Shell-model study of ^{58}Ni using quantum computing

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arXiv:2402.15577

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Objective

Achieve *high precision* in determining *low-lying energy* levels of ^{58}Ni using a *problem-based ansatz* and the shell-model interaction *JUN45*.

Methodology

- Utilizing a simulated quantum computing approach employing the Variational Quantum Eigensolver (VQE) method.
- A problem-specific ansatz tailored for the investigation into the shell-model energy levels of ^{58}Ni.

Purpose

- Exact reproduction of ground state and first and second excited state energy values.
- Comparison between classical shell model values, qubit-mapped diagonalization, and noiseless simulated ansatz+VQE simulation validating method of correctness.
- Accuracy of simulation showing the suitability of the ansatz for full reconstruction of the nuclear wave function.

Nuclear Shell Model

J. Suhonen, From Nucleons to Nucleus: Concepts of Microscopic Nuclear Theory (Springer Berlin, Heidelberg, 2007) (Ch. 8)

Hamiltonian

$$H = \sum_{i=1} \epsilon_i \hat{a}_i^\dagger \hat{a}_i + \frac{1}{2} \sum_{i,j,k,l} V_{ijkl} \hat{a}_i^\dagger \hat{a}_j^\dagger \hat{a}_l \hat{a}_k$$

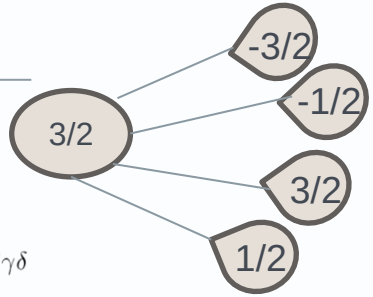
ϵ = single-particle energy term
V_{ijkl} = Two-body interaction term

Interaction

JUN45 interaction is used involving $1p_{3/2}$, $0f_{5/2}$, and $1p_{1/2}$ orbitals.

Transformation

J-scheme ⟹ *M*-scheme



$$\langle ab; JT|V|cd; JT\rangle = N \sum C\, \overline{v}_{\alpha\beta\gamma\delta}$$

Here, *a,b,c, and d* are the single-particle orbitals $|a> = |n_a, l_a, j_a>$. The α,β,γ,δ are the nucleon states as a complete set of quantum numbers $|\alpha> = |n_\alpha, l_\alpha, j_\alpha, m_\alpha, m_{t\alpha}>$.

Qubit mapping

Represent 12 neutron single-particle orbitals with 12 qubits, following a specific combination of total angular momentum (j), projection on the z-axis (m_α), and third component of isospin ($m_{t\alpha}$) as illustrated in Table, $m_{t\alpha}$ is 1/2 for all qubits to represent the neutron.

qubit(α)	0	1	2	3	4	5	6	7	8	9	10	11
n	1	1	1	1	0	0	0	0	0	0	1	1
l	1	1	1	1	3	3	3	3	3	3	1	1
j	3/2	3/2	3/2	3/2	5/2	5/2	5/2	5/2	5/2	5/2	1/2	1/2
m_α	−3/2	3/2	−1/2	1/2	−5/2	5/2	−3/2	3/2	−1/2	1/2	−1/2	1/2

Variational Quantum Eigensolver

*Peruzzo A. et al., Nat. Commun. **5**, 4123 (2014).*

Quantum algorithm for finding the ground state energy of a given Hamiltonian.

