QCSH: A full quantum computer nuclear shell-model package

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The nuclear system is a promising area for demonstrating practical quantum advantage. A comprehensive computation of a nuclear system in a classical computer is beyond the capacity of current classical computers. With the rapid development of hardware, the prospect of using quantum computers in nuclear physics is close at hand. In this paper, we report a full quantum package, QCSH, for solving a nuclear shell model in a quantum computer. QCSH uses the linear combination of the unitary formalism of quantum computing and performs all calculations in a quantum computer. The complexities of qubit resource and the number of basic gates of QCSH are both polynomials to the number of nucleons in nuclei. For example, QCSH is used to calculate the binding energies of 12 light nuclei (i.e., $^2$H, $^3$H, $^3$He, $^4$He, $^6$Li, $^7$Li, $^{12}$C, $^{14}$N, $^{16}$O, $^{17}$O, $^{23}$Na, and $^{40}$Ca). Moreover, we experimentally demonstrate the calculation of deuteron binding energy using a superconducting quantum processor. The result indicates that QCSH can provide meaningful results already in near-term quantum devices.

quantum simulation, nuclear shell model, linear combination of unitary operations, quantum gradient descent

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1 Introduction

The nucleus is an important layer of a material, and a quantum many-body system composed of protons and neutrons. The calculation in nuclear physics is tremendously difficult due to the large state space involved. The study of nuclear systems is even more difficult than ordinary quantum many-body systems because the complexities and uncertainties of nuclear interactions [1, 2].

In practice, nuclear forces are considered effective interaction potentials in relativistic models to describe the properties of nuclei (e.g., energy levels, electromagnetic transition rates, and reaction cross sections). The nuclear shell model is a typical example of this type of relativistic model. In the nuclear shell model, each nucleon moves independently in an effective average field, and the nucleons interact with each other via residual interactions. The shell model achieves great success nowadays in explaining the formation of magic numbers and nuclear collective motion [3-5]. Specifically, advanced shell model codes (e.g., the NuShellX [6]) are extensively used for various calculations.

Similar to any other quantum many-body systems, full calculation of the nuclear shell model, with all nucleons and all shells involved, in a conventional computer is intractable, because of the limitations of computational resources. For instance, the NuShellX code can treat a matrix with a dimension in the order of 100 million, namely, $1 \times 10^8$. Currently, calculations of the nuclear shell model are performed with
several restrictions. For instance, only valence shells are considered, and the inner shells are treated as frozen. Even with such restrictions, the shell model can only calculate the structure of light nuclei. For medium and heavy nuclei, calculations using valence nucleons remain impossible. Only one type of valence nucleon can be treated in medium and heavy nuclei, for example, \( N = 50 \) isotones or \( Z = 64 \) is treated as a sub-shell. The combined uncertainties in the nuclear interaction and calculation due to approximations make the study of nuclear systems extremely difficult and with a large uncertainty when compared with the experimental data.

Meanwhile, rapid development in quantum computing is attracting worldwide attention \([7, 8]\). For a given quantum many-body system with \( N \) nucleons, a classical computer has to use \( O(2^N) \) resources, while a quantum computer only consumes \( O(poly(N)) \) resources. Over the past two decades, quantum computer hardware has advanced a lot. Rudimentary quantum computers with 100 qubits are now available, and the size and quality of quantum computers are continuously improving. Although they are still far from the sophisticated fault-tolerant quantum computers, they can already complete useful tasks \([9-12]\).

The prospect of using quantum computers to examine quantum systems is more than ever close. In the chemistry field, a variational quantum eigensolver (VQE) \([13, 14]\) and a full quantum eigensolver (FQE) \([15]\) have been proposed to find the eigenvalues and wavefunctions of molecules. In a quantum-classic hybrid model (i.e., VQE), the computation process is switched iteratively between classical and quantum computers. The VQE has been applied to calculate the binding energy of the deuteron nucleus \([16, 17]\).

Conversely, the FQE is a full quantum computer algorithm \([15]\), which is based on the linear combination of unitary formalism \([18]\). It performs all calculations on a quantum computer, avoiding the slow and tedious switching between classic and quantum computers. The FQE has been demonstrated in chemistry calculation \([15]\), and has attracted attention in recent years \([19-26]\).

Therefore, we present a full quantum computer package, namely, QCSH, for solving the nuclear shell model in a quantum computer. First, we present the framework of the quantum computer nuclear shell model. Then, we demonstrate the use of QCSH by applying it to find the binding energies of 12 light nuclei (i.e., \( ^2\text{H}, ^3\text{H}, ^3\text{He}, ^4\text{He}, ^7\text{Li}, ^7\text{Li}, ^{12}\text{C}, ^{14}\text{N}, ^{16}\text{O}, ^{17}\text{O}, ^{25}\text{Na}, \) and \(^{40}\text{Ca}\)). We verify that QCSH achieves identical results as those from the exact diagonalization in a classical computer in some examples. To estimate the influence of imperfection of near-term quantum computers, we also perform QCSH calculations with quantum noises.

2 QCSH framework

2.1 Hamiltonian and model

We use a nuclear shell model with an effective average field having spin-orbit coupling \([2, 3]\). In addition to the average field, the nucleons interact through the residual interaction. For a given nucleus \(^Z\text{X}\), the Hamiltonian can be written in first quantization formalism as:

\[
H = \sum_{i=1}^{Z} \frac{p_i^2}{2M_p} + \sum_{j=j+1}^{A} \frac{p_j^2}{2M_n} + \sum_{k=1}^{A} V(r_k) + \sum_{1 \leq i \leq Z} \frac{e^2}{4\pi\varepsilon_0 |\mathbf{r}_i - \mathbf{r}_k|} + \frac{1}{2} \sum_{k_1, k_2} v(k_1, k_2),
\]

(1)

where \( M_p = 938.3 \text{ MeV}/c^2 \), \( M_n = 939.6 \text{ MeV}/c^2 \) are the masses of proton and neutron. \( V(r_k) \) is the average field; and \( v(k_1, k_2) \) is the residual two-body interaction. The first two terms are kinetic energies of protons and neutrons, respectively, and the fourth term is the Coulomb potential between protons. To transform the Hamiltonian from first into second quantization, we choose single particle orbits for protons and neutrons \( \{\psi_{\pi,\alpha}\}_{j=1}^{N_\pi} \) and \( \{\psi_{\nu,\beta}\}_{j=1}^{N_\nu} \), respectively. Here \( N_\pi \) and \( N_\nu \) are the number of single-particle orbits taken in the calculations.

