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

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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

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

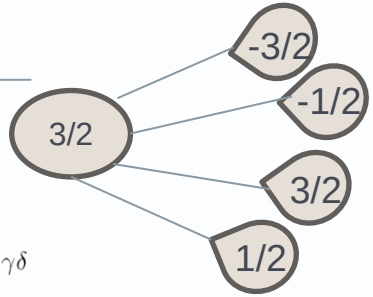
$\epsilon$ = single-particle energy term
$V_{ijkl}$ = Two-body interaction term

## 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 $|\alpha> = |n_\alpha, l_\alpha, j_\alpha>$. The $\alpha,\beta,\gamma,\delta$ 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

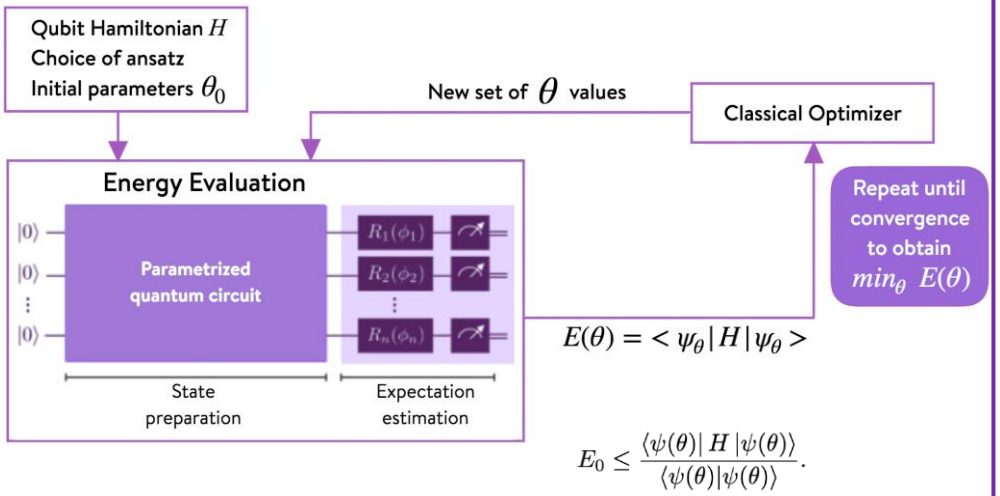
Represent 12 neutron single-particle orbitals with 12 qubits, following a specific combination of total angular momentum (j), projection on the z-axis ($m_\alpha$), and third component of isospin ($m_{t\alpha}$) as illustrated in Table, $m_{t\alpha}$ is 1/2 for all qubits to represent the neutron.

| qubit($\alpha$) | 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 |
| $m_\alpha$ | −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.




$$E_0 \leq \frac{\langle \psi(\theta) | H | \psi(\theta) \rangle}{\langle \psi(\theta) | \psi(\theta) \rangle}.$$

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

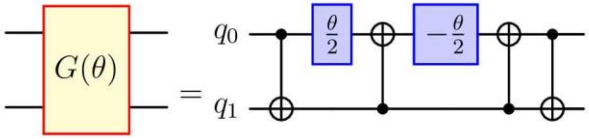
Spin-lowering

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

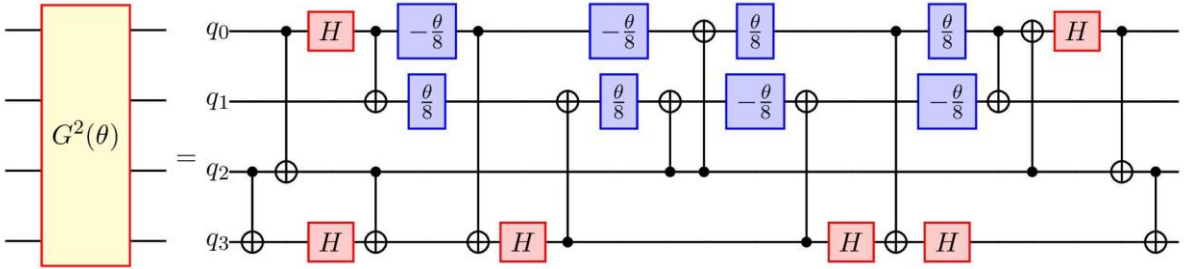
# Single and double excitation

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.