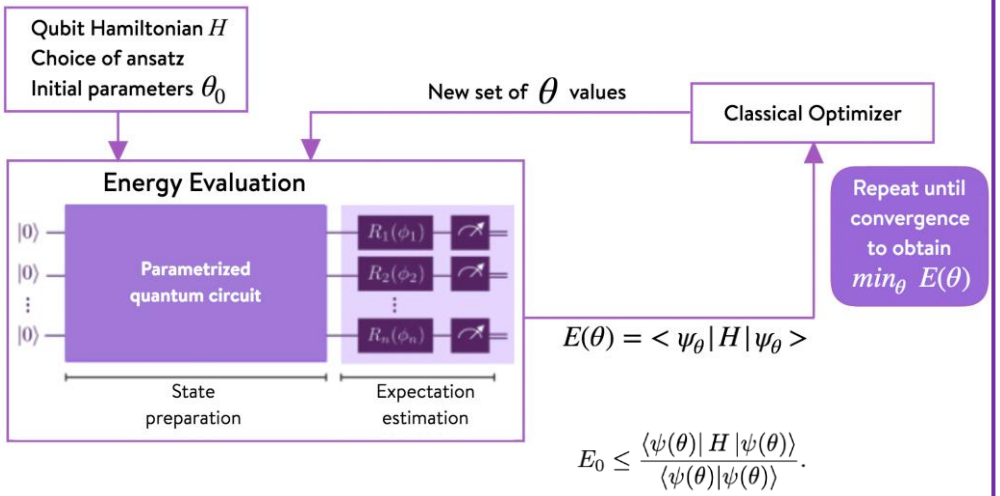


Image Credit: 1QBit

Jordan-Wigner Mapping

Maps fermionic creation and annihilation operators onto Pauli spin matrices.

|0>

$\hat{n}_j = a_j^\dagger a_j$ Spin ½ operators (qubit)

$$a_j \mapsto \left(\prod_{k=1}^{j-1} \sigma_k^z\right) \sigma_j^-, \quad a_j^\dagger \mapsto \left(\prod_{k=1}^{j-1} \sigma_k^z\right) \sigma_j^+$$

$$\sigma_j^+ = \tfrac{1}{2}(\sigma_j^x + i\sigma_j^y),\ \sigma_j^- = \tfrac{1}{2}(\sigma_j^x - i\sigma_j^y)$$

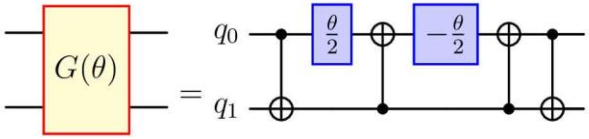
Spin-raising Spin-lowering

$\prod_{k=1}^{j-1} \sigma_k^z$ = For the preservation of fermionic anti-commutation relations.

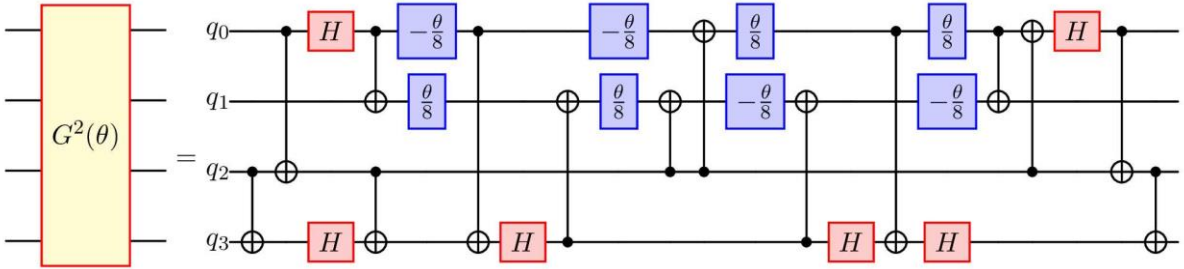
Single and double excitation

J. M. Arrazola *et al.*, Quantum 6, 742 (2022)
G.-L. R. Anselmetti *et al.*, New Journal of Physics 23, 113010 (2021).

- Enable access to specific configurations in ^{58}Ni with correct M values.
- Preserve particle number, ensuring consistency within the Fock space.
- Parameterized for flexibility to explore various configurations and find the lowest energy state.



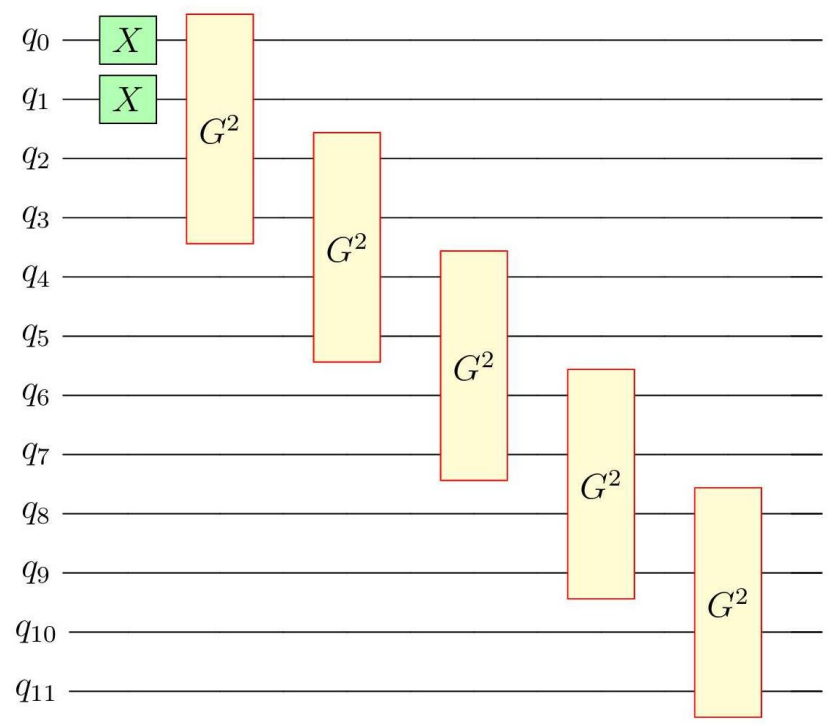
- Achieved through creation and annihilation operators ($a^\dagger_i a_j$).
- Conservation of m_α ensured by selecting nucleon spins appropriately.



