Ab initio nuclear mass model and the emergence of nuclear magicity

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Frontiers in Nuclear Lattice EFT: From *Ab Initio* Nuclear Structure to Reactions
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Contents

Background and Motivation

01

Revisit the nuclear magicity

The nuclear magicity: For specific proton or neutron numbers, the nuclei exhibit enhanced stability.

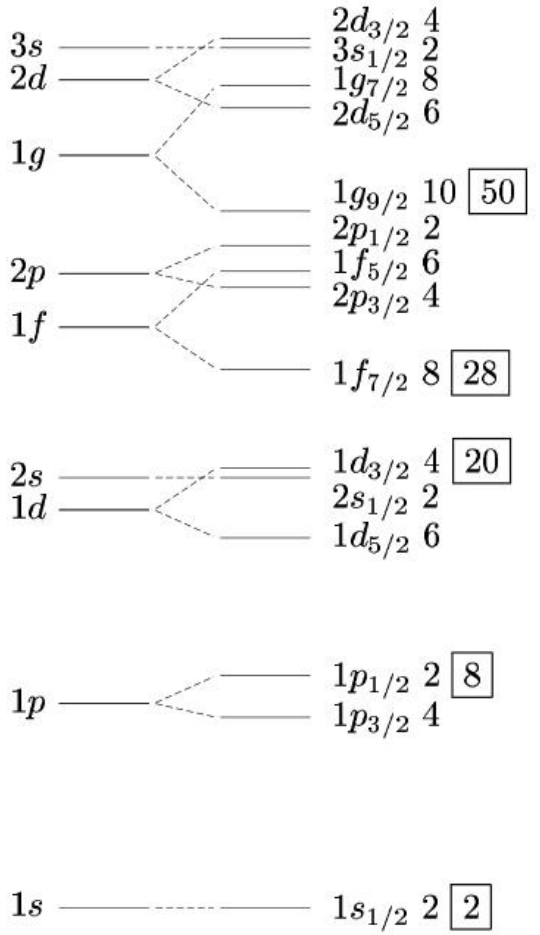
Mayer & Jensen. Nuclear shell model. (1963 Nobel Prize)

"Protons & neutrons in a nucleus move in regular orbits"

$$V = -\lambda \frac{1}{r}\frac{dV}{dr}\boldsymbol{L}\cdot\boldsymbol{S}$$

The introduction of the **spin-orbit coupling term** successfully explains the existence of the **magic numbers** 2, 8, 20, 28, 50, 82, and 126.

Magic numbers emerge at the **shell closures**.



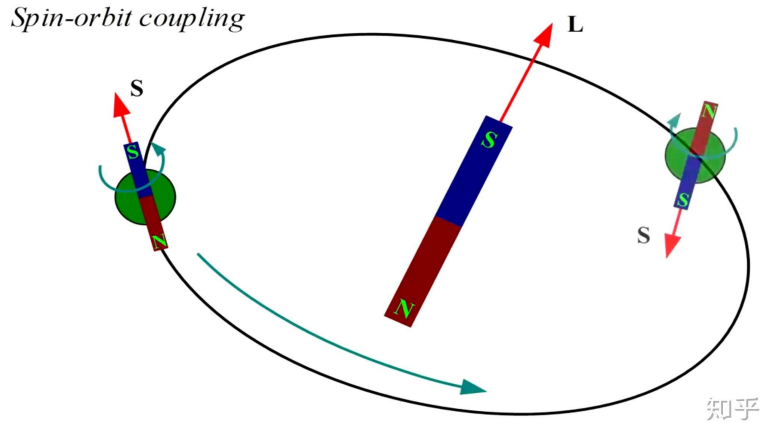
Emergence of nuclear shell structures

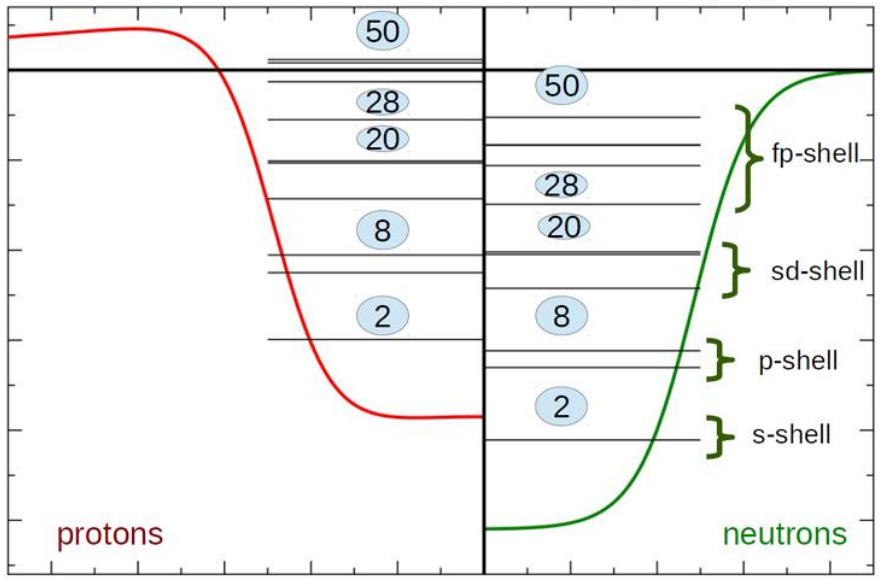
How to trace the **microscopic origin** of this critical spin-orbit coupling ?

- Mean-field models generate **single particle orbits** via variational principles; however, the interactions are **effective** ones dressed in the medium

- ***Ab initio* calculations** start from **bare nuclear forces in the vacuum** and solve the many-body Schrödinger equation directly, with all correlation taken into account

- Shell structure emerge from the intricate interplay between **nuclear force** and **many-body correlations**





Nuclear *ab initio* calculations

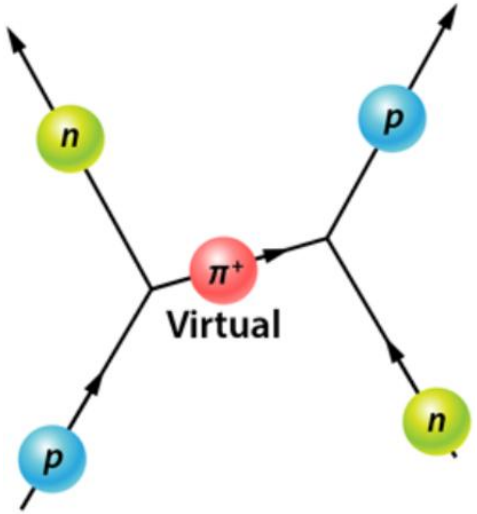
- **Shell-model based methods**
  - **No-Core Shell Model** PPNP 69, 131 (2013)
  - **In-medium Similarity Renormalization Group** Phys. Rept. 621, 165 (2016)
  - **Coupled Cluster** Rep. Prog. Phys. 77, 096302 (2014)
  - **…**
- **Coordinate/Momentum space methods**
  - **Green's Function Monte Carlo** RMP 87, 1067 (2015)
  - **Self-Consistent Green's Function** PPNP 52, 377 (2004)
  - **Nuclear Lattice Effective Field Theory** PPNP 63, 117 (2009)
  - **…**