After the single-particle orbits have been selected, the Hamiltonian can be written in the second quantization form as:

\[
H = \sum_{\alpha \beta} g_\pi(\alpha', \alpha) a_\pi^{\dagger} a_\pi \otimes I_v + \sum_{\alpha_1 \alpha_2} g_\nu(\alpha_1', \alpha_2') a_\nu^{\dagger} a_\nu \otimes I_v + \sum_{\beta_1 \beta_2} g_{\beta}(\beta_1', \beta_2') 1_i \otimes a_\beta^{\dagger} a_\beta + \sum_{\beta_1 \beta_2} h_{\beta}(\beta_1', \beta_2') I_v \otimes \alpha_\beta \otimes \alpha_\beta^{\dagger}
\]

\[
+ \sum_{\alpha_1' \alpha_2'} h_{\pi}(\alpha_1', \alpha_2') a_\pi^{\dagger} a_\pi \otimes \alpha_\beta \otimes \alpha_\beta^{\dagger},
\]

(2)

where \( \alpha, \alpha', \alpha_1, \beta, \beta_1, \beta_2 \) \in \{1, 2, ..., N_\pi\}, \( \beta', \beta_1', \beta_2' \) \in \{1, 2, ..., N_\nu\}. \( \alpha \), \( \alpha' \), \( \alpha_1 \), \( \beta \), \( \beta_1 \), \( \beta_2 \), \( \beta_1' \), \( \beta_2' \) are the creation and annihilation operators acting on a single-particle state. The operators of protons and neutrons are denoted by subscript \( \pi \) and \( \nu \), respectively. The one and two-body interactions in the Hamiltonian can be calculated by

\[
g_\pi(\alpha', \alpha) = \langle \psi_{\pi,\alpha'} | \frac{p^2}{2M_p} + V(\mathbf{r}) | \psi_{\pi,\alpha} \rangle,
\]

\[
g_{\beta}(\beta', \beta) = \langle \psi_{\nu,\beta'} | \frac{p^2}{2M_n} + V(\mathbf{r}) | \psi_{\nu,\beta} \rangle,
\]
age field can also be calculated from relativistic mean field protons and neutrons in a single-particle state. The state of a nucleus with Fermions obey the Pauli principle; henceforth, one qubit is and \( M \) is the orbital angular momentum operators, and \( s \) and \( l \) are the single-particle spin and orbital angular momentum operators, respectively. Further, \( s \) and \( l \) take the positive and negative signs, respectively. Further, the\( s \) and \( I \) are the single-particle spin and orbital angular momentum operators, and \( s \cdot I = l/2 \) for \( j = l + 1/2 \) and \(- (l + 1)/2 \) for \( j = l - 1/2 \). The average field can also be calculated from relativistic mean field approach [27].

A major component of the two-body interaction \( v(k_1, k_2) \) is the pair correlation, which can be directly written as [2]:

\[
H_{\text{pair}} = - \frac{G}{4} \sum_{j,m,m'} (-1)^{j+m+m'} a_{j,m}^\dagger a_{j-m,m'}^\dagger a_{j,m} a_{j-m,m'} \otimes I_y + \sum_{j,m,m'} (-1)^{j+m+m'} I_y \otimes a_{j,m}^\dagger a_{j,m}^\dagger a_{j,m} a_{j,m}^\dagger \right],
\]

where \( G = 0.25 \text{ MeV} \). Thus, in the nuclear shell model, we can first provide a Hamiltonian in the form of eq. (2), taking the average potential to calculate single-particle orbits, and adopt a form of residual interactions from either a microscopic or from phenomenological model. Then, we calculate the matrix elements using eq. (3). In the examples of this paper, we take the interaction as given in eq. (2).

### 2.2 Encoding the quantum states into qubits

Fermions obey the Pauli principle; henceforth, one qubit is enough to represent possession (1) or absence (0) of a nucleon in a single-particle state. The state of a nucleus with \( Z \) protons and \( N \) neutrons could be written as the superposition of the basis states,

\[
N_z \text{ qubits } N_n \text{ qubits}
\]

\[
|0100...101)0101...110),
\]

where \( N_z \) and \( N_n \) are the proton and neutron single-particle orbits, respectively. After encoding quantum states on the qubits, we use the Jordan-Wigner (J-W) transformation [28] to map the creation and annihilation operators into the Pauli operators by

\[
a_k^\dagger = c_k(1) k(0) = c_k^2 (X_k - iY_k)
\]

\[
= \frac{1}{2} Z_1 \otimes Z_2 \otimes ... Z_{k-1} \otimes (X_k - iY_k) \otimes I_{k+1} \otimes ..., \]

\[
a_k = c_k(0) k(1) = \frac{c_k^2}{2} (X_k + iY_k)
\]

\[
= \frac{1}{2} Z_1 \otimes Z_2 \otimes ... Z_{k-1} \otimes (X_k + iY_k) \otimes I_{k+1} \otimes ..., \]

where subscript \( k \) denotes the single-particle state labeling; \( c_k = (-1)^{n_1+n_2+...+n_{k-1}} \in \{-1, +1\} \) and \( n_1, n_2, ..., n_{k-1} \in \{0, 1\} \) are the particle number in each single-particle state, and \( X, Y, Z \) are the Pauli gates. The nucleus contains both protons and neutrons, and the transformation is carried out for protons and neutrons separately. The operators should also be labeled with the type of nucleons such as \( a_{x,k}^\dagger, a_{x,k}, a_{v,k}^\dagger, a_{v,k} \), \( I_y, \) and \( I_z \).