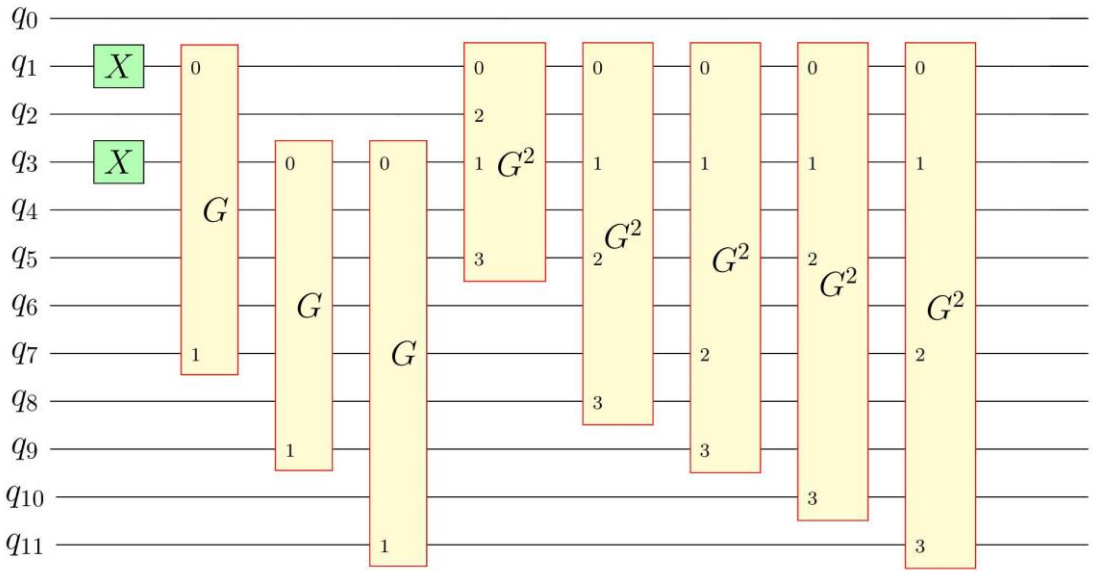
- Simultaneously promote two nucleons to different orbitals ($a^\dagger_i a^\dagger_j a_k a_l$).
- Maintain constant total angular momentum projection along the z-axis.

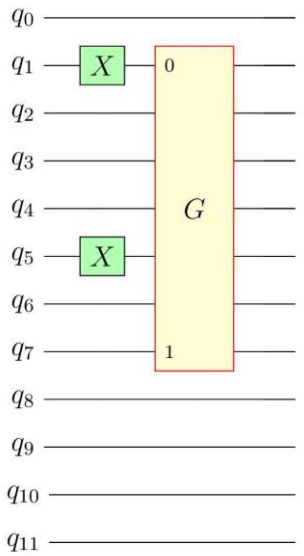
Quantum circuit for the ground state

- All qubits are active in the ground state wave function.
- The ground state ansatz uses pairwise excitations from the starting configuration always to ± m levels.
- The double excitations are: {0,1,2,3}, {2,3,4,5}, {4,5,6,7}, {6,7,8,9}, {8,9,10,11}, for M=0.