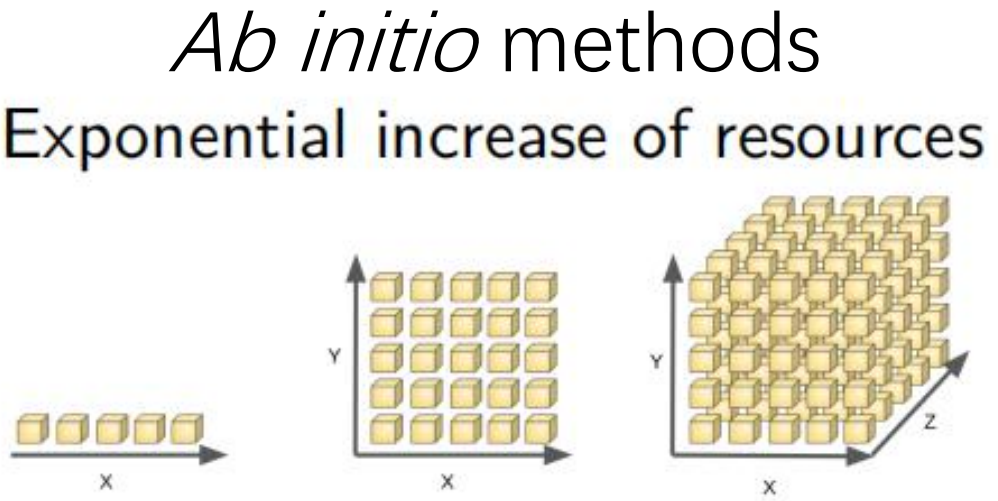
Solve the nuclear forces directly

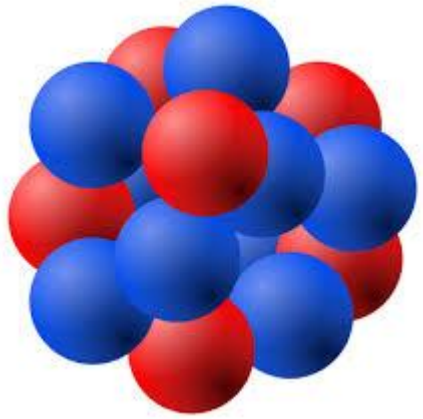
shell structure / nuclear clustering / symmetry breaking / shape fluctuation

All emerge naturally without assumptions

Nuclear *ab initio* calculations





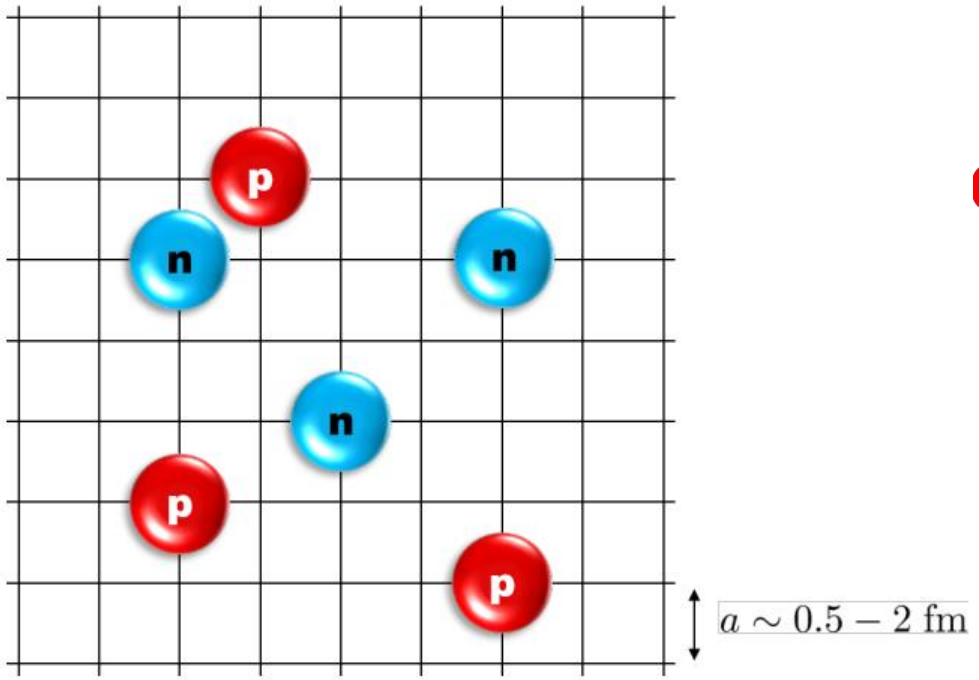


- Connect **bare nuclear forces** with macroscopic nuclear properties (such as nuclear magicity).
- **Strategy: Combine the *ab initio* computations** with **simplified interactions** that capture the **essential elements** of nuclear binding.

Nuclear Lattice Effective Field Theory

Nuclear lattice effective field theory is a Monte Carlo method based on discretizing space-time into a **lattice** combined with **effective field theory**.

Review: Dean Lee, Prog. Part. Nucl. Phys. 63, 117 (2009),
Lähde, Meißner, "Nuclear Lattice Effective Field Theory", Springer (2019)



Euclidean time projection:

$$|\Psi_{g.s.}\rangle \propto \lim_{\tau\to\infty} \exp(-\tau H)|\Psi_A\rangle$$

Core chanllenge : Sign prolem

When handling integrands involving high-order phase oscillations, significant statistical errors may arise — the fermionic **Sign Problem**.

