied to any other interactions including microscopically derived ones as far as one considers similar systems with same-species nucleons under the methods described below. Diagonalization with these interactions can be repro-

duced using publicly available codes such as KSHELL [31] or NUCLEARTOOLKIT.JL [32].

Once the Hamiltonian is defined, one can diagonalize the Hamiltonian in a given model space by means of variants of configuration interaction (CI) methods, known as the nuclear shell model in nuclear physics community. In this work, full configuration interaction (FCI) refers to exact diagonalization within the selected valence space, following the convention of quantum chemistry (rather than the no-core shell-model definition often used in nuclear physics).

A useful truncation of CI is the doubly occupied configuration interaction (DOCI) method, equivalent to restricting the shell-model space to zero-seniority configurations, i.e., considering only time-reversed nucleon pairs as active degrees of freedom. In even-neutron systems, DOCI often provides a good approximation to FCI and is exact for two-valence-neutron $J = 0$ states. This DOCI method has been also used in nuclear physics and proven to be a good approximation to even-number neutron systems [36]. Thus, DOCI serves as an important benchmark in this work.

Another viable method for approximating FCI and/or DOCI is the use of pair coupled-cluster methods and their extensions [27–29,37–39]. Whereas the methods have been successfully applied to pairing Hamiltonians (also known as BCS Hamiltonians) in the nuclear physics context, their applications to more general shell-model Hamiltonians remain limited and warrant further exploration.

In the case of electronic structure calculations, the natural assumption on the *pair* degree of freedom is to consider the spin-up and spin-down electrons as a pair. Detailed derivations of such zero-seniority Hamiltonian for electronic structure calculations can be found in Ref. [38]. For nuclear many-body methods, one has more freedom involved in the system, so one can consider the pairs of nucleons with different spins and/or different orbitals. For this reason, we will detail the way to introduce the paired form of a nuclear shell-model Hamiltonian.

The HCB representation provides a natural way to introduce paired degrees of freedom by folding each time-reversed single-particle pair $(i, \bar{i})$ into a single bosonlike site that can be occupied or empty but forbids multiple occupancy. Similar mappings have been employed in various contexts within quantum chemistry and nuclear physics [17,19,22,26,27,30,40,41]. Depending on whether one emphasizes the underlying degrees of freedom or the commutation relations of the operators, this construction is referred to by various names—geminal, hard-core-boson antisymmetrized geminal power, seniority-zero, quasiparticle representations, etc.—but the underlying idea is similar.

Here, we summarize the derivation of the HCB representation for nuclear shell-model Hamiltonians. Figure 1 illustrates this mapping for ^{22}O on top of the ^{16}O inert core: The valence single-particle states are grouped into pair orbitals, which reduces the number of active degrees of freedom (and hence qubits). The single-particle states in the original fermionic representation are specified by the quantum numbers $\{n, l, j, j_z, t_z\}$, leading to 12 single-particle states for both protons and neutrons in the sd shell. In the HCB representation, these 12 single-particle states form six pair orbitals

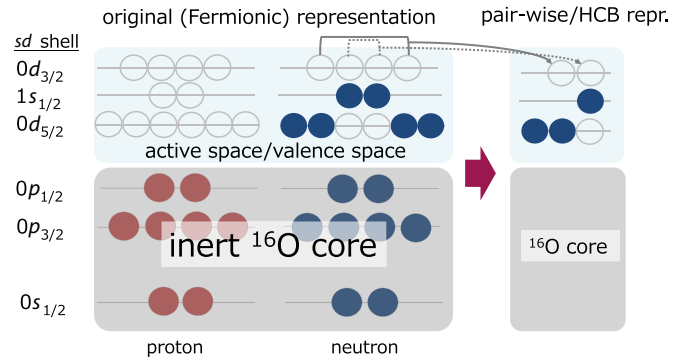


FIG. 1. Schematics of the hard-core-boson (HCB) representation. This example shows a configuration of ^{22}O nucleus on top of the inert core ^{16}O . The active (valence) space consists of $1s_{1/2}$, $0d_{3/2}$, and $0d_{5/2}$ single-particle states.

for neutrons, each represented by a qubit. Focusing on even-number neutron systems and terms involving time-reversed pairs, the shell-model Hamiltonian can be expressed as

$$H = \sum_{i<0} \varepsilon_i (a_i^\dagger a_i + a_{\bar{i}}^\dagger a_{\bar{i}}) + \sum_{i<0} V_{i\bar{i}\bar{i}i} a_i^\dagger a_{\bar{i}}^\dagger a_{\bar{i}} a_i + \sum_{i \neq j < 0} V_{i\bar{i}j\bar{j}} a_i^\dagger a_{\bar{i}}^\dagger a_j a_{\bar{j}} + \frac{1}{4} \sum_{i,j \notin \{i,\bar{i}\}} V_{ijij} n_i n_j, \quad (2)$$

where $i < 0$ denotes single-particle states with negative j_z values and $\bar{i}$ is the time-reversal partner of the single-particle state i . The last term, absent in the valence two-neutron systems studied previously [26], can be regarded as a mean-field contribution from other occupied pairs. Then, the Hamiltonian can be expressed in terms of the paired operators defined below:

$$A_{\bar{i}}^\dagger = a_i^\dagger a_{\bar{i}}^\dagger, \quad (3)$$

$$A_{\bar{i}} = a_{\bar{i}} a_i, \quad (4)$$

$$N_{\bar{i}} = \frac{1}{2}(n_i + n_{\bar{i}}) = \frac{1}{2}(a_i^\dagger a_i + a_{\bar{i}}^\dagger a_{\bar{i}}), \quad (5)$$

where $A_{\bar{i}}^\dagger$ and $A_{\bar{i}}$ are, respectively, the pair creation and annihilation operators, $N_{\bar{i}}$ is the pair occupation number operator, and $\bar{i}$ denotes the pair index corresponding to the single-particle states i and $\bar{i}$. Then, the Hamiltonian in Eq. (2) can be rewritten as