Quantum circuit for the first and second excited state

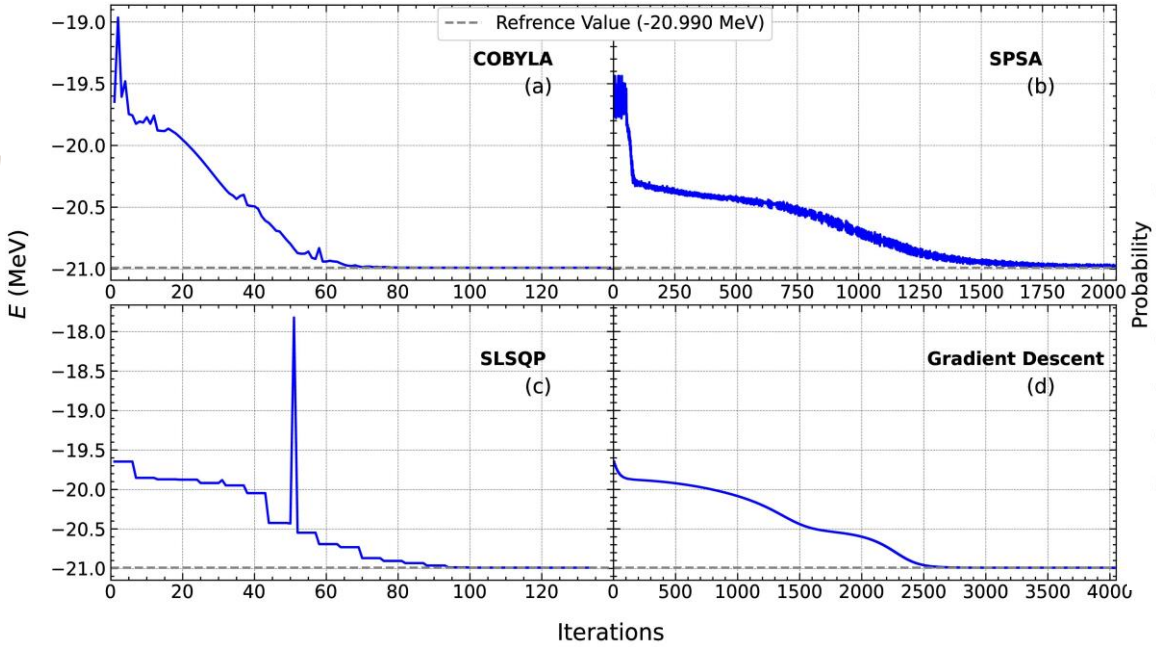


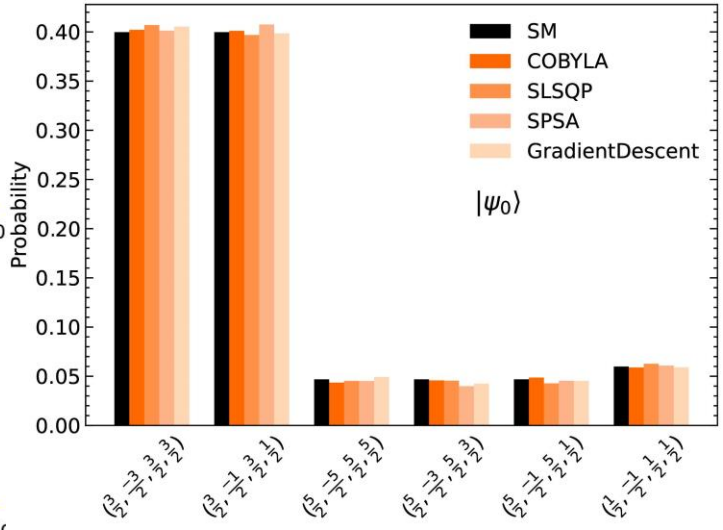


- The system is initialized in the state |1, 3>.
- Double excitations: {1,3,5,8}, {1,3,5,10}, {1,3,2,5}, {1,3,7,9}, {1,3,7,11}.
- Single excitations: {3,9}, {3,11}, and {1,7}.
- Pair-wise excitation and pair-breaking mechanisms are combined

- The system is initialized in the state |1, 5 >, with the single excitation {1,7}.