After the J-W transformation, the Hamiltonian in the second quantization formalism is represented by

\[
H = \sum_{k=0}^{M-1} a_k H_k^\dagger.
\]

where \( H_k^\dagger \) is unitary operator comprising Pauli operators (Figure 1). Eq. (8) can be expressed as a linear combination of unitary operators as given in ref. [29].

### 2.3 Quantum gradient descent iteration

Rather than diagonalizing the Hamiltonian directly, we use

\[
\begin{align*}
\left| \psi_k \right\rangle & \quad 0 \quad 1 \quad \ldots \quad M - 1 \\
H^\dagger & \quad H^\dagger & \quad \ldots \quad H^\dagger \\
\left| \phi(0) \right\rangle & \quad H_0^\dagger & \quad \ldots \quad H_{M-1}^\dagger
\end{align*}
\]

Figure 1 Quantum circuit of QCSH. Here, \( H \) is the Hadamard gate, and \( H_k^\dagger \) are the unitary operators composed of Pauli operators.
the gradient descent iteration as in the FQE approach [15] using the LCU formalism [18] in QCSH. In classical computing, by starting from the initial state \( X^{(0)} \in \mathbb{R}^N \) and evolving along the objective function’s gradient direction to the next state as:

\[
X^{(t+1)} = X^{(t)} - \gamma \nabla f(X^{(t)}).
\]  

The gradient descent algorithm can obtain the minimum value of the objective function \( f(X) \). We start from a trial wavefunction \( |\phi(0)\rangle \), and the average energy of the system is \( \langle E^{(t)} \rangle = \langle \phi^{(t)}|H|\phi^{(t)}\rangle \). Taking the gradient of the average energy, we have \( \nabla \langle \phi^{(t)}|H|\phi^{(t)}\rangle = 2H|\phi^{(t)}\rangle \). Using eq. (9), the next step is iterated as:

\[
|\phi^{(t+1)}\rangle \propto (I-2\gamma H)|\phi^{(t)}\rangle,
\]  

where \( \gamma \) is a scaling factor that characterizes the amount of the step in the iteration, often \( \gamma > 0 \). The determination of the value of \( \gamma \) is briefly discussed in the following section.

Denoting the iteration operator \( T = I - 2\gamma H = \sum_{k=0}^{d-1} \beta_k H_k^2 \).

In general, \( T \) is not unitary, but it can be implemented using the LCU formalism [29]. Explicitly, we add an ancillary register with \( m = \lceil \log_2 M \rceil \) qubits in state \( |\psi_0\rangle = \frac{1}{\sqrt{2}} \sum_{k=0}^{M-1} \beta_k |k\rangle \), where \( \mathbb{C} = \sqrt{\sum_{k=0}^{M-1} |\beta_k|^2} \) is a normalization constant and \( |k\rangle \) is the computational basis. We denote the state of the entire composite system as \( |\Phi\rangle = |\psi_0\rangle|\phi^{(t)}\rangle \). We implement the ancillary qubit-controlled operations \( \sum_{k=0}^{M-1} |k\rangle \langle k| \otimes H_k^2 \) on the work qubits. The quantum state evolves to

\[
|\Phi\rangle \rightarrow \frac{1}{\mathbb{C}} \sum_{k=0}^{M-1} \beta_k |k\rangle H_k^2 |\phi^{(t)}\rangle.
\]  

Then, we perform Hadamard gates on each qubit in the ancillary register, and the state of the entire system in the subspace where the ancillary register in state \( |0\rangle \) evolves to

\[
|\Phi^*\rangle = \frac{1}{\sqrt{2^m}} \sum_{k=0}^{M-1} \beta_k H_k^2 |\phi^{(t)}\rangle,
\]  

which is exactly the desired state. Then, we measure the auxiliary register. If \( |0\rangle \) is the result, then the iteration succeeds, and we obtain the desired state. This happens with a probability

\[
P_s = \|T|\phi^{(t)}\rangle\|^2 / \mathbb{C}^2 M.
\]  

Any initial state can be decomposed in terms of the linear superposition of eigenstates of the system, denoted as

\[
|\phi^{(0)}\rangle = \sum_{k=0}^{d-1} c_k |u_k\rangle.
\]  

Consecutively implementing the generate iteration operator \( T = I - 2\gamma H \) on the quantum state, we obtain

\[
|\phi^{(t)}\rangle = \frac{1}{\mathbb{D}} \sum_{k=0}^{d-1} c_k (1 - 2\gamma \lambda_k) |u_k\rangle,
\]  

where \( \mathbb{D} = \sqrt{\sum_{k=0}^{d-1} |c_k (1 - 2\gamma \lambda_k)|^2} \) is a normalization constant. Hence, finding that \( |\phi^{(t)}\rangle \) approach to \( |u_{k^*}\rangle \), which satisfies

\[
k^* = \text{argmax}_{i \in \{0, 1, \ldots, d-1\}} \{1 - 2\gamma \lambda_k\}.
\]  