$$H_{\text{HCB}} = \sum_{\bar{i}} (\varepsilon_{\bar{i}} + V_{\bar{i}\bar{i}}^P) N_{\bar{i}} + \sum_{\bar{i} \neq \bar{j}} V_{\bar{i}\bar{j}}^P A_{\bar{i}}^\dagger A_{\bar{j}} + \sum_{\bar{i} \neq \bar{j}} V_{\bar{i}\bar{j}}^M N_{\bar{i}} N_{\bar{j}}, \quad (6)$$

$$\varepsilon_{\bar{i}} \equiv 2\varepsilon_i = \varepsilon_i + \varepsilon_{\bar{i}}, \quad (7)$$

$$V_{\bar{i}\bar{j}}^P \equiv V_{i\bar{i}j\bar{j}}, \quad (8)$$

$$V_{\bar{i}\bar{j}}^M \equiv V_{ijij} + V_{i\bar{j}i\bar{j}} + V_{i\bar{j}j\bar{i}} + V_{i\bar{i}j\bar{j}}, \quad (9)$$

where V^P and V^M are introduced to emphasize the pairing and monopole nature of the interactions, respectively. The factor $1/2$ in Eq. (5) is sometimes omitted (as in our earlier work [26]), but is retained here to interpret $N_{\bar{i}}$ as the occupation number of a pair degree of freedom. More details on this

derivation are provided in the Supplemental Material [42]. The paired-neutron operators satisfy bosonic commutation relations, as detailed in Refs. [26,27,38], but multiple occupancy of the same pair is forbidden, leading to the term hard-core boson. A key advantage of the HCB representation—beyond the qubit reduction—is the elimination of long strings of Pauli-Z operators. From Jordan-Wigner mappings, Pauli-Z terms appear to maintain the anticommutation relations of the fermionic operators. In some literature, these Pauli-Z terms are omitted on purpose, which is referred to as qubit excitation in Refs. [43,44], as a hardware-efficient mapping. However, in the HCB representation, those Pauli-Z terms naturally cancel out. Hence, one can map the Hamiltonian to the Pauli operators into simple forms as

$$H_{\text{HCB};q} = \sum_i \frac{\varepsilon_i + V_{ii}}{2} (I_i - Z_i) + \frac{1}{4} \sum_{i \neq j} V_{ij} (X_i X_j + Y_i Y_j) + \frac{1}{4} \sum_{i \neq j} V_{ij}^m (I_i - Z_i)(I_j - Z_j), \quad (10)$$

where i denotes the pair index of single-particle states in the valence space specified by n (principal quantum number), l (orbital angular momentum), j (total angular momentum), $|j_z|$ (absolute value of the angular momentum projection on the z axis), and t_z (isospin projection) quanta.

All terms of the Hamiltonian [Eq. (10)] except the second are diagonal in the computational basis and can be measured directly by measuring the expectation values of the Pauli-Z operators. One needs additional circuits to measure the non-diagonal terms $XX + YY$, which will be discussed later in Sec. II C.

B. Ansatz

The ansatz, circuit for state preparation, plays a central role in quantum algorithms in both the NISQ and FTQC regimes. In practice, the ansatz must satisfy two requirements: (1) It should be implementable on available quantum hardware and (2) it should be expressive enough to approximate, e.g., the true ground state with high fidelity.

In this work, we employ the pUCCD ansatz within the HCB representation, which is particularly well suited for systems with an even number of valence neutrons. The pUCCD ansatz is a quantum version of the pair coupled-cluster doubles method. A seminal work on the pUCCD ansatz in the context of quantum computing is found in Ref. [27], where strategies for measurement and postselection were also proposed. In chemistry, pUCCD has been successfully applied to systems of paired electrons with spin up and spin down [27–29]. For nuclear systems, the pUCCD ansatz has been considered in a few theoretical studies [19], but to our knowledge, no experimental implementation has been reported so far.

The pUCCD ansatz is expressed as

$$|\psi_{\text{pUCCD}}\rangle = \exp(T - T^\dagger)|\text{ref.}\rangle \equiv U|\text{ref.}\rangle, \quad (11)$$

where T is the cluster operator and $|\text{ref.}\rangle$ is a reference state. For paired-neutron excitations, the unitary operator takes the

form

$$U = \exp \left[\sum_{ph} t_h^p (A_p^\dagger A_h - A_h^\dagger A_p) \right], \quad (12)$$

with t_h^p the cluster amplitudes and $A_p^\dagger, A_h$ the pair creation and annihilation operators [Eqs. (3) and (4)], respectively. The indices p and h denote the particle and hole states, respectively. Mapping to Pauli operators yields

$$U_{\text{qubit}} = \exp \left[\sum_{ph} \frac{it_h^p}{2} (X_p Y_h - Y_p X_h) \right], \quad (13)$$

$$\approx \prod_{ph} \exp \left[\frac{it_h^p}{2} (X_p Y_h - Y_p X_h) \right], \quad (14)$$

where the last expression corresponds to a first-order Trotter approximation with a single step, which we adopt in this work. Each term in Eq. (14) can be implemented as a Givens rotation gate acting on qubits p and h :

$$G(2\theta) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \cos \theta & -\sin \theta & 0 \\ 0 & \sin \theta & \cos \theta & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}. \quad (15)$$

Thus, the pUCCD ansatz can be implemented as a sequence of Givens rotations on top of a reference state, e.g., initially prepared by applying X gates to the qubits corresponding to occupied pair orbitals. Figure 2 illustrates two circuit layouts for preparing the pUCCD ansatz, taking ^{22}O nucleus as an example. (1) pUCCD(GS): optimized for devices with limited connectivity (e.g., IBM heavy-hexagon architectures), using Givens rotations followed by swap gates (GS) [27]. The basic idea behind the circuit is detailed in Ref. [45]. (2) pUCCD(G): one realization for all-to-all connectivity (e.g., trapped-ion devices) using only Givens rotations (G). In both cases, the number of parameters is the same as the number of particle-hole pairs.