Nuclear Lattice Effective Field Theory

Core challenge : Sign problem

$$1 \quad \sigma_1 \cdot \sigma_2$$

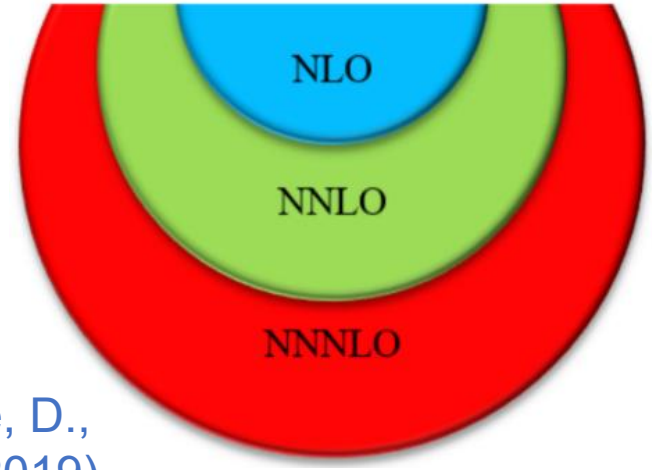
$$q^2 \quad q^2(\tau_1 \cdot \tau_2) \quad q^2(\sigma_1 \cdot \sigma_2) \quad q^2(\sigma_1 \cdot \sigma_2)(\tau_1 \cdot \tau_2)$$

$$j(q \times k) \cdot (\sigma_1 + \sigma_2)/2 \quad (\sigma_1 \cdot q)(\sigma_2 \cdot q) \quad (\sigma_1 \cdot q)(\sigma_2 \cdot q)(\tau_1 \cdot \tau_2)$$

Non-perturbative – Monte Carlo

"Improved LO"

Perturbative corrections



Example: "Essential Element"
Lu, B.-N., Li, N., Elhatisari, S., Lee, D., Epelbaum, E., & Meißner, U.-G. (2019).

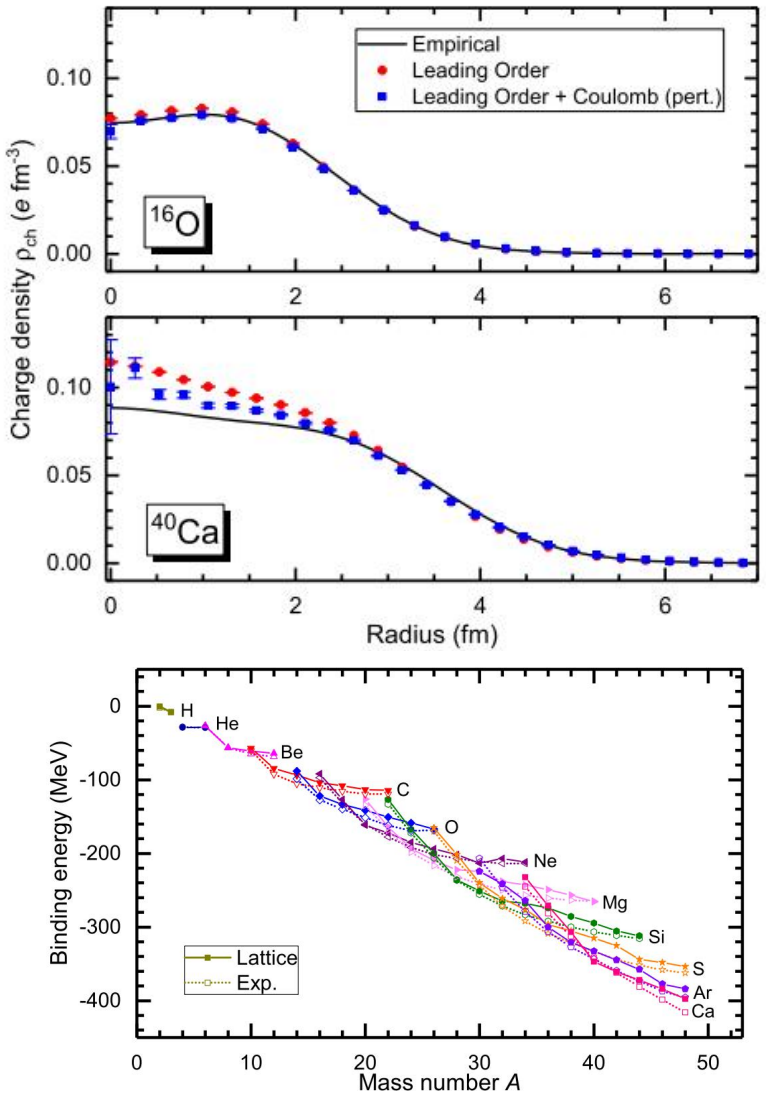
Use a simplified sign-free Hamiltonian serving as the leading-order term while **other components are handled perturbatively.**

Borasoy, B., Epelbaum, E., Krebs, H., Lee, D., & Meißner, U.-G. (2007). EPJA, 31(1), 105-123.Lu B. N., Li N., Elhatisari S., et al. PRL 128, 242501 (2022).

Methods

02

Lattice SU(4) model



The spin- and isospin independent interactions obey Wigner's SU(4) symmetry[1].

$$H_{\mathrm{SU(4)}} = H_{\mathrm{free}} + \frac{1}{2!}C_2 \sum_{\boldsymbol{n}} \tilde{\rho}(\boldsymbol{n})^2 + \frac{1}{3!}C_3 \sum_{\boldsymbol{n}} \tilde{\rho}(\boldsymbol{n})^3$$

$$\tilde{\rho}(\boldsymbol{n}) = \sum_i \tilde{a}_i^\dagger(\boldsymbol{n})\tilde{a}_i(\boldsymbol{n}) + s_L \sum_{|\boldsymbol{n}'-\boldsymbol{n}|=1} \sum_i \tilde{a}_i^\dagger(\boldsymbol{n}')\tilde{a}_i(\boldsymbol{n}')$$

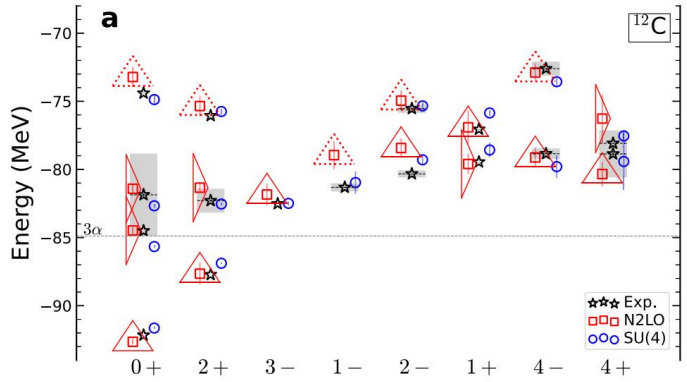
$$\tilde{a}_i(\boldsymbol{n}) = a_i(\boldsymbol{n}) + s_{NL} \sum_{|\boldsymbol{n}'-\boldsymbol{n}|=1} a_i(\boldsymbol{n}')$$

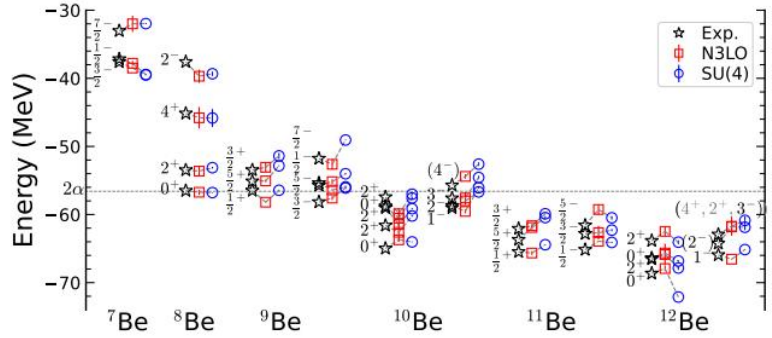
The **SU4 interaction**[2] gives good predictions of nuclear properties, such as **energy spectrum, charge density distribution and so on.** And it is **without sign problem.**

[1] E. Wigner, Phys. Rev. 51, 106 (1937).
[2] Lu, B.-N., Li, N., Elhatisari, S., Lee, D., Epelbaum, E., & Meißner, U.-G. (2019).