If we intended to obtain the ground state of the system, we show that this can be achieved by reasonably selecting the value of \( \gamma \). First, we estimate an upper bound of the smallest and largest eigenvalues by \( \lambda_0 < q, \lambda_{d-1} < Q \). Second, we have \( |\frac{\gamma Q Q}{2\gamma} - \lambda_k| \geq |\frac{\gamma Q Q}{2\gamma} - \lambda_{d-1}| \) for any \( k \in \{0, 1, \ldots, d - 1\} \). To ensure that \( |u_{k_0}\rangle \) is the target state of iteration, \( |1 - 2\gamma \lambda_{k_0}| \) must be the largest among \( \{|1 - 2\gamma \lambda_k| \}_{k=0}^{d-1} \); that is, \( \frac{1}{\gamma Q} \geq \frac{\gamma Q Q}{2\gamma} \) should be satisfied, which derives

\[
\gamma \in \left\{ \begin{array}{ll}
0, & q + Q > 0, \\
\frac{1}{q + Q}, & q + Q = 0, \\
-\infty, & q + Q < 0.
\end{array} \right.
\]  

Because \( \lambda_0 \leq \lambda_{d-1} \), we can always choose \( q = Q \). Estimating an upper bound of \( \lambda_0 \) is dispensable. For efficiency, the closer \( q \) and \( Q \) are to the exact bound, the higher the iteration efficiency. When the ground state is degenerate, this algorithm cannot distinguish the degenerate states, but calculating the ground state energy remains reliable. To reach the ground state of the nuclear many-body system, we must continuously apply the iterative operator \( T \) on the quantum state. For every iteration, an adaptive mechanism can be added on the selection of \( \gamma \) to accelerate the process, or reach the ground state faster in the update rule

\[
\gamma^{(t+1)} = \frac{\gamma^{(t)}}{1 + \gamma^{(t)}(\langle E^{(t)} \rangle - \langle E^{(t-1)} \rangle)}.
\]  

An evident problem of this algorithm is the probability of success in each iteration. This is because quantum computers could not directly perform any non-unitary evolution similar to the operator \( T \) above, while the probability can be estimated under several reasonable assumptions.

Choosing \( \gamma = \frac{1}{\sqrt{M}} \), and supposing \( \frac{\lambda_0 + \lambda_{d-1}}{2} < \frac{\gamma Q}{2} < \lambda_{d-1} \), the upper and lower bounds of \( P_s \) are available. However,
before that, we present the upper bound of \( \| T|\phi^{(0)} \| \) at first

\[
| T|\phi^{(0)} \rangle \| ^2 = \sum_{k=0}^{d-1} 4\gamma^2 |c_k|^2 \left( \frac{q + Q}{2} \right)^2 - \lambda_k \right)^2
\]

\[
\leq \sum_{k=0}^{d-1} 4\gamma^2 |c_k|^2 \left( \frac{q + Q}{2} \right)^2 - \lambda_0 \right)^2
\]

\[
\approx 4\gamma^2 |c_0|^2 \left( \frac{q + Q}{2} \right)^2 - \lambda_0 \right)^2.
\]

Similarly, the lower bound of \( \| T|\phi^{(0)} \| \) is

\[
| T|\phi^{(0)} \rangle \| ^2 = \sum_{k=0}^{d-1} |c_k|^2 \left( 1 - 2\gamma\lambda_k \right)^2
\]

\[
\geq |c_0|^2 \left( 1 - 2\gamma\lambda_0 \right)^2
\]

\[
= 4\gamma^2 |c_0|^2 \left( \frac{q + Q}{2} - \lambda_0 \right)^2
\]

\[
\approx 4\gamma^2 |c_0|^2 \left( \lambda_{d-1} - \lambda_0 \right)^2.
\]

(18)

Because the Hamiltonian of the nuclear many-body system has been written as in eq. (8), regardless of the assumption that \( H_0 = I \), then the \( C^2 \) in eq. (13) can be simplified as:

\[
C^2 = \sum_{k=0}^{M-1} |\phi_k|^2 = (1 - 2\gamma\alpha_0)^2 + 4\gamma^2 \sum_{k=1}^{M-1} |\alpha_k|^2.
\]

(20)

Using eqs. (18)-(20), the probability of success \( P_s \) in each iteration is limited to the following range:

\[
P_s \leq \frac{1}{M} \left( \frac{\lambda_{d-1} - \lambda_0}{\alpha_0} \right)^2 + \sum_{k=1}^{M-1} |\alpha_k|^2,
\]

\[
P_s \geq \frac{|c_0|^2}{4M} \left( \frac{\lambda_{d-1} - \lambda_0}{\alpha_0} \right)^2 + \sum_{k=1}^{M-1} |\alpha_k|^2.
\]

(21)

An alternative approach to increase the success probability is to implement amplitude amplification [30] before making measurement on the auxiliary register.

3 Results

3.1 Basis states and interactions

We adopt the harmonic oscillator basis

\[ \psi_{nlm}(r) = R_{nl}(r)Y_{lm}(\theta, \phi), \]

\[ R_{nl}(r) = N_{nl} e^{-a r^2/2} (ar)^{l+1/2} L_{n+l+1/2}(a^2 r^2), \]

\[ N_{nl} = \sqrt{\frac{2^{l-n+1} (2l + 2n + 1)! a^3}{\pi^{1/2} n! (2l + 1)!}} \]

(22)

to fit the wave function, where \( R_{nl}(r) \) and \( Y_{lm}(\theta, \phi) \) are the radial wave function and spherical harmonic function. \( a = 1.1/\text{A}^{1/6} \text{fm}^{-1} \), respectively. Further, \( L_{n+l+1/2}^{l+1/2} \) is the Laguerre polynomial, \( n \) is the principal quantum number, and \( l \) and \( m \) represent the orbital angular momentum and its projection on the \( z \)-axis, respectively. Considering also the spin part, the eigenstates of the total angular momentum are adopted

\[
|n, l, j, m_j \rangle = \sum_{m=-m_j}^{m_j} \langle l, m; 1/2, m_j | \phi_{nlm} \rangle |1/2, m_j \rangle.
\]

(23)

where \( \langle l, m; 1/2, m_j | \phi_{nlm} \rangle \) is the Clebsch-Gordan coefficient.