However, the circuit depth and number of two-qubit gates slightly differ. While pUCCD(GS) has a nearly unique circuit layout, pUCCD(G) admits many realizations depending on the choice of initial configuration and ordering of Givens rotations. We will therefore present simulator results for pUCCD(G) as distributions over multiple circuit realizations in Sec. III.

In what follows, we use a single deterministic realization for both pUCCD(GS) and pUCCD(G) unless otherwise noted. The qubits are aligned by ascending order of j , total angular momentum of the corresponding single-particle states. This is not the optimal lowest-filling configuration; however, we verified that initializing qubits strictly in ascending SPE order is not necessarily superior. The present ordering is therefore a simple and reasonable choice among equivalent alternatives. One can further confirm that this choice does not give an outlier result by comparing with multiple random realizations, as will be shown later in Sec. III.

As a related study, it should be noted that a work by Sarma *et al.* [15] considered oxygen isotopes in the sd shell on a trapped-ion quantum computer, IonQ Aria, using a variant of UCCD ansatz. Their UCCD ansatz was applied only to

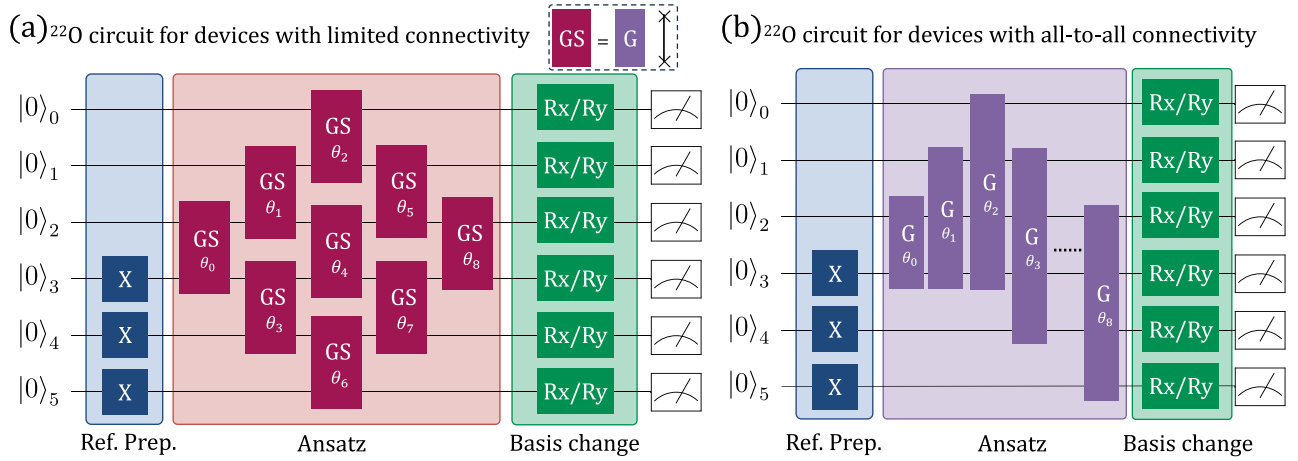


FIG. 2. Sketched quantum circuits for preparing the pUCCD ansatz taking ^{22}O as an example. Original single-particle states in the sd shell consist of twelve states for neutrons, which are now represented by six qubits in the HCB representation. (a) Circuit layout suitable for devices with heavy-hexagon connectivity. (b) Circuit layout for all-to-all connectivity. First, the reference state is prepared by applying X gates to qubits. Then, Givens rotations are applied to take into account particle-hole excitations of nucleon pairs. Single-qubit rotations are applied as needed prior to measuring Hamiltonian expectation values.

time-reversal nucleon pairs [denoted by UCCD ($\nu = 0$) in the following where ν is the seniority]. Although formally equivalent to DOCI, their implementation yielded ground-state errors of 3%–13% relative to FCI, depending on the isotope. One limitation arises from the scaling of circuit parameters: The number of Givens rotations to express the excitations/deexcitations of nucleon pairs grows rapidly with system size, making direct application to heavier isotopes impractical.

By contrast, the pUCCD ansatz with a single Trotter step scales more favorably, as

$$N_{\text{param}} = N_{\text{occ.}}(N_q - N_{\text{occ.}}), \quad (16)$$

where $N_{\text{occ.}}$ is the number of occupied pairs and N_q is the number of qubits in the HCB representation. This scaling is significantly milder than that of UCCD ($\nu = 0$), as summarized in Table II. Note that the FCI dimension is also shown in the table for reference, and these show the number of configurations in the so-called M scheme; i.e., the basis states are labeled by the sum of the j_z values of the single-particle states. For even number of neutrons, all the states with different total angular momentum J are included in the $M = 0$ subspace leading to the FCI dimension shown in the table.

C. Measurement of energy expectation values

Once the ansatz circuit is prepared, the next task is to evaluate the expectation value of the Hamiltonian. First, we discuss our optimization approach; then, we detail the measurement strategies. In this work, the parameters of the pUCCD ansatz were optimized on state vector simulators using the Adam optimizer with PennyLane [46]. This is still an idealized setting, but good starting point to evaluate the ansatz quality and measurement strategies, and to benchmark hardware results. The strategy to optimize the ansatz circuit on a real device is left as a future issue. Optimization directly on quantum hardware remains an open problem, for which gradient-free sequential approaches [47] may offer a promising path.

Once the ansatz circuit is prepared, the next task is to evaluate the expectation value of the Hamiltonian. For noise-free simulations, one does not need to care about the measurement strategy, but it is a crucial point to be considered for noisy simulations and experiments on hardware.