Application of Lattice SU(4) interactions

^{12}C and Be isotope excitation spectra

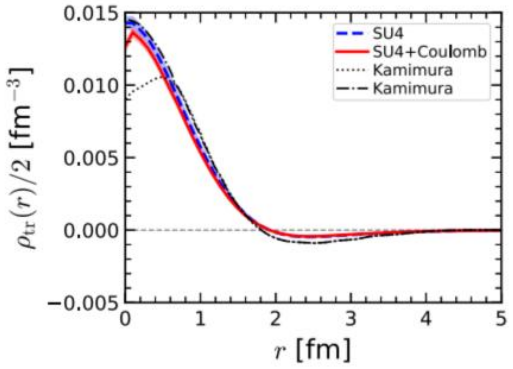




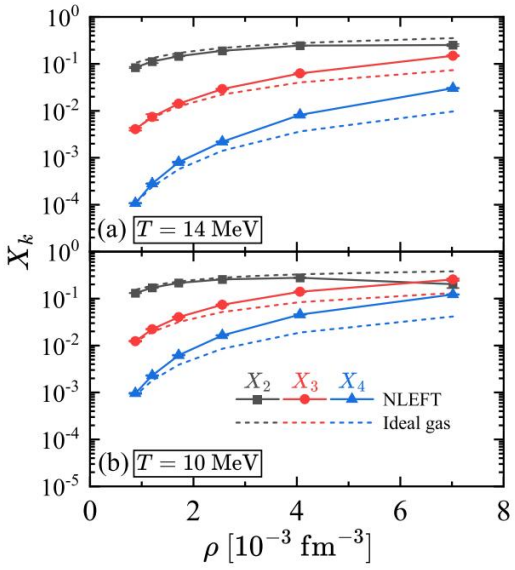
Shihang Shen, Serdar Elhatisari, et al. nat. comm, 14(1):2777, 2023.

Shihang Shen, Serdar Elhatisari, Lee D, et al. arXiv:2411.14935, 2024.

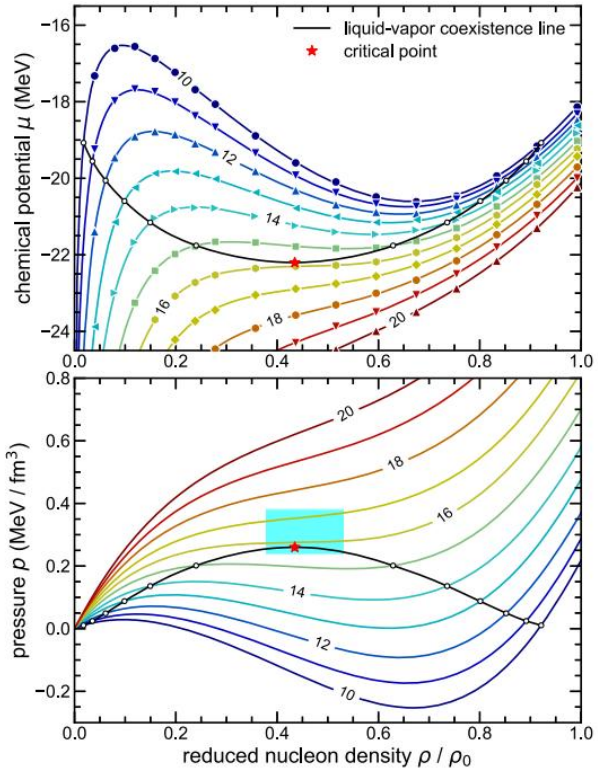
Alpha-Particle Monopole Transition



Clustering at finite temperature



Ab initio nuclear thermodynamics



Z Ren, Serdar Elhatisari, Lähde T A, et al. PLB, 1000,2024.

U G Meißner, Shihang Shen, Serdar Elhatisari, et al. PRL, 132(6): 062501,2024.

Bing-Nan Lu, Ning Li, et al. PRL, 125(19): 192502,2020.

Nuclear force model

To better describe shell evolution, we **non-perturbatively** introduce the **spin-orbit coupling interaction** with no sign problem.

$$H = H_{\text{free}} + \frac{1}{2!}C_2\sum_{\vec{n}}\tilde{\rho}(\vec{n})^2 + \frac{1}{3!}C_3\sum_{\vec{n}}\tilde{\rho}(\vec{n})^3 + \boxed{C_{sl}V_{\frac{i}{2}(\mathbf{q}\times S)\cdot\mathbf{k}}}$$

$$\tilde{\rho}(\vec{n}) = \sum_i \tilde{a}_i^\dagger(\vec{n})\tilde{a}_i(\vec{n}) + s_L \sum_{|n'-\vec{n}|=1}\sum_i \tilde{a}_i^\dagger(\vec{n}')\,\tilde{a}_i(\vec{n}')$$

Nonlocal density operator :

$$\tilde{a}_i(\vec{n}) = a_i(\vec{n}) + s_{NL}\sum_{|\vec{n}'-\vec{n}|=1} a_i(\vec{n}')$$

The Hamiltonian is defined on a L^3 cubic lattice with integer coordinates $n = (n_x, n_y, n_z)$.

Nuclear mass Model

$$H = H_{\text{free}} + \frac{1}{2!}C_2 \sum_{\vec{n}} \tilde{\rho}(\vec{n})^2 + \frac{1}{3!}C_3 \sum_{\vec{n}} \tilde{\rho}(\vec{n})^3 + \boxed{C_{sl} V_{\frac{i}{2}(\mathbf{q}\times S)\cdot\mathbf{k}}}$$

Under **small coupling constants** and appropriate auxiliary field transformations, the introduction of the spin-orbit coupling term does not lead to sign problems.

$$:\exp(-\frac{1}{2}C_2\rho^2 - C_{sl}V_{\frac{i}{2}(\mathbf{q}\times S)\cdot\mathbf{k}}) =: \exp\left[-\frac{1}{2}C_2(\rho+\rho')^2 + \frac{1}{2}C_2\rho'^2\right] :$$

Rewrited as a **perfect square form** so that there is no phase oscillation in the interaction.