We define each \( m_j \), the projection of the total angular momentum single-particle state, as an orbit. Therefore, the single-particle orbit ordering is \( 1s_{1/2}, 1d_{3/2}, 1p_{3/2}, 1p_{1/2}, 1d_{5/2}, 1f_{7/2}, 1p_{1/2}, 1f_{5/2} \), and \( 1d_{5/2} \).

In most cases, the Hartree-Fock state is a good approximation to the ground state of light nuclei. In our calculation, the initial state is selected as a superposition of the Hartree-Fock state with an excited state, to clearly demonstrate the iterative process of QCSH.

We take the interaction as given in eq. (1). All the interactions are fixed except for those in the Wood-Saxon potential in eq. (4). The average field in nuclei is the sum of the action fields of other nucleons on a single nucleon, and actually, extra calculations are required to obtain its exact form. Our algorithm can serve as a subroutine to fit the parameters for nuclear models (see Appendix for details). However, to briefly illustrate the scheme of QC-SH, we choose the depth of the Wood-Saxon potential by fitting the binding energy calculated close to the experimental data (Table 1). The iterative process of QCSH is shown in Figure 2 for the four typical nucleons in this paper and for the calculations of the remaining eight nuclei (see Appendix for details).

3.2 QCSH results

3.2.1 Numerical results

We calculated the ground state energies of 12 light nuclei (i.e., \( ^2\text{H}, ^3\text{H}, ^3\text{He}, ^4\text{He}, ^6\text{Li}, ^7\text{Li}, ^{12}\text{C}, ^{14}\text{N}, ^{16}\text{O}, ^{17}\text{O}, ^{23}\text{Na}, \) and \(^{40}\text{Ca}\)). The numbers of proton and neutron single particle orbits are given in Table 1. For instance, we chose four single-particle orbits for both proton and neutrons to calculate \(^3\text{H}\), namely, \( 1s_{1/2}, 1s_{1/2}, 1p_{3/2}, 1p_{3/2} \). For \(^3\text{H}\), the Hartree-Fock state \( 1s_{1/2}^2 1p_{1/2}^{1/2} 1s_{1/2}^{1/2} \) is a good approximation to the ground state. In terms of qubit representation (6), it is written as \( |1000\rangle_z |1100\rangle_y \). This is a good approximation in that almost no iteration is made to converge to the final state if we start directly from the Hartree-Fock state. To demonstrate the iterative process of QCSH, we chose a superposition of the Hartree-Fock state with an excited state component, \( C(|1000\rangle_z |1100\rangle_y + 0.1|1010\rangle_z |1100\rangle_y) \). Here,
Table 1  The number of single-particle orbits for protons and neutrons \((N_p, N_n)\), the dimension of the matrix to be diagonalized in the classical shell model calculation (shell model dimensions), the number of qubits used in QCSH (QCSH Qubits), experimental binding energy (Exp.), and QCSH calculated binding energy.

| \( \delta X \) | \((N_p, N_n)\) | Shell model dimensions | \(U_0\) (MeV) | QCSH qubits | Binding energy (MeV) |
|----------------|-----------------|------------------------|---------------|-------------|---------------------|
|                |                 |                        |               |             | Exp.                |
|                |                 |                        |               |             | QCSH                |
| \(^2\text{H}\) | (4, 4)          | \(2^8 \times 2^8\)    | \(-48.0\)     | 15          | \(-2.22\)          |
| \(^3\text{H}\) | (4, 4)          | \(2^8 \times 2^8\)    | \(-45.4\)     | 15          | \(-8.48\)          |
| \(^3\text{He}\) | (4, 4)         | \(2^8 \times 2^8\)    | \(-45.4\)     | 15          | \(-7.72\)          |
| \(^4\text{He}\) | (4, 4)          | \(2^8 \times 2^8\)    | \(-42.9\)     | 15          | \(-28.30\)         |
| \(^6\text{Li}\) | (6, 6)          | \(2^{12} \times 2^{12}\) | \(-40.6\)     | 21          | \(-31.99\)         |
| \(^7\text{Li}\) | (6, 6)          | \(2^{12} \times 2^{12}\) | \(-40.6\)     | 21          | \(-39.24\)         |
| \(^{12}\text{C}\) | (8, 8)          | \(2^{16} \times 2^{16}\) | \(-38.9\)     | 27          | \(-92.16\)         |
| \(^{14}\text{N}\) | (8, 8)          | \(2^{16} \times 2^{16}\) | \(-38.9\)     | 27          | \(-104.66\)        |
| \(^{16}\text{O}\) | (10, 10)        | \(2^{20} \times 2^{20}\) | \(-38.9\)     | 32          | \(-127.61\)        |
| \(^{17}\text{O}\) | (12, 12)        | \(2^{24} \times 2^{24}\) | \(-38.4\)     | 37          | \(-131.76\)        |
| \(^{23}\text{Na}\) | (14, 14)       | \(2^{28} \times 2^{28}\) | \(-37.5\)     | 42          | \(-186.56\)        |
| \(^{40}\text{Ca}\) | (22, 22)        | \(2^{34} \times 2^{34}\) | \(-37.6\)     | 61          | \(-342.05\)        |

Figure 2  (Color online) Iterative process to the ground-state energy by QCSH for \(^2\text{H}, ^4\text{He}, ^{16}\text{O}\) and \(^{40}\text{Ca}\). The initial state is a superposition of the Hartree-Fock state and an excited state. The exact classical diagonalization results (red line), the QCSH without noise (blue line), QCSH with a Gaussian noise (orange line), and QCSH with random noise (green line) are also presented.