Diagonal terms in the computational basis, i.e., operators involving $\{I, Z_i, Z_i \otimes Z_j\}$, can be obtained by measuring the ansatz circuit in the computational basis. In this case, postselection techniques are naturally applicable: Bitstrings violating the particle number of the target system are discarded.

TABLE II. Comparison of Hilbert-space dimension and ansatz parameter counts. For each nucleus, we list the number of qubits N_q in both Fermionic and HCB representations, the FCI dimension in the $M = 0$ sector, the number of variational parameters required by UCCD ($\nu = 0$) (unitary coupled-cluster doubles restricted to zero-seniority/paired configurations), and the number of parameters for the pUCCD ansatz implemented with a single Trotter step.

Nucleus	N_q Fermionic/HCB	Dimensions		
		FCI	UCCD ($\nu = 0$)	pUCCD
$^{18}\text{O}, ^{26}\text{O}$	12/6	14	5	5
$^{20}\text{O}, ^{24}\text{O}$		81	14	8
^{22}O		142	19	9
$^{42}\text{Ca}, ^{58}\text{Ca}$	20/10	30	9	9
$^{44}\text{Ca}, ^{56}\text{Ca}$		565	44	16
$^{46}\text{Ca}, ^{54}\text{Ca}$		3952	119	21
$^{48}\text{Ca}, ^{52}\text{Ca}$		12 022	209	24
^{50}Ca		17 276	251	25
$^{58}\text{Ni}, ^{76}\text{Ni}$	22/11	19	10	10
$^{60}\text{Ni}, ^{74}\text{Ni}$		365	54	18
$^{62}\text{Ni}, ^{72}\text{Ni}$		3103	164	24
$^{64}\text{Ni}, ^{70}\text{Ni}$		12 240	329	28
$^{66}\text{Ni}, ^{68}\text{Ni}$		23 884	461	30

In contrast, nondiagonal terms $\{X_i \otimes X_j, Y_i \otimes Y_j\}$ require additional circuits. Both XX and YY terms are local, i.e., free from Z strings, and contribute equally to the energy expectation value. Thus, all $X_p X_q$ terms can be evaluated by a single additional circuit, ansatz followed by Hadamard gates on all qubits prior to measurement, and $\langle Y_p Y_q \rangle$ terms can be evaluated by doubling the $\langle X_p X_q \rangle$ results. This approach will be referred to as the *Hadamard* method in the following. While straightforward, this method does not preserve particle-number symmetry, limiting the use of postselection. The other approach employed in this work is one to be referred to as *basis rotations*, which involves diagonalizing $XX + YY$ terms in the computational basis prior to measurement [27,48]:

$$\langle \psi | X_p X_q + Y_p Y_q | \psi \rangle = \langle \psi | \mathcal{U}_{p,q}(\pi/4)(Z_p - Z_q)\mathcal{U}_{p,q}^\dagger(\pi/4) | \psi \rangle, \quad (17)$$

where $\mathcal{U}_{p,q}(\theta)$ can be implemented as a Givens rotation $G(2\theta)$ on qubits p and q . In accordance with the discussion in Ref. [48], the required terms can be grouped such that only $2\lfloor N_q/2 \rfloor$ additional circuits are needed to measure all the $XX + YY$ terms, where N_q is the number of qubits. Importantly, this strategy preserves particle-number symmetry, enabling effective postselection.

Note that since we measure diagonal and off-diagonal contributions in separate circuits, the summed estimate of the energy is not strictly variational even after postselection. However, in practice, we observed that the energy estimates were distributed around the noise-free values from state vector simulations; hence, nonvariational nature does not pose significant issues in this work.

D. Implementation of Givens rotation gates

To construct the pUCCD ansatz circuits (Fig. 2) and to perform basis rotations for diagonalizing the $XX + YY$ terms, it is necessary to implement Givens rotation gates. Several approaches are known in literature and we examined the following three methods:

- (1) Magic-gate method (Ref. [49])—implements Givens rotation using a sequence of “magic” gates.
- (2) $\sqrt{\text{SWAP}}$ -based method (Ref. [45])—uses $\sqrt{\text{SWAP}}$ gates to construct the Givens rotation.
- (3) Controlled- R_y method (Ref. [50])—equivalent to a breakdown of controlled R_y followed by cnot gates.

At the raw circuit level, these methods require two, four, and three cnot gates per Givens rotation, respectively. However, we found that the number of corresponding two-qubit native gates for the transpiled/compiled circuits is equivalent to each other. As a result, the total number of the two-qubit gates for pUCCD(GS) and pUCCD(G) ansatzes scales as $3N_G$ and $2N_G$, respectively. Here, N_G is the number of Givens rotations. Thus, the choice of the implementation method can be made based on convenience and the first method was adopted in this work.

Quantum circuits submitted to the hardware are transformed to native gate sets of the adopted hardware. On the RIKEN-Quantinuum’s Reimei device, two-qubit native gates are ZZPhase gates, $\exp(-i\pi\alpha/2(Z_p \otimes Z_q))$. Here, we follow the notation of pytket [51], i.e., angle parameter is given in

TABLE III. Calibration data of the Reimei device. The values are from data on 2025-05-09 via the Quantinuum’s Nexus [52] platform.

Error type	Value	Uncertainty
One-qubit gate error P_1	4.22×10^{-5}	5.23×10^{-6}
Two-qubit gate error P_2	1.39×10^{-3}	5.92×10^{-5}
SPAM error (0)	2.73×10^{-3}	1.57×10^{-4}
SPAM error (1)	5.25×10^{-3}	2.18×10^{-4}
Crosstalk error	3.21×10^{-5}	1.89×10^{-6}
Memory error	2.83×10^{-4}	2.32×10^{-5}

the unit of $\pi/2$. In practice, the compiled circuit uses exactly twice as many ZZPhase gates as there are Givens rotations.