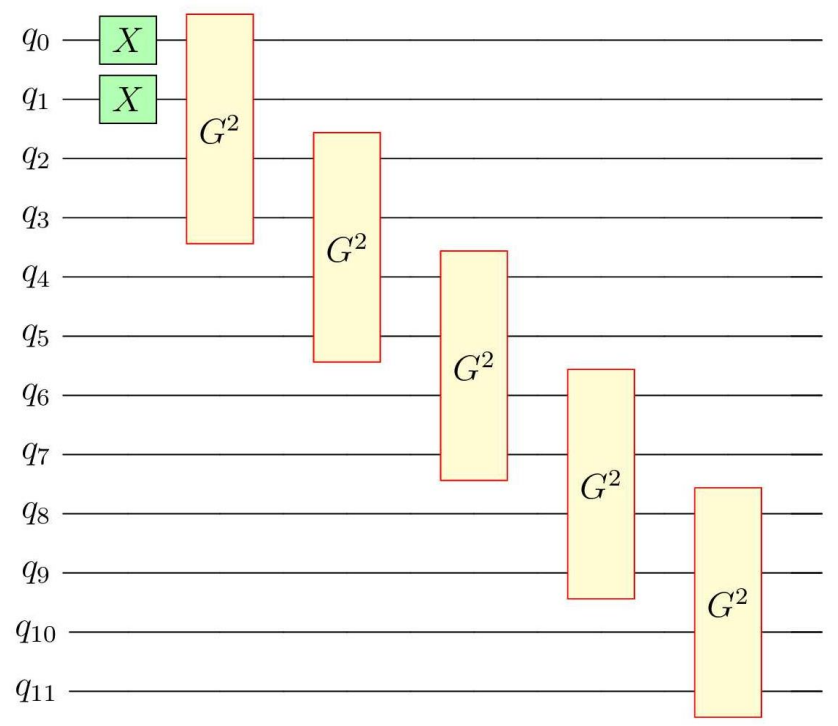

- Achieved through creation and annihilation operators ($a^\dagger_i a_j$).
- Conservation of $m_\alpha$ ensured by selecting nucleon spins appropriately.



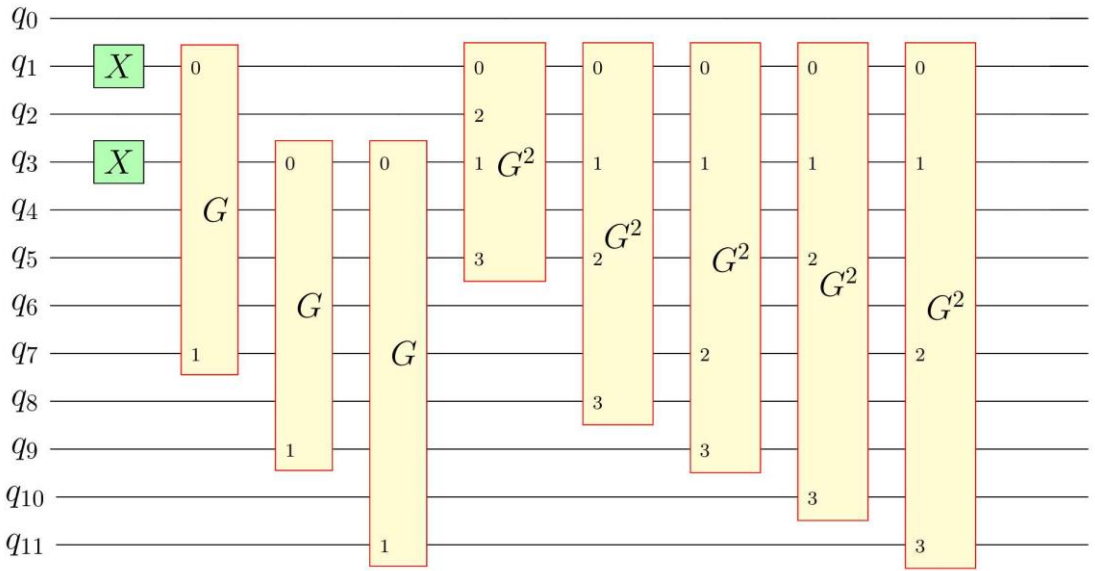

- Simultaneously promote two nucleons to different orbitals ($a^\dagger_i a^\dagger_j a_k a_l$).
- Maintain constant total angular momentum projection along the $z$-axis.