\(C\) is the normalization constant. For relatively heavy nuclei, their quantum circuits with dozens of qubits are difficult to simulate using a classical computer. We reduced the dimensions of the Hilbert space through particle number conservation, making the simulation in classical computers possible. However, simulation in classical computers remains challenging for nuclei \(^{23}\text{Na}\) and \(^{40}\text{Ca}\). We have to freeze some lower single-particle orbits of these nuclei. In details, we froze \(1s_1/2, 1p_3/2\) and \(1p_1/2\) to simulate the nucleus \(^{23}\text{Na}\).

\(\gamma\) is the normalization constant. For relatively heavy nuclei, their quantum circuits with dozens of qubits are difficult to simulate using a classical computer. We reduced the dimensions of the Hilbert space through particle number conservation, making the simulation in classical computers possible. However, simulation in classical computers remains challenging for nuclei \(^{23}\text{Na}\) and \(^{40}\text{Ca}\). We have to freeze some lower single-particle orbits of these nuclei. In details, we froze \(1s_1/2, 1p_3/2\) and \(1p_1/2\) to simulate the nucleus \(^{23}\text{Na}\).

Meanwhile, \(1s_{1/2}, 1p_{3/2}, 1p_{1/2}, 1d_{5/2}\), and \(1d_{3/2}\) were frozen for simulating the nucleus \(^{40}\text{Ca}\). The experimental binding energies were obtained from the real experiment in nuclear physics [31].

We performed the quantum gradient descent iteration of eq. (11) and obtained the ground state energies through numerical simulation. The results are marked as noiseless in Figure 2 and shown on the right-most column in Table 1.

To simulate the noises in the practical quantum com-
puting device, we added a noise term $\sum_k \delta \alpha_k Z_k$ into the Hamiltonian of the system and a perturbation $|\delta \psi\rangle$ to the quantum state $|\psi(t)\rangle$. That is, the quantum state is truly $|\tilde{\psi}(t)\rangle = (|\psi(t)\rangle + |\delta \psi\rangle)/(|\psi(t)\rangle + |\delta \psi\rangle)|\delta \psi\rangle$. $\delta \alpha_k$ and $|\delta \psi\rangle$ were chosen both as Gaussian distribution, $P(\alpha) = e^{-(\alpha-\mu)^2/2\sigma^2} / \sqrt{2\pi\sigma}$ with $\mu = 0$, $\sigma = 0.1/3$, which are marked as Gaussian noise in Figure 2; or both as uniform distribution with an amplitude of 0.02, which are marked as random noise in Figure 2, respectively. In this case, the iteration operator is $\tilde{T} = I - 2\gamma(H + \sum_k \delta \alpha_k Z_k)$. Because the measurement at the final step may obtain wavefunctions with different numbers of particles, a projection was performed to conserve the proton and neutron particle numbers.

The QCSH finds the eigenvalue through iteration quickly. As shown in Figure 2, it takes less than 20 iterations to reach the ground state. We compared the results of QCSH with the exact diagonalization of the noiseless Hamiltonian in a classical computer. The exact conventional results are given as diagonalization in Figure 2. The results of our quantum algorithm without noise are consistent with those of classic diagonalization. For cases with a given strength of noise, the results of QCSH converge to the exact energy of diagonalization within an error of about 1 keV, which is within the accuracy of nuclear structure physics. In fact, QCSH converges more quickly if the initial state is taken as the Hartree-Fock state. This noise analysis demonstrated that QCSH is robust against noises and is quite promising to be realized in NISQ quantum computers in the near future.

### 3.2.2 Experimental results

We carried out the experiment of simulating deuteron on a quantum cloud based on a superconducting circuit. Our results are based on cloud access to the Quafu platform (http://quafu.baqis.ac.cn/), which consists of 10 superconducting qubits (see Appendix for details). Due to the limitation of the quantum qubits of the Quafu platform, a simplified Hamiltonian was selected to simulate deuteron, which is almost the lightest nucleus [16].

$$H_2 = 5.9067091 + 0.218291Z_0 - 6.125Z_1 - 2.143304(X_0X_1 + Y_0Y_1).$$

(24)

We chose $|n\rangle = |10\rangle$ as the initial state and $\gamma = 0.02$. We obtain $(I - 2\gamma H_2)|n\rangle = (I - 2\gamma H_0)|n\rangle = 2\gamma H_{xy}|n\rangle$, where $H_0 = 5.9067091 + 0.218291Z_0 - 6.125Z_1$ and $H_{xy} = -2.143304(X_0X_1 + Y_0Y_1)$. The output state of $H_{xy}|n\rangle$ can be calculated by the following quantum circuit in Figure 3(b). Here, $q_0$ and $q_2$ are work qubits, and $q_1$ is an ancillary qubit. We measured all three qubits and only focused on the probability of output state, where $q_1$ is in state 0. Assume that the output quantum state of the work system is $|n\rangle_{out}$ and the experimentally-measurable distribution of $P_{01} = \langle 01|n\rangle_{out}$ and $P_{10} = \langle 10|n\rangle_{out}$. We can reconstruct $|n\rangle_{out}$ as the initial state of next iteration by $R_{\theta}(q_0)$, where $\theta = 2\arccos(P_{01})$. The quantum circuit was implemented iteratively eight times to converge to the ground state. To mitigate the effect of noise, we performed 10000 measurements for each calculation. The experiment was repeated three times to obtain error bars. The results are presented in Figure 3(a), indicating that the binding energy $E(H_2) = -1.744 \pm 0.001$ MeV, agree with the exact energy of $-1.749$ MeV within uncertainties.