A Coulomb interaction is then taken into account perturbatively

$$V_C(r) = \frac{e^2}{r}\,\mathrm{erf}\left(\frac{\Lambda_{cou} r}{2}\right) \qquad \Lambda_{cou} = 180\,\mathrm{MeV}$$

Optimization of the nuclear force model

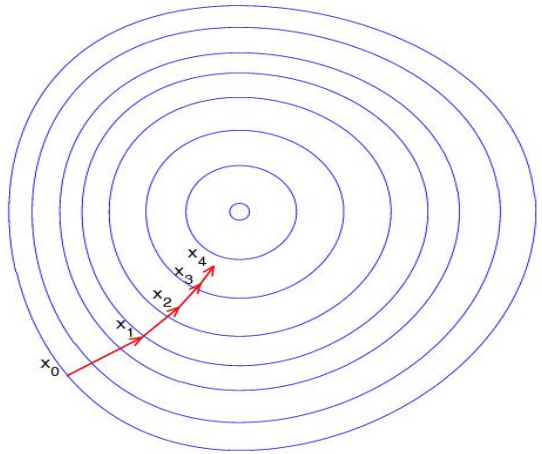
Experimental data is required to determine **five parameters.**

$$H = H_{\text{free}} + \frac{1}{2!}C_2\sum_{\vec{n}}\tilde{\rho}(\vec{n})^2 + \frac{1}{3!}C_3\sum_{\vec{n}}\tilde{\rho}(\vec{n})^3 + \boxed{C_{sl}V_{\frac{i}{2}(\mathbf{q}\times S)\cdot\mathbf{k}}}$$

$$\tilde{a}_i(\vec{n}) = a_i(\vec{n}) + s_{NL}\sum_{|\vec{n}'-\vec{n}|=1} a_i(\vec{n}') \qquad \tilde{\rho}(\vec{n}) = \sum_i \tilde{a}_i^\dagger(\vec{n})\tilde{a}_i(\vec{n}) + s_L\sum_{|n'-\vec{n}|=1}\sum_i \tilde{a}_i^\dagger(\vec{n}')\,\tilde{a}_i(\vec{n}')$$

Loss function : $\chi^2 = \chi^2(s_L, s_{NL}, C_2, C_3, C_{sl}) = \sum_A \left(\frac{E(A) - E(A)_{\text{exp}}}{\epsilon}\right)^2$

Determine the parameters by **minimizing** the loss function.



Difficulties

1. A single Monte Carlo calculation consumes **hundreds to thousands of times** more resources than a mean-field calculation, with consumption rising as precision and nucleon count increase.

2. The **magnitude differences** in parameters make it difficult for the system to converge to the minimum.

3. Monte Carlo calculations have statistical errors, making it **difficult to compute accurate derivatives**. Implementing efficient gradient descent in NLEFT is challenging.

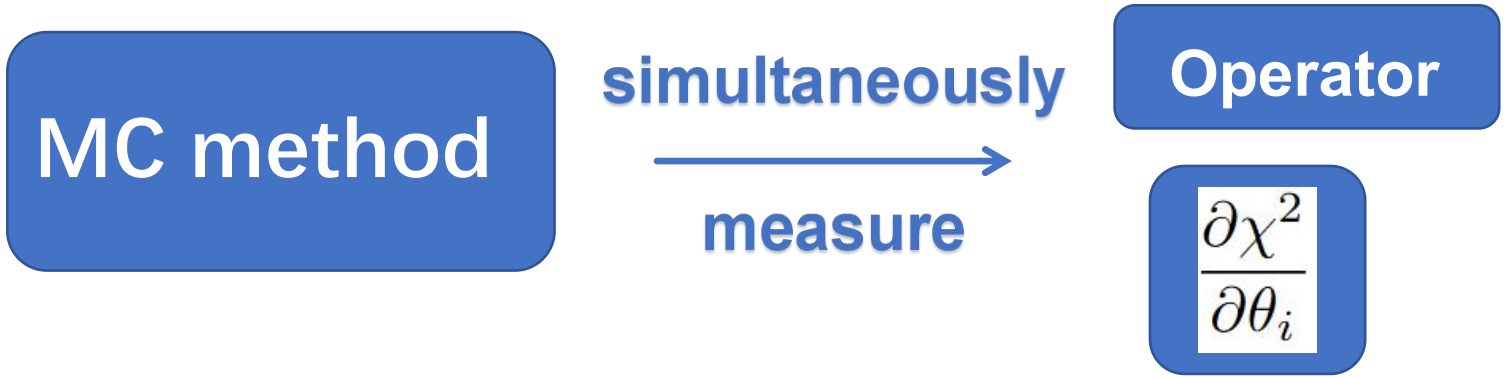
Accurate evaluation of derivatives

According to the chain rule, we only need to calculate the derivative with respect to each nucleus.

$$\chi^2 = \sum_A \left(\frac{E(A) - E(A)_{\text{exp}}}{\varepsilon} \right)^2 \longrightarrow \frac{\partial \chi^2}{\partial \theta_i} = \sum_A \left[2 \left(\frac{E(A) - E(A)_{\text{exp}}}{\varepsilon^2} \right) \frac{\partial E(A)}{\partial \theta_i} \right]$$

where θ_i is the fitting parameters.

Therefore, we can directly **measure** $\frac{\partial E}{\partial \theta_i}$ as an operator in the Monte Carlo calculations, providing an exact derivative.



So, we consider using **the gradient descent method**.

The Gradient Descent Method

Implementation: We implemented the Gradient Descent algorithm simply by introducing strategies such as **feature scaling** and **adaptive learning rates**.