E. Hardware information

We now describe the quantum hardware used in this work. The Reimei is based on Quantinuum’s H-1 series trapped-ion quantum computer, and has 20 qubits with all-to-all connectivity. The Reimei device was installed in RIKEN’s Wako campus, and started its operation in February 2025. Table III summarizes the calibration data of the Reimei device, which were measured on 2025-05-09. The reported metrics include single- and two-qubit gate errors, state preparation and measurement (SPAM) errors, crosstalk, and memory error rates. These parameters provide a baseline for evaluating the quality of quantum circuits executed on the device. In particular, the relatively low one- and two-qubit gate error rates, combined with the all-to-all connectivity of trapped-ion hardware, enable the accurate implementation of the pUCCD ansatz circuits described in this work.

The experiments on the Reimei trapped-ion quantum computer of this work were carried out via the Quantinuum Nexus [52] platform, which enables users to run quantum simulations on various backends, including noise-free state vector simulators, emulators, and real devices.

III. RESULTS

In this section, we present the results of the pUCCD ansatz both on noise-free state vector simulators and on the Reimei quantum hardware for the ground-state energies of oxygen, calcium, and nickel isotopes. The former allows us to assess the intrinsic accuracy of the pUCCD ansatz, while the latter demonstrates the feasibility of executing the pUCCD ansatz on real quantum hardware.

A. Ideal simulation results of the pUCCD ansatz

We first assess the performance of the pUCCD ansatz on a noiseless state vector simulator, thereby probing its intrinsic accuracy in approximating ground-state energies of the target isotopes. FCI provides the exact ground-state energies within the valence space, serving as a benchmark for evaluating the accuracy of approximate methods. DOCI is another approximate method that restricts the configuration space to zero-seniority configurations, i.e., states in which all nucleons are paired as time-reversed partners. In noise-free simulations, any deviation from FCI obtained with the pUCCD ansatz reflects intrinsic limitations of the ansatz itself, independent

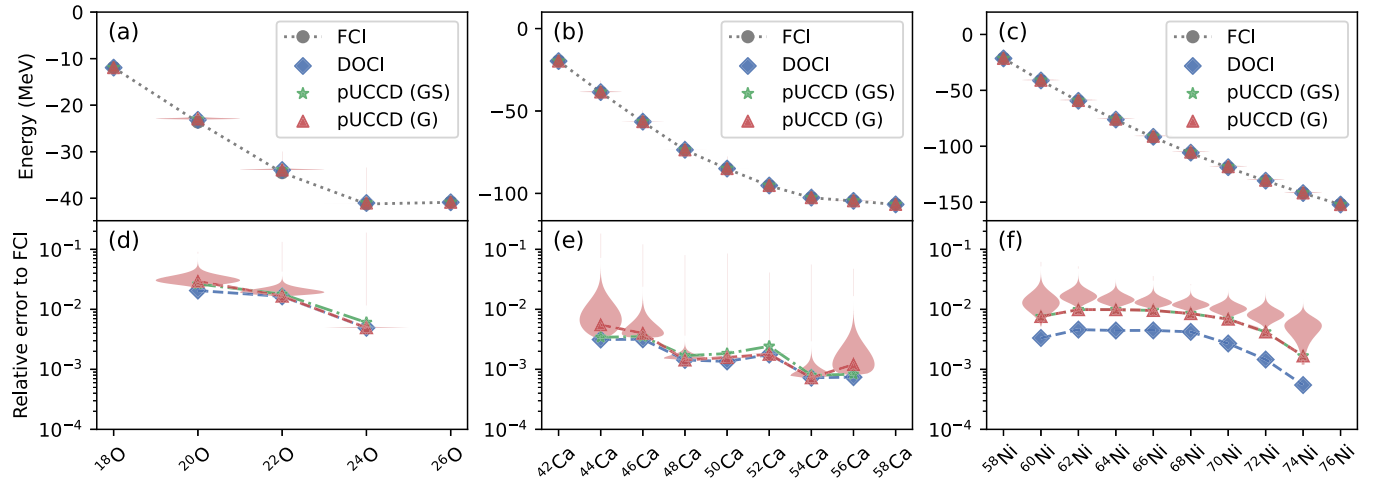


FIG. 3. Ground-state energies of target isotopes on noise-free state vector simulators. (a)–(c) Ground-state energies of oxygen, calcium, and nickel isotopes, respectively. Full configuration interaction (FCI, dotted lines with gray circles) and doubly occupied configuration interaction (DOCI, blue diamonds) are compared with state vector simulations using the pUCCD(GS) ansatz (green stars) and the pUCCD(G) ansatz (red triangles). (d)–(f) Differences between the pUCCD ansatz results and the DOCI results are shown relative to FCI in logarithmic scale. Uncertainty bands for pUCCD(G) are obtained by random sampling over circuits with different initial configurations and Givens rotation orderings.

of hardware noise or statistical noise due to the finite number of measurement shots.

In what follows, we consider two types of pUCCD ansatz, named pUCCD(GS) and pUCCD(G). The (GS) represents Givens plus swap, which consists of only nearest-neighbor Givens rotations and is thereby more suitable for hardware with a limited connectivity [27,48]. On the other hand, (G) stands for Givens rotations, where all-to-all connectivity is assumed. In experiments on the Reimei device, we will focus on the pUCCD(G) ansatz.

Figure 3 shows ground-state energies for the target isotopes, obtained with pUCCD(G) and pUCCD(GS) on noise-free state vector simulators compared to FCI and DOCI results. The upper panels (a)–(c) display the ground-state energies. At this scale, all curves are nearly indistinguishable. The lower panels (d)–(f) show the differences between pUCCD and DOCI results relative to FCI in logarithmic scale. Results for two-neutron (or two-neutron-hole) systems are omitted in the lower panels where both DOCI and pUCCD exactly reproduce FCI in these cases. This is because the HCB representation with paired operators can exactly represent the ground states of single pair systems without approximation [26].