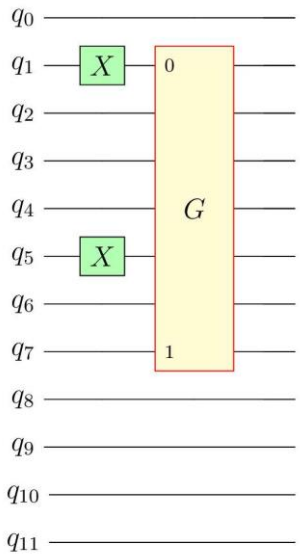
# Quantum circuit for the ground state

- 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

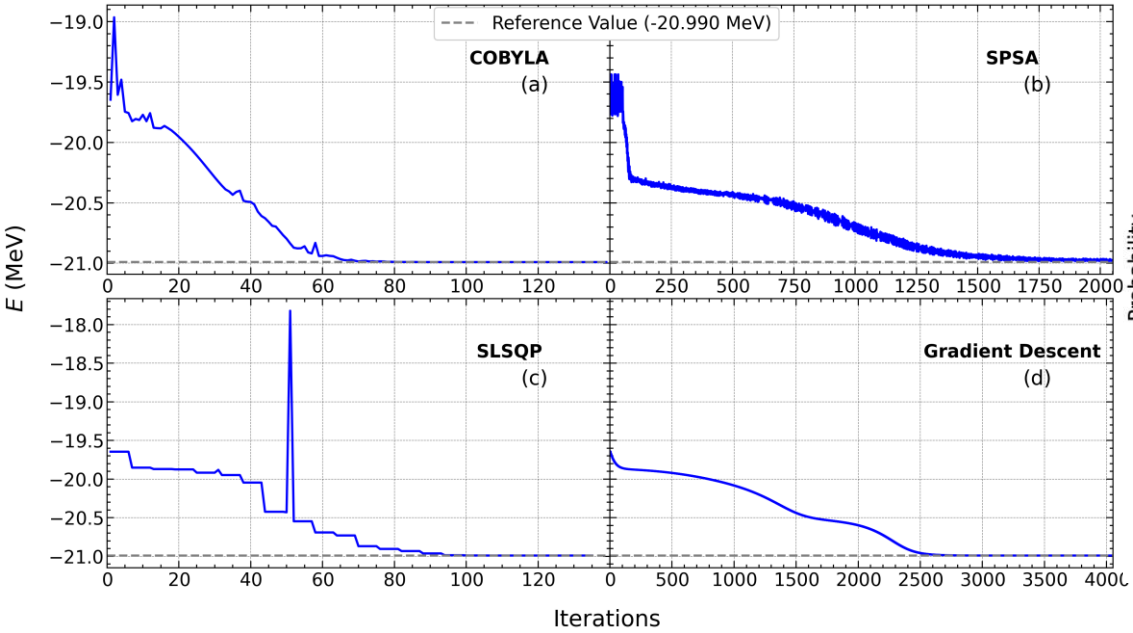


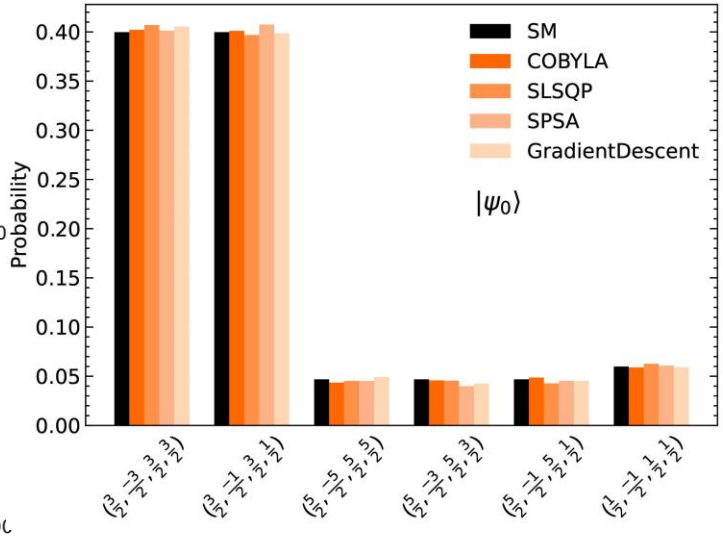




- The system is initialized in the state |1, 3>.
- Double excitations: {1,3,5,8}, {1,3,5,10}, {1,3,2,5}, {1,3,7,9}, {1,3,7,11}.
- Single excitations: {3,9}, {3,11}, and {1,7}.
- Pair-wise excitation and pair-breaking mechanisms are combined

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