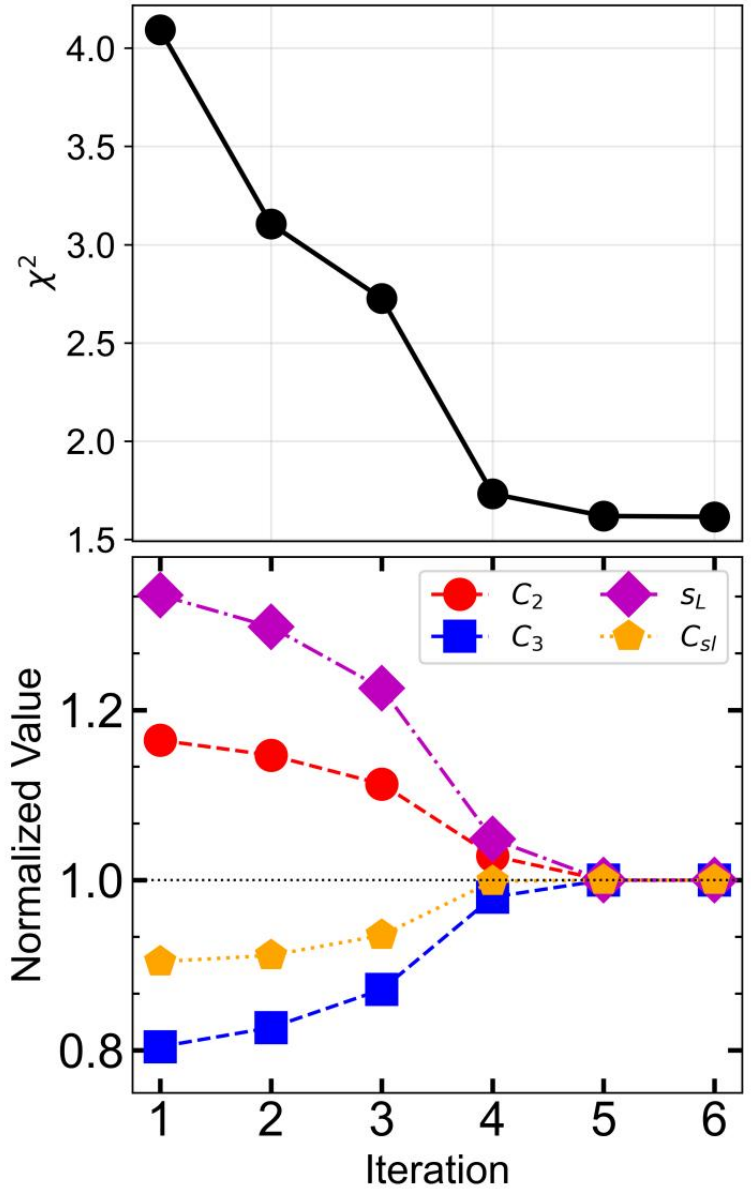
Target nuclei ^{4}He, ^{16}O, ^{24}Mg, ^{28}Si, ^{32}S, ^{40}Ca

The loss function and all parameters **converge rapidly** with iterations.

Final parameters:

$$s_L = 8.082 \times 10^{-2}, s_{NL} = 0.45, C_2 = -4.410 \times 10^{-7}$$

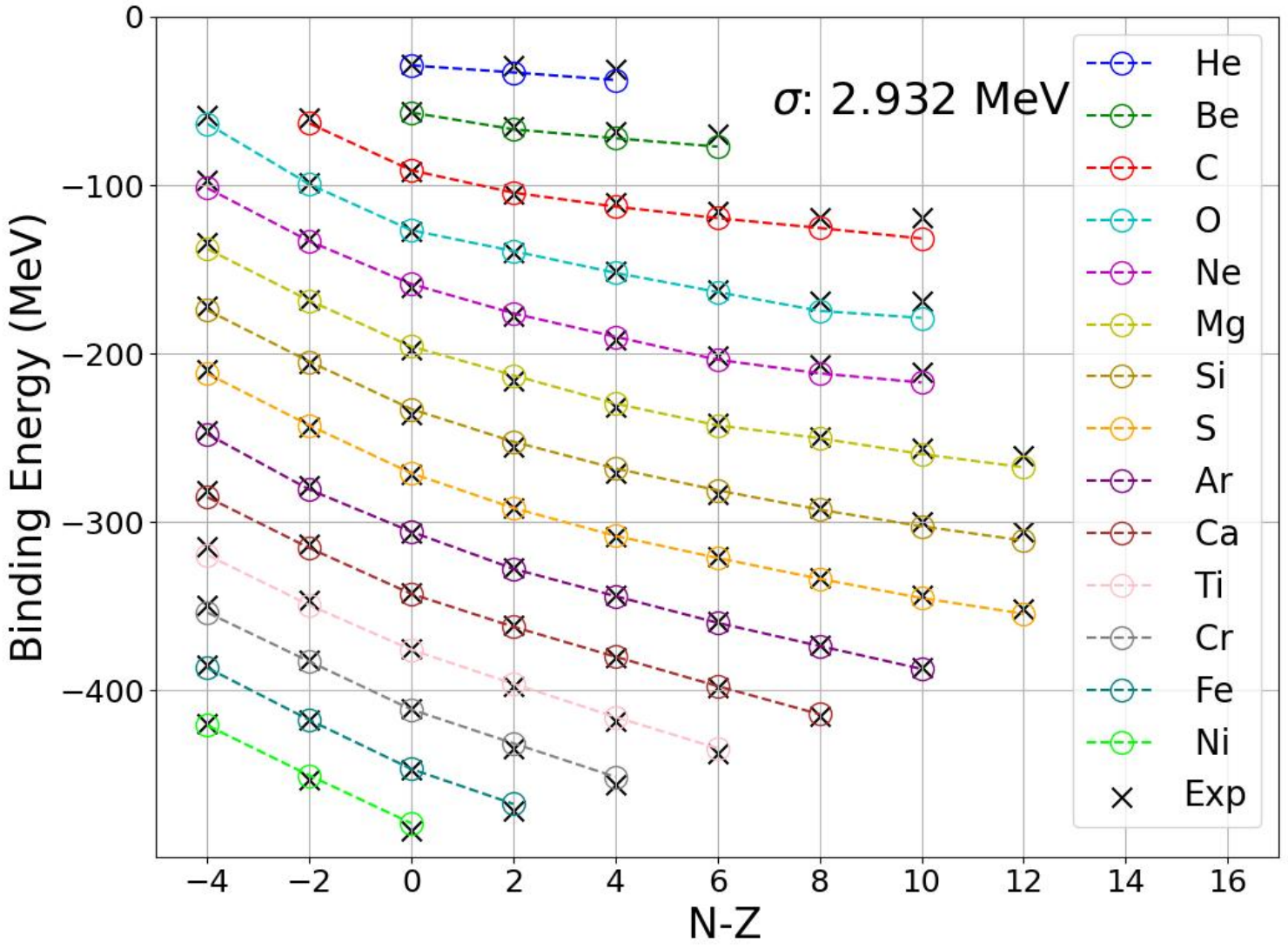
$$C_3 = 1.561 \times 10^{-15},\ C_{sl} = 8.590 \times 10^{-12}$$



Results

03

Binding energy of even-even nuclei with N, Z ≤ 28



$$\sigma = \sqrt{\frac{1}{N}\sum_{i=1}^{N}(x_i - \bar{x})^2}$$

Method	Standard deviation	parameter numbers
Liquid drop [1]	1.15 MeV	> 30
Relativistic mean-field[2]	2.25 MeV	11
Skyrme [3]	3.41 MeV	12
Lattice SU4	10.21MeV	4
This work	2.93 MeV	5