For the pUCCD ansatz, the symbols show the results of one representative realization of the ansatz, and the uncertainty bands are plotted for the pUCCD(G) ansatz. We generated many pUCCD(G) realizations by varying the initial configuration and the order of Givens rotations in the ansatz circuit. The resulting energies from a skewed distribution around the representative realization, and the uncertainty bands are constructed by fitting Gamma distributions to the histograms of sampled energies. More technical details are provided in the Supplemental Material [42].

Most importantly, pUCCD reproduces DOCI energies with an error of mostly less than 1%, while using far fewer parameters, demonstrating its compact yet accurate description. For reference, DOCI itself reproduces FCI ground-state energies

within 0.1%–1%, with deviations smaller than the typical uncertainties (a few percent) of modern nuclear many-body methods [53]. The residual differences depend on the target system: Ca isotopes in the pf shell are well described within the zero-seniority space, whereas oxygen isotopes show larger contributions from higher-seniority configurations, leading to slightly larger deviations from FCI. Nickel isotopes in the $jj45$ shell exhibit larger discrepancies between DOCI and pUCCD compared to oxygen and calcium isotopes. This arises from the factors intrinsic to the $jj45$ shell. The valence space of the $jj45$ shell consists of four jj -coupling orbitals ($1p_{1/2}$, $1p_{3/2}$, $0f_{5/2}$, $0g_{9/2}$), and the configuration mixing among these orbitals is pronounced in Ni isotopes even for ground states since their effective single-particle energies are close to each other [35]. The results imply that the dominant pairing correlations in the same-species nucleons are expressed rather separable manner, and that one may need to consider more expressive ansatzes, e.g., by increasing the number of Trotter steps or including higher-order excitations, to further improve the accuracy for systems with strong configuration mixing.

B. Results on RIKEN-Quantinuum's Reimei trapped-ion quantum device

We now report the hardware results for ground-state energies of oxygen, calcium, and nickel isotopes using the pUCCD(G) ansatz on Reimei. Table IV summarizes exact FCI energies, the ideal pUCCD results from noise-free state vector simulations, and the experimentally measured energies with two measurement strategies along with percent errors relative to the ideal pUCCD results and valid ratios. The valid ratio indicates the ratio of bitstrings that preserve the correct particle number of the target nucleus after measurement, reflecting the hardware fidelity in preparing the desired state. The num-

TABLE IV. Summary of pUCCD results on the RIKEN-Quantinuum Reimei device. FCI and ideal pUCCD are classical results. Reimei columns list results obtained on the Reimei device using two measurement strategies. “Rel. error” columns show the absolute value of the relative error of the hardware results to the ideal pUCCD results, and the “Std.” columns list typical 1σ statistical uncertainties (in %) from bootstrap analyses. Valid ratio is the fraction of bitstrings passing particle-number postselection. All energies and their standard deviations are in MeV and relative errors are in %.

Nuclide	FCI	Ideal pUCCD	Reimei: Hadamard			Reimei: Basis rotation			Valid ratio (%)
	Energy	Energy	Energy	Std.	Rel. error	Energy	Std.	Rel. error	
¹⁸ O	−11.932	−11.932	−11.802	(0.209)	1.09	−11.893	(0.099)	0.33	0.98
²⁰ O	−23.632	−22.939	−22.383	(0.234)	2.42	−22.854	(0.140)	0.37	0.98
²² O	−34.498	−33.924	−33.560	(0.222)	1.07	−33.829	(0.152)	0.28	0.97
²⁴ O	−41.225	−41.021	−40.985	(0.194)	0.09	−41.027	(0.150)	0.02	0.97
²⁶ O	−40.869	−40.869	−40.613	(0.176)	0.63	−40.940	(0.106)	0.18	0.96
⁴² Ca	−19.734	−19.734	−19.727	(0.126)	0.04	−19.775	(0.053)	0.21	0.97
⁴⁴ Ca	−38.675	−38.462	−38.540	(0.162)	0.20	−38.424	(0.073)	0.10	0.97
⁴⁶ Ca	−56.667	−56.440	−56.414	(0.143)	0.05	−56.565	(0.062)	0.22	0.96
⁴⁸ Ca	−73.662	−73.556	−73.538	(0.131)	0.02	−73.489	(0.080)	0.09	0.95
⁵⁰ Ca	−85.055	−84.921	−85.135	(0.151)	0.25	−85.007	(0.087)	0.10	0.94
⁵² Ca	−95.360	−95.190	−95.038	(0.146)	0.16	−95.149	(0.095)	0.04	0.94
⁵⁴ Ca	−102.632	−102.557	−102.622	(0.127)	0.06	−102.648	(0.081)	0.09	0.94
⁵⁶ Ca	−104.589	−104.462	−104.620	(0.143)	0.15	−104.325	(0.082)	0.13	0.94
⁵⁸ Ca	−106.666	−106.666	−106.885	(0.132)	0.20	−106.668	(0.058)	<0.01	0.94
⁵⁸ Ni	−21.447	−21.447	−21.207	(0.149)	1.12	−21.291	(0.071)	0.73	0.93
⁶⁰ Ni	−41.276	−40.961	−40.752	(0.197)	0.51	−40.992	(0.094)	0.07	0.94
⁶² Ni	−59.602	−59.013	−58.703	(0.228)	0.52	−59.015	(0.110)	<0.01	0.93
⁶⁴ Ni	−76.444	−75.687	−76.027	(0.261)	0.45	−75.765	(0.116)	0.10	0.92
⁶⁶ Ni	−91.941	−91.059	−90.552	(0.245)	0.56	−90.695	(0.138)	0.40	0.93
⁶⁸ Ni	−106.140	−105.237	−105.169	(0.263)	0.06	−105.288	(0.133)	0.05	0.92
⁷⁰ Ni	−119.034	−118.215	−118.189	(0.253)	0.02	−118.158	(0.115)	0.05	0.91
⁷² Ni	−130.930	−130.379	−130.511	(0.223)	0.10	−130.397	(0.092)	0.01	0.95
⁷⁴ Ni	−141.932	−141.694	−141.565	(0.197)	0.09	−141.715	(0.074)	0.02	0.93
⁷⁶ Ni	−152.103	−152.103	−151.986	(0.133)	0.08	−152.054	(0.053)	0.03	0.94

bers are from ansatz measurements, hence independent of the measurement strategy for $XX + YY$ terms.