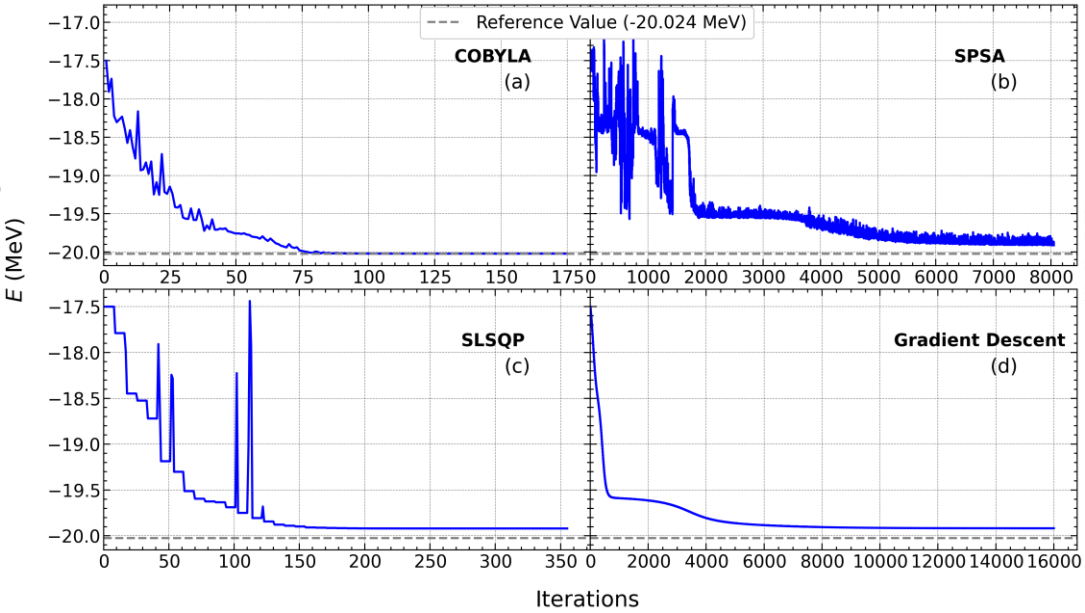
# Result for the ground state ($0^+$)

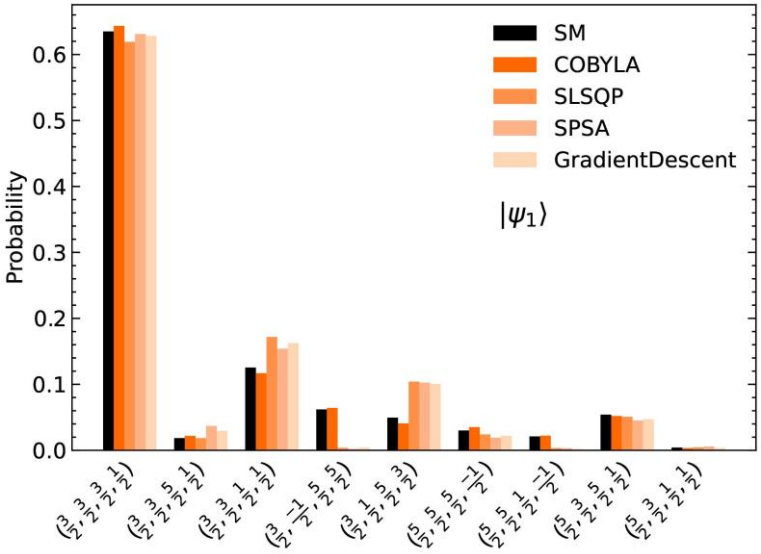



- Convergence achieved with all optimizers, with COBYLA demonstrating the fastest convergence within 80 iterations.
- COBYLA and SLSQP optimizers converge quickly, achieving $10^{-3}$ MeV accuracy.
- Other optimizers require over 2000 iterations for convergence with less accurate expectation values.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