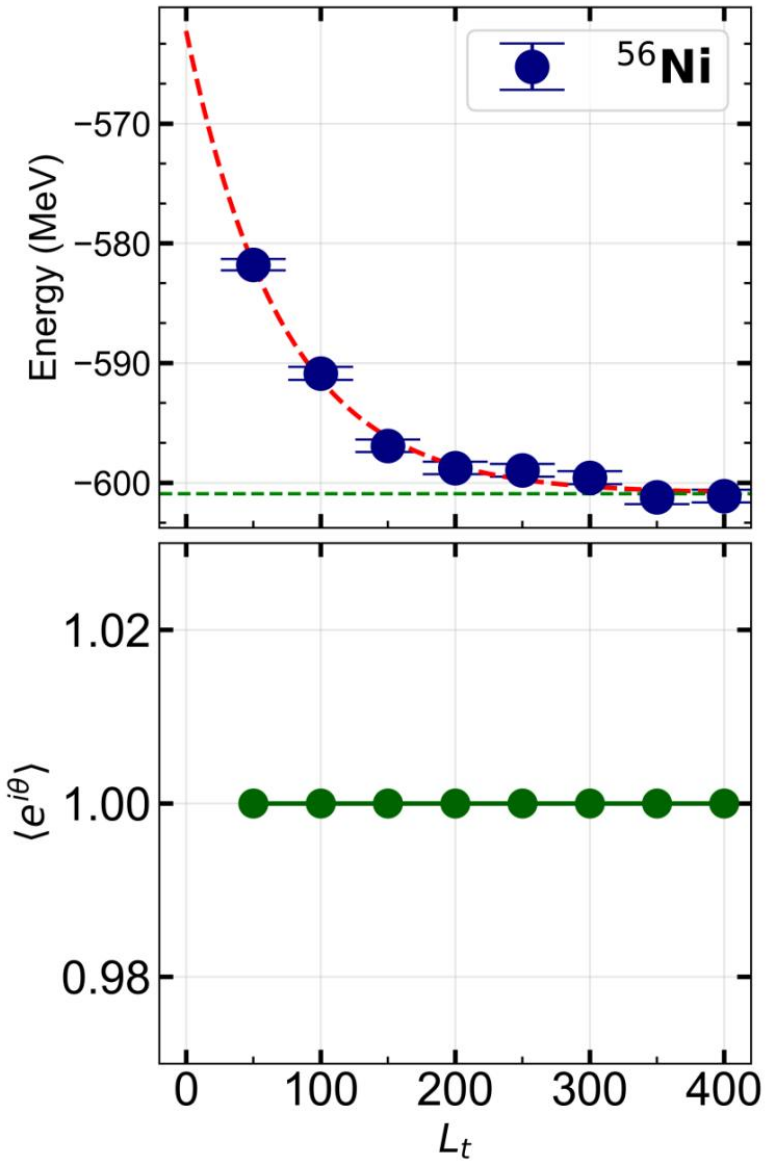
Deviation from experiment is calculated for 76 nuclei with N, Z<=28.

[1]P. Möller, A.J. Sierk, T. Ichikawa, and H. Sagawa. ADANDT, 109-110:1–204, 2016.

[2]Zhang, K., Cheoun, M.-K., et al. ADANDT, 144:101488, 2022.

[3]M. Kortelainen, J. McDonnell, et al. PRC, 85:024304, Feb 2012.

Imaginary time extrapolation and sign problems



Get interacting ground state from imaginary time projection.

$$|\Psi_{g.s.}\rangle \propto \lim_{\tau\to\infty} \exp(-\tau H)|\Psi_A\rangle$$

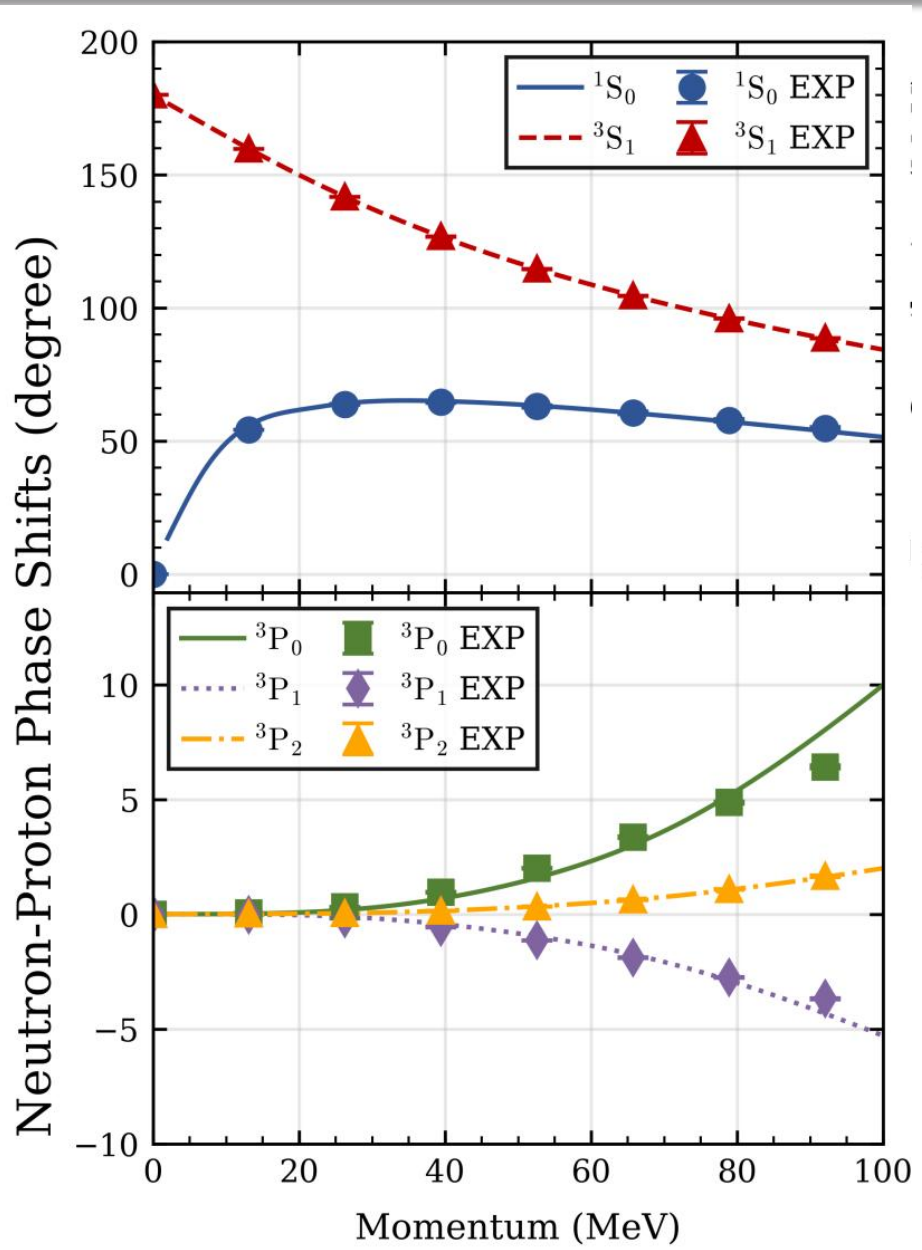
Total energies at the large τ follow

$$E_A(\tau) = E_A(\infty) + c\exp(-\Delta E\tau)$$

$e^{i\theta}$ characterize whether there is a phase oscillation in the current transfer matrix.