As a whole, the hardware results agree closely with the noise-free simulations, showing relative errors mostly below 0.3% to the ideal pUCCD results, and at most a few percent relative to FCI. These results demonstrate the capability of current quantum hardware to accurately capture nuclear pairing correlations.

This trend is further supported by bootstrapping analyses. Figure 4 displays the relative errors of ground-state energies obtained on Reimei for oxygen, calcium, and nickel isotopes, using both measurement strategies. Error bars represent 1σ statistical uncertainties evaluated by bootstrapping with 500 resamplings of datasets obtained from 1024 measurement shots. The shaded band corresponds to a 0.3% error for reference. Most data points fall within this range.

Note again that the difference between Hadamard and basis-rotation methods lies only in the measurement of $XX + YY$ terms, while diagonal terms are measured in the same way for both methods. Between the two measurement strategies, the basis-rotation method consistently outperforms the Hadamard method, yielding results closer to ideal simulations. Lighter isotopes exhibit larger uncertainties because $XX + YY$ terms contribute to the total energy relatively larger in lighter isotopes. In contrast, for heavier isotopes, the mass-dependent scaling commonly applied to two-body matrix

elements in phenomenological shell-model interactions reduces the absolute size of the $XX + YY$ contributions (e.g., TBMEs for ⁵⁸Ca and ⁷⁸Ni are multiplied by ~ 0.9 compared with ⁴²Ca and ⁵⁸Ni), which further diminishes their relative contribution to the total energy.

Next, we further examine the statistical uncertainties by separating the total energy into diagonal and $XX + YY$ contributions. As an illustration, Fig. 5 shows the distribution of the ground-state energy of ⁶⁶Ni obtained by resampling the data 500 times. The energy is separated into contributions from diagonal terms (top panel) and $XX + YY$ terms (bottom panel). Vertical dashed lines indicate the corresponding noise-free state vector results for comparison.

The accuracy on the diagonal term depends primarily on occupation numbers, while the $XX + YY$ terms are more sensitive to both occupation numbers and relative phases between configurations. As shown in the lower panel of Fig. 5, the distribution obtained using the Hadamard method is noticeably broader than that obtained with basis rotations.

We emphasize, however, that this analysis does not account for systematic errors inherent to the Reimei device. Therefore, our results do not imply that the basis-rotation method always outperforms the Hadamard method in practice. Nonetheless, the observed trends (see also Fig. 4) suggest that basis rotations tend to yield more stable

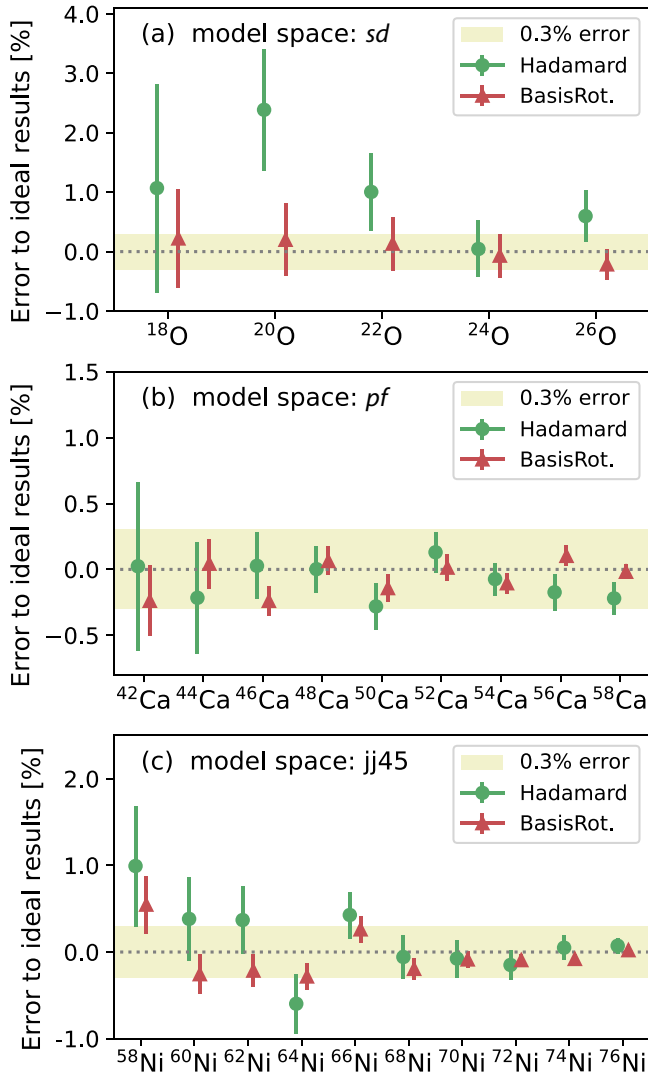


FIG. 4. Relative errors in ground-state energies on the RIKEN-Quantum Reimei device. The results are shown for oxygen [panel (a)], calcium [panel (b)], and nickel [panel (c)] isotopes, using two measurement strategies: Hadamard and basis rotation. The error bars represent 1σ statistical uncertainties evaluated by bootstrapping, and the shaded band corresponds to a 0.3% error.

estimates of energy expectation values for the systems studied here.