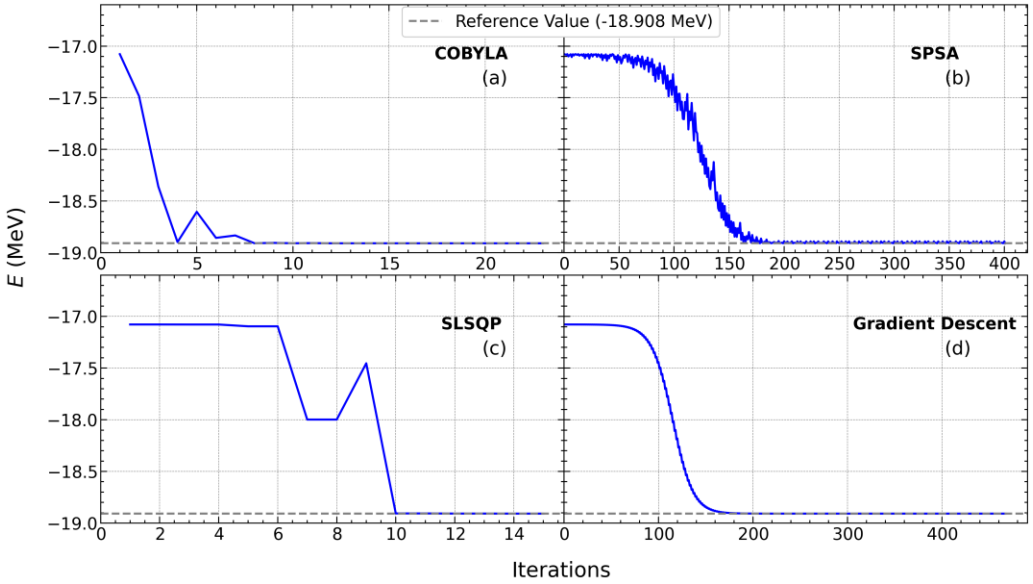
# Result for the first excited state ($2^+$)

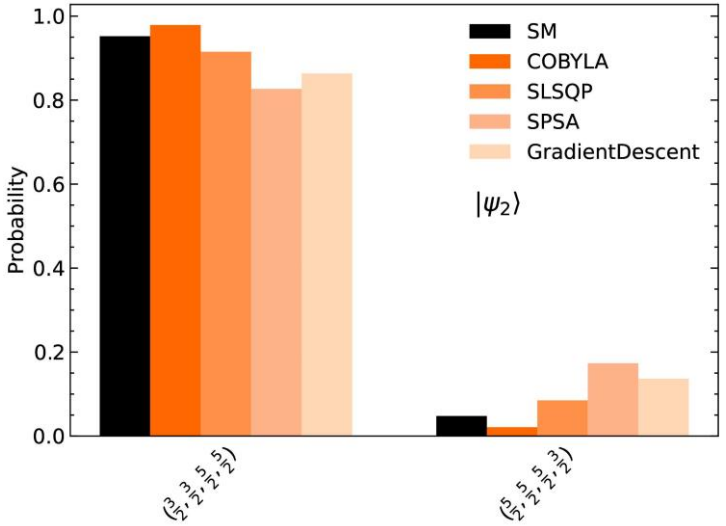



- COBYLA optimizer demonstrates the fastest convergence, achieving it in 105 iterations with $10^{-2}$ MeV accuracy.
- SPSA and Gradient Descent take longer (more iterations) to converge, similar to the ground state calculations.
- Other optimizers provide reasonable results but miss correct distributions 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. | 8 | 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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