### 3.3 Computational complexity of QCSH

We first analyzed the qubit resource complexity. In a nucleus, if a proton occupies $N_p$ single-particle states and a neutron occupies $N_n$ single-particle states, the number of qubits that represent the quantum state of the system is $N_p + N_n$. For simplicity, we set $N_p = N_n = N$ to characterize the system scale. The number of Pauli product terms from one-body interaction is $N_p + N_n + 1$ due to the orthogonality between orbitals. The number of Pauli product terms from two-body integrals is no more than $3(N_p + N_n) + C_{N_p}^2 + \sum_{k=3}^{4} 2^k C_{N_p}^k + 1$. Therefore, the number of required ancillary qubits is

$$m = \lceil \log_2 M \rceil$$

$\leq \lceil \log_2(4(N_p + N_n) + C_{N_p}^2 + \sum_{k=3}^{4} 2^k C_{N_p}^k + 1) \rceil$. (25)

Thus, the total number of required qubits is $N_p + N_n + m$, whose complexity is $O(N)$. For gate complexity, we must decompose the many-qubit control gates $\bigotimes_{k=0}^{M-1} |k\rangle \otimes H_k$ into basic qubit gates. If

![Figure 3](https://example.com/figure3.png)

**Figure 3** (Color online) (a) Iteration process of calculating the deuteron binding energy. The initial state is the Hartree-Fock state $|n\rangle = |10\rangle$. (b) Quantum circuit for calculating $H_{xy}|n\rangle$. $q_0$, $q_2$ denote the work qubits, and $q_1$ is the ancillary qubit.
we restrict to only one and two-body interactions, an $m$-qubit controlled Pauli gate $C^m(U)$ can be decomposed of $M_k = 32(m - 1) + 4$ basic gates \[O(N_k^2 + \frac{N_k^2}{2} + \frac{C_2^{N_k^2}}{2}) + \sum_{k=3}^{4} (M_k + k)2^k C_{N_k^2}. \] Conversely, diagonalizing a $2^N$-dimension symmetric matrix on a classic computer using the symmetric Gaussian elimination takes the $O(2^N)$ steps. Therefore, in the circumstance iteration steps $k \propto O(polyN)$, QCSH achieves an exponential speedup compared with a classical shell model.

4 Discussion and conclusion

QCSH provides an efficient quantum algorithm to calculate the nuclear structure. The gate complexity and qubit resources are both polynomials to the number of selected single particle states. With the wavefunctions at hand, we can directly calculate the transition rates, and reaction cross section.

In QCSH, we often obtain the target state with a certain probability, as is true for an LCU algorithm. The convergence rate depends on the appropriate choice of the step size factor, $\gamma$, and the initial state. Selecting the Hartree-Fock state as the initial state can significantly accelerate the convergence, and mitigate errors. Another effective method is to apply amplitude amplification to increase the success probability, and it will be useful when the depth of quantum circuits becomes larger.

We demonstrated QCSH by applying it to 12 light nuclei. The results are consistent with those from exact diagonalization on a classic computer using the symmetric Gaussian elimination. For each iteration, only for shallow gate operations, it can already perform some meaningful tasks. Most importantly, recent progress in hardware still has errors and can work on only for shallow gate operations, it can already perform some meaningful tasks. Most importantly, recent progress in hardware is rapid and accelerated. The QCSH application can be smoothly transformed into future large-scale fault-tolerant quantum computers due to its full quantum computing nature.

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Appendix

A1 Numerical calculations of the remaining eight nuclei

Here, we show the iterative process of QCSH for eight typical nuclei in Figures a1 and a2. The initial state is chosen as a superposition of the Hartree-Fock state and an excited state. The exact classical diagonalization results (red line), the QCSH without noise (blue line), QCSH with Gaussian noise (orange line), and QCSH with random noise (green line) are also shown.

A2 Fitting parameters for nuclear models

Our algorithm can serve as a subroutine to fit the parameters for nuclear models. When the form of a nuclear structure model is obtained through theoretical analysis, the parameters of this model should be well selected to conform to the experimental results. As the simulation of nuclei on classic computers is intractable, the process of adjusting parameters is highly complex. However, employing quantum computation to adjust the parameters can raise the efficiency of this process.

As discussed in the main text, we directly used the average field depth $U_0$ with properly fixed parameters to examine the feasibility of our algorithm by calculating $^3\text{H}$, $^3\text{He}$, $^6\text{Li}$, $^{12}\text{C}$, and $^{14}\text{N}$. Here we show an approximate method to obtain the parameters above based on our algorithm. Then, we use the parameters fitted to predict the ground state energy of $^7\text{Li}$ and $^{16}\text{O}$. A comparison between theory and experiments is introduced, and the results indicate the applicability of the nuclear shell model.

To fit the parameters in $U_0 = (u + a \cdot (N - Z)/A + b \cdot Z + c \cdot N + d/(N + Z))$ MeV, for each $^2X$ in $[^3\text{H}, ^3\text{He}, ^6\text{Li}, ^{12}\text{C}, ^{14}\text{N}]$, we vary the value of $U_0$ and calculate the ground state energy corresponding to a specific $U_0$ using FQE. We denote the value of $U_0$ as $U^*$, when the theoretical result obtained by the FQE is equal to the ground state energy obtained in experiments. We obtain $U^*$ for every nucleon and use them to fit the parameters through linear regression. Meanwhile, we record the upper and lower bound of $U_0$ with the allowable error 0.3 MeV/nucleon, that is, when $U_0$ is within this value range, the difference between the prediction of the shell model and experiments is less than 0.3 MeV average to each nucleus.

Results are presented in Table a1, indicating that the appropriate average field depth roughly increases with the number of nucleons.

To obtain the parameters efficiently, we set a loss function for linear regression, and optimize the parameters by minimizing this loss function

\[
\text{Loss} = \sum_k [(u+a\cdot(N_k-Z_k)/A_k+b\cdot Z_k+c\cdot N_k+d/A_k)-U_0^*]^2. \tag{a1}
\]

where $k \in \{^3\text{H}, ^3\text{He}, ^6\text{Li}, ^{12}\text{C}, ^{14}\text{N}\}$.