IV. SUMMARY AND OUTLOOK

Quantum many-body systems have become a central focus of quantum-computing research over the past decade, driven by rapid progress in algorithms and hardware. However, demonstrating genuine quantum advantage in interacting many-body physics remains an open challenge, requiring advances in all components of the algorithmic workflow: ansatz design, quantum algorithms, measurement strategies, optimization techniques, and so on. This work concentrated on the ansatz and measurement aspects, from the standpoint of nuclear structure, where exceptionally strong correlations make the choice of ansatz especially critical.

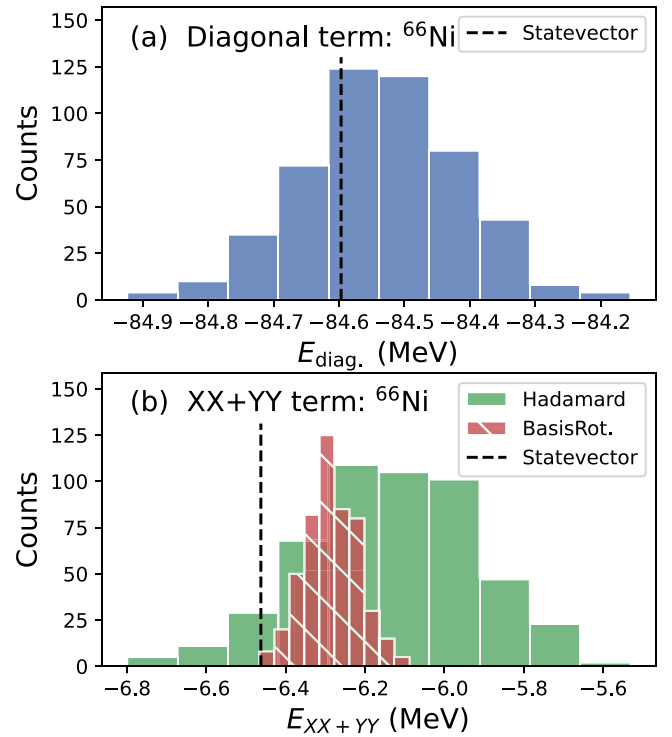


FIG. 5. Bootstrapping of hardware results for ^{66}Ni . (a) Diagonal terms. (b) $XX + YY$ terms evaluated by two measurement strategies: Hadamard (green) and basis rotation (red with hatching). The vertical dashed line shows the ideal state vector simulation result. The bin width is automatically determined by the Freedman-Diaconis rule.

By combining a hard-core-boson mapping of the nuclear shell-model Hamiltonian with a pUCCD ansatz, we demonstrated accurate ground-state calculations of oxygen, calcium, and nickel isotopes on the RIKEN-Quantum Reimei trapped-ion quantum computer. Our results achieve subpercent agreement with noise-free state vector simulations, setting a benchmark for nuclear-structure simulations on real NISQ hardware.

While the pUCCD parameters in this work were optimized on classical simulators, this proof-of-principle study shows that compact, physically motivated ansatzes can achieve high accuracy with modest qubit counts and circuit depths. Such strategies can guide the design of efficient variational forms for larger systems where classical preoptimization is infeasible. Optimization for classically intractable systems remains an open challenge, and hardware-suitable optimization methods are needed. Our previous study [26] demonstrated that a sequential, gradient-free optimization scheme [47] can effectively optimize a similar ansatz for two-valence-neutron systems. Although those systems were still classically tractable, the results suggest that sequential methods may be viable for optimizing or refining ansatzes on quantum hardware. For larger problems, hybrid approaches that combine classical preoptimization in a reduced subspace with subsequent quantum refinement could also be explored.

It remains an open question how best to extend the present framework to include proton-neutron interactions, which are essential for a complete description of nu-

clei. While several studies have investigated proton-neutron pairing alongside like-particle pairing [19,22], a practical quantum ansatz must be able to capture more general, non-local correlations beyond simple pair excitations. Developing such ansatzes and evaluating their resource and measurement requirements will be necessary to treat mixed-species correlations robustly. Nonetheless, our results demonstrate that pUCCD provides a compact and accurate description of pairing correlations in single-species systems (multineutron or multiproton), establishing a foundation for future extensions to more complex nuclear systems, and footsteps toward heavier systems such as neutron drops or neutron-rich isotopes.

As an illustration of possible extensions, entropy-driven entanglement forging [54] has recently been proposed to localize correlations in Adapt-VQE circuits; similar ideas including Ref. [55] could be combined with pUCCD, for instance, by monitoring generalized seniority. In addition, hybrid qubit encoding schemes [56] could be extended to nuclear systems.

Beyond ansatz design, algorithmic paradigms merit exploration. Quantum subspace diagonalization techniques [57–61], including quantum Krylov and related methods, use quantum devices to generate subspace states while delegating diagonalization to classical post-processing. These approaches provide access to excited states and transition properties such as electromagnetic transitions. Such hybrid methods, in combination with physically motivated ansatzes and developing efficient schemes for time evolution and

measurement, may offer a promising path toward realistic quantum simulations of nuclear systems beyond the reach of classical methods.

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DATA AVAILABILITY

The data that support the findings of this article, including circuits and encoded Hamiltonians, are openly available from the GitHub repository and the Zenodo archive [62]. For classical calculations, the exact diagonalization results can be reproduced by using the NUCLEAR TOOLKIT.JL package [32] with the interaction files available through KSHELL [31]. We utilized the QISKIT [63], PENNY-LANE [46], and PYTKET [51] for quantum computations. Experiments on the Reimei device were carried out using the Quantinuum’s Nexus [52] platform.

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