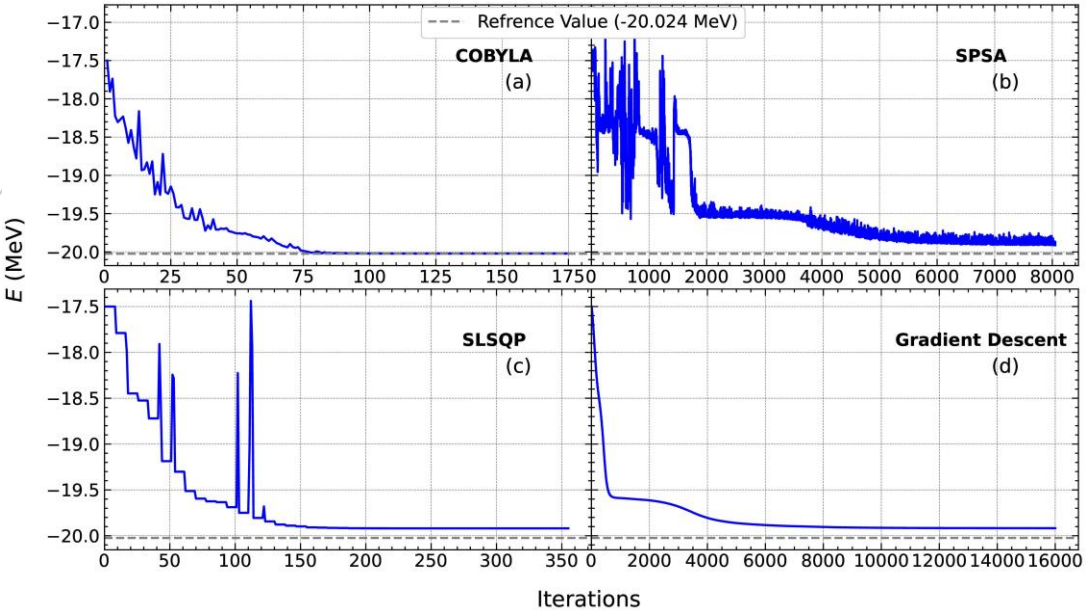
Result for the ground state (0^+)

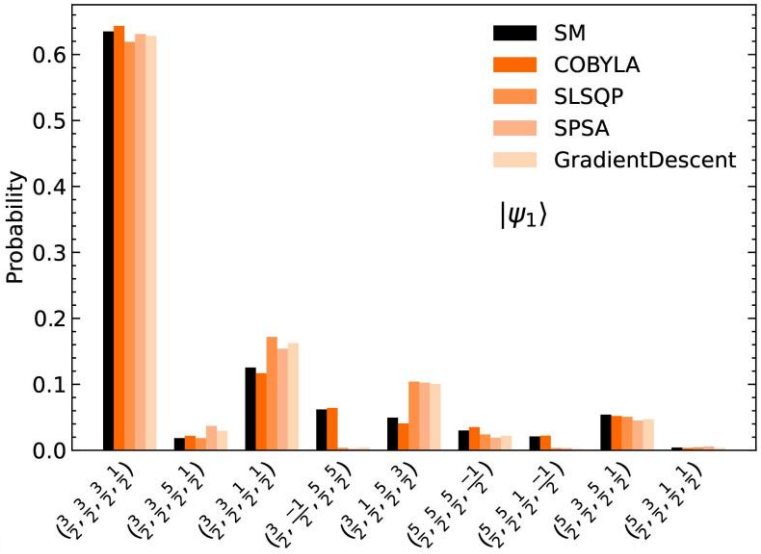




- Convergence achieved with all optimizers, with COBYLA demonstrating the fastest convergence within 80 iterations.
- COBYLA and SLSQP optimizers converge quickly, achieving 10^{-3} MeV accuracy.
- Other optimizers require over 2000 iterations for convergence with less accurate expectation values.
- ^{58}Ni, above magic nuclei ^{56}Ni (Z = 28, N=28), exhibits single-particle nature, evident in the ground state wavefunction.

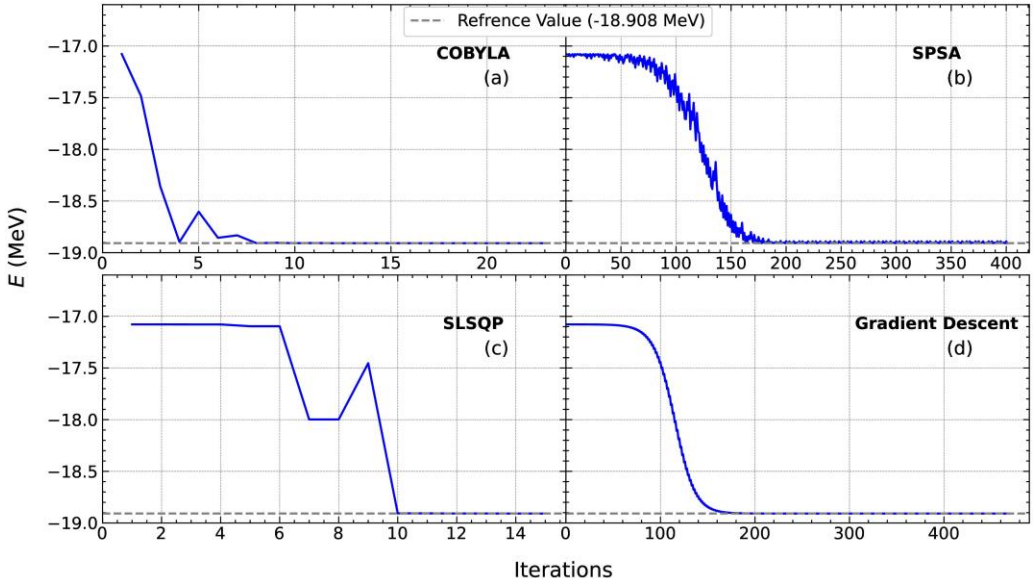
Result for the first excited state (2^+)