After fitting the parameters of the average field, we use the formula fitted to calculate $U_0$ for $^7\text{Li}$ and $^{16}\text{O}$, and compare the results of the average filed approximation and experiments in Table a1 and Figure a3. The simulation results show that predictions of ground state energy for $^7\text{Li}$ and $^{16}\text{O}$ are also within the error range compared to experiments in nuclear physics (Figure a3 with red points). With the parameters fitted using experimental data of a few nuclei, the nuclear

| $^2X$ | $E_0$ (MeV) | $(E_0/A)$ (MeV) | $U^*$ (MeV) | Allowable depth (MeV) |
|-------|-------------|-----------------|-------------|-----------------------|
| $^3\text{H}$ | -8.48 | -2.83 | -45.30 | -45.78 – 44.83 |
| $^3\text{He}$ | -7.72 | -2.57 | -45.47 | -45.94 – 44.99 |
| $^6\text{Li}$ | -31.99 | -5.33 | -40.71 | -41.10 – 40.32 |
| $^{12}\text{C}$ | -92.16 | -7.68 | -38.61 | -38.97 – 38.26 |
| $^{14}\text{N}$ | -104.66 | -7.48 | -38.57 | -38.95 – 38.22 |
shell model can make a good prediction of more complex nuclei. Our quantum algorithm, as a subroutine, provides an economical method to fit the parameters for nuclear models.

The details for the Woods-Saxon potential in different nuclei are shown in Figure a4.

A3 Computational complexity and the choice of the initial state

Here we list the qubits resources and gate complexity for simulating the nucleus in Figure a5.
The choice of the initial state is also a crucial issue that should be addressed. Even if we choose a reasonable $\gamma$, the condition $c_0 = \langle u_0 | \phi^{(0)} \rangle \neq 0$ should be satisfied, or we could not obtain the ground state. Fortunately, the Hartree-Fock state $|HF\rangle$ is already a good approximation to the ground state, which often satisfies $\langle u_0 | HF \rangle \neq 0$. However, for some nuclei with mixed configurations, $|HF\rangle$ might not be a good choice, because the efficiency of iteration will be extremely low (Figure a6). In this case, other configurations should be added with a sizable weight.

A4 Details about the superconducting quantum cloud

Quafu is an open cloud platform for quantum computation. It provides four specifications of superconducting quantum
Table a2  Device parameters. Here, \( \omega_j \) shows the maximum frequency of \( Q_j \). \( \omega_j^{10} \) corresponds to the idle frequency of \( Q_j \). \( \omega_j^{r} \) shows the resonant frequency of \( Q_j \) during readout. \( \eta_j \) corresponds to the anharmonicity of \( Q_j \). \( g_{j,j+1} \) is the coupling strength between nearest-neighbor qubits, and \( T_{1,j} \) and \( T^*_{2,j} \) represent the relaxation and coherence times of \( Q_j \). Further, \( F_{0,j} \) and \( F_{1,j} \) are the readout fidelities of \( Q_j \) in \( |0\rangle \) and \( |1\rangle \), and \( F_{j,j+1} \) represents the fidelity of the CZ gate composed of \( Q_i \) and \( Q_j \), which is obtained by randomized benchmarking.

| Qubit | \( Q_1 \) | \( Q_2 \) | \( Q_3 \) | \( Q_4 \) | \( Q_5 \) | \( Q_6 \) | \( Q_7 \) | \( Q_8 \) | \( Q_9 \) | \( Q_{10} \) |
|-------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|
| \( \omega_j/2\pi \) (GHz) | 5.536  | 5.069  | 5.660  | 4.742  | 5.528  | 4.929  | 5.451  | 4.920  | 5.540  | 4.960  |
| \( \omega_j^{10}/2\pi \) (GHz) | 5.456  | 4.424  | 5.606  | 4.327  | 5.473  | 4.412  | 5.392  | 4.319  | 5.490  | 4.442  |
| \( \omega_j^{r}/2\pi \) (GHz) | 5.088  | 4.702  | 5.606  | 4.466  | 5.300  | 4.804  | 5.177  | 4.697  | 5.474  | 4.819  |
| \( \eta_j/2\pi \) (GHz) | 0.250  | 0.207  | 0.251  | 0.206  | 0.251  | 0.203  | 0.252  | 0.204  | 0.246  | 0.208  |
| \( g_{j,j+1}/2\pi \) (MHz) | 12.07  | 11.58  | 10.92  | 10.84  | 11.56  | 10.00  | 11.74  | 11.70  | 11.69  | –      |
| \( T_{1,j} \) (\( \mu \)s) | 20.0   | 52.5   | 15.9   | 16.3   | 36.9   | 44.4   | 30.8   | 77.7   | 22.8   | 25.0   |
| \( T^*_{2,j} \) (\( \mu \)s) | 8.60   | 1.48   | 9.11   | 2.10   | 12.8   | 2.73   | 15.7   | 1.88   | 4.49   | 2.05   |
| \( F_{0,j} \) (%) | 98.90  | 98.32  | 98.67  | 95.30  | 97.00  | 95.47  | 97.00  | 96.37  | 98.33  | 97.13  |
| \( F_{1,j} \) (%) | 92.90  | 92.30  | 92.97  | 91.53  | 86.17  | 87.93  | 93.40  | 93.37  | 94.63  | 92.07  |
| \( F_{j,j+1} \) (%) | 94.2   | 97.8   | 96.6   | 97.3   | 96.8   | 97.0   | 94.5   | 93.2   | 96.0   | –      |

Figure a7  (Color online) Topological structure of quantum processor P-10. Each qubit is capacitively coupled to its nearest neighbors.