$e^{i\theta}$ = 1 means **no sign problem** at all.

The first reason for introducing spin-orbit coupling is reasonable



Our nuclear mass model is based on a simplified version of pionless EFT.

$$1 \quad \sigma_1 \cdot \sigma_2$$

$$q^2 \quad q^2(\tau_1 \cdot \tau_2) \quad q^2(\sigma_1 \cdot \sigma_2) \quad q^2(\sigma_1 \cdot \sigma_2)(\tau_1 \cdot \tau_2)$$

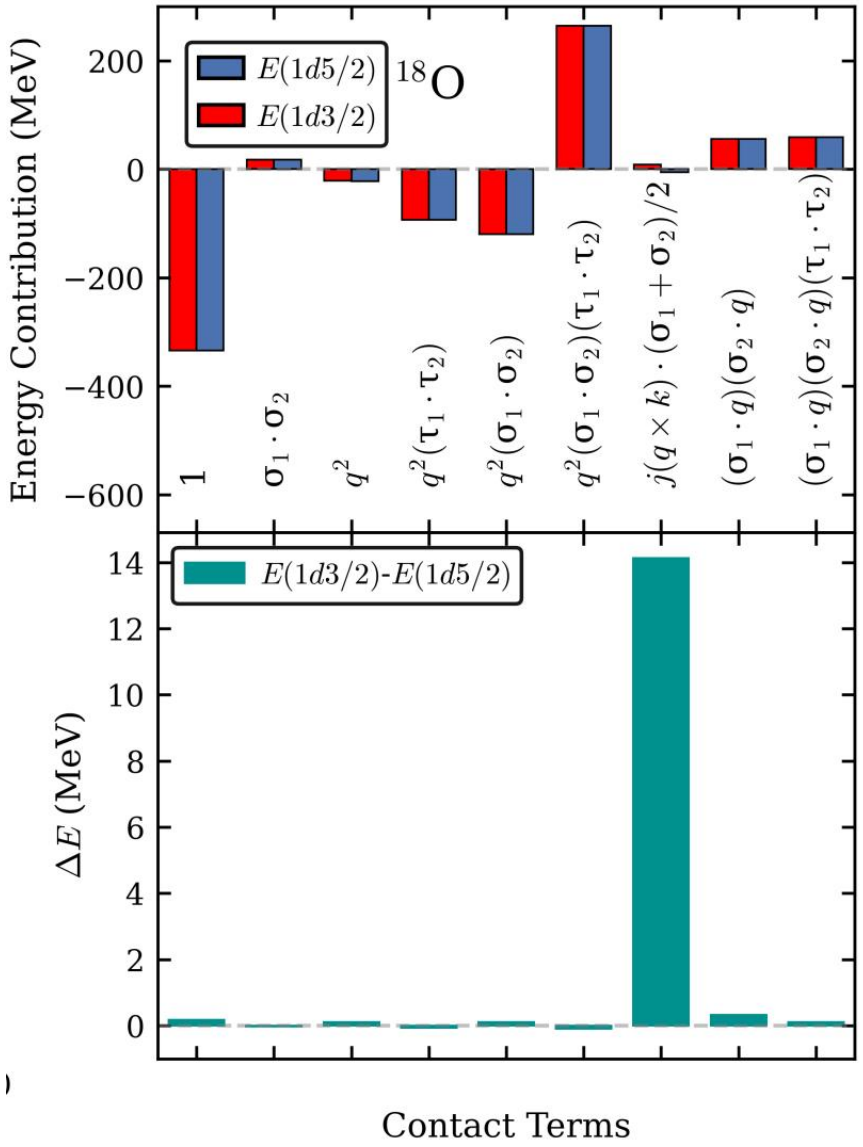
$$j(q \times k) \cdot (\sigma_1 + \sigma_2)/2 \quad (\sigma_1 \cdot q)(\sigma_2 \cdot q) \quad (\sigma_1 \cdot q)(\sigma_2 \cdot q)(\tau_1 \cdot \tau_2)$$

By fitting the scattering phase shifts at Next-Leading-Order(NLO), we get spin-orbit coupling constant: $C_{j(q\times k)\cdot(\sigma_1+\sigma_2)/2} = 9.09 \times 10^{-12}\ \mathrm{MeV}^{-4}$

Comparing with the coupling constant fitting bound energy

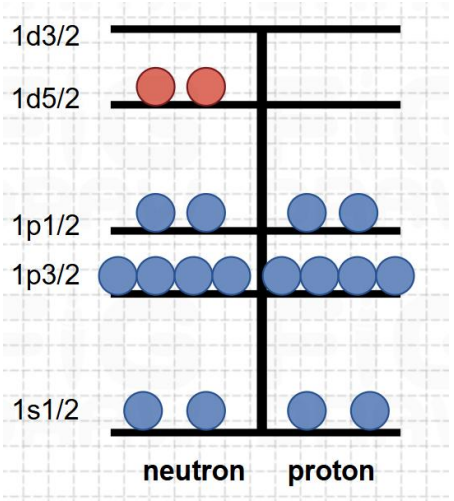
$$C_{j(q\times k)\cdot(\sigma_1+\sigma_2)/2} \simeq C_{sl} = 8.59 \times 10^{-12}\ \mathrm{MeV}^{-4}$$

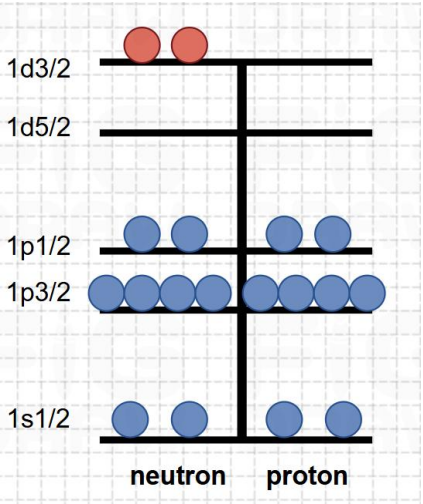
The second reason for introducing spin-orbit coupling is reasonable



For justifying the splitting of the $1d_{3/2}$ and $1d_{5/2}$ orbitals as predicted by the shell model:

Expectation values of the nine NLO operators using the shell model wavefunctions.