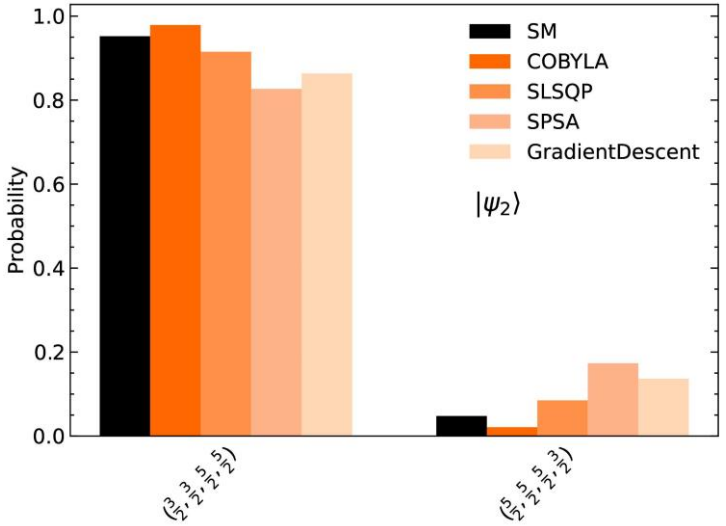




- COBYLA optimizer demonstrates the fastest convergence, achieving it in 105 iterations with 10^{-2} MeV accuracy.
- SPSA and Gradient Descent take longer (more iterations) to converge, similar to the ground state calculations.
- Other optimizers provide reasonable results but miss correct distributions across certain configurations.

Result for the second excited state (4^+)





- COBYLA and SLSQP demonstrate particularly fast convergence, achieving convergence in approximately 10 iterations.
- SPSA optimizer's perturbation parameter tuned to 0.01 for improved convergence, mitigating oscillatory behaviour observed at default calibration.

Circuit property

Properties of ansatz used for the ground state, first and second excited state with the number of parameters, CNOT gates(2-qubit), RY gates(1-qubit), H gate(1-qubit), X gate(1-qubit) and circuit depth.

State	No. parameters	2-qubit	1-qubit	Depth
G.S.	5	70	72	96
1^{st} e.s.	7	82	78	108
2^{nd} e.s.	1	4	4	7

Comparison between results

Summary of the results for the ground state, first excited state, and second excited state alongside the shell model value for ^{58}Ni in *pf* model space. The exact result, obtained with exact diagonalization of the Hamiltonian and the E_{UCC} energy is obtained by minimizing the Hamiltonian using ansatz.

			E_{UCC}			
State	SM	E_{exact}	COBYLA	SLSQP	SPSA	GD
G.S.	-20.990	-20.990	-20.990	-20.990	-20.988	-20.990
1^{st} e.s.	-20.024	-20.024	-20.022	-19.919	-19.912	-19.918
2^{nd} e.s.	-18.908	-18.908	-18.908	-18.908	-18.908	-18.908

Conclusions

- Provides a robust framework for calculating properties of atomic nuclei within a defined model space of single-particle states.
- By mapping single-particle states to qubits and employing tailored ansatz with the VQE algorithm, we successfully extended simulated quantum computation to ^{58}Ni, obtaining exact results for its lowest 0^+, 2^+, and 4^+ states.
- Straightforward extension to other nuclei in the *fp* shell, requiring no additional qubits but potentially more complex circuits.
- Possibility of circuit simplification through compilation or approximation techniques.
- Potential extension to heavier nuclei, where classical shell model calculations face challenges due to exponential increases in the size of the Hilbert space.

Thanks!

Do you have any questions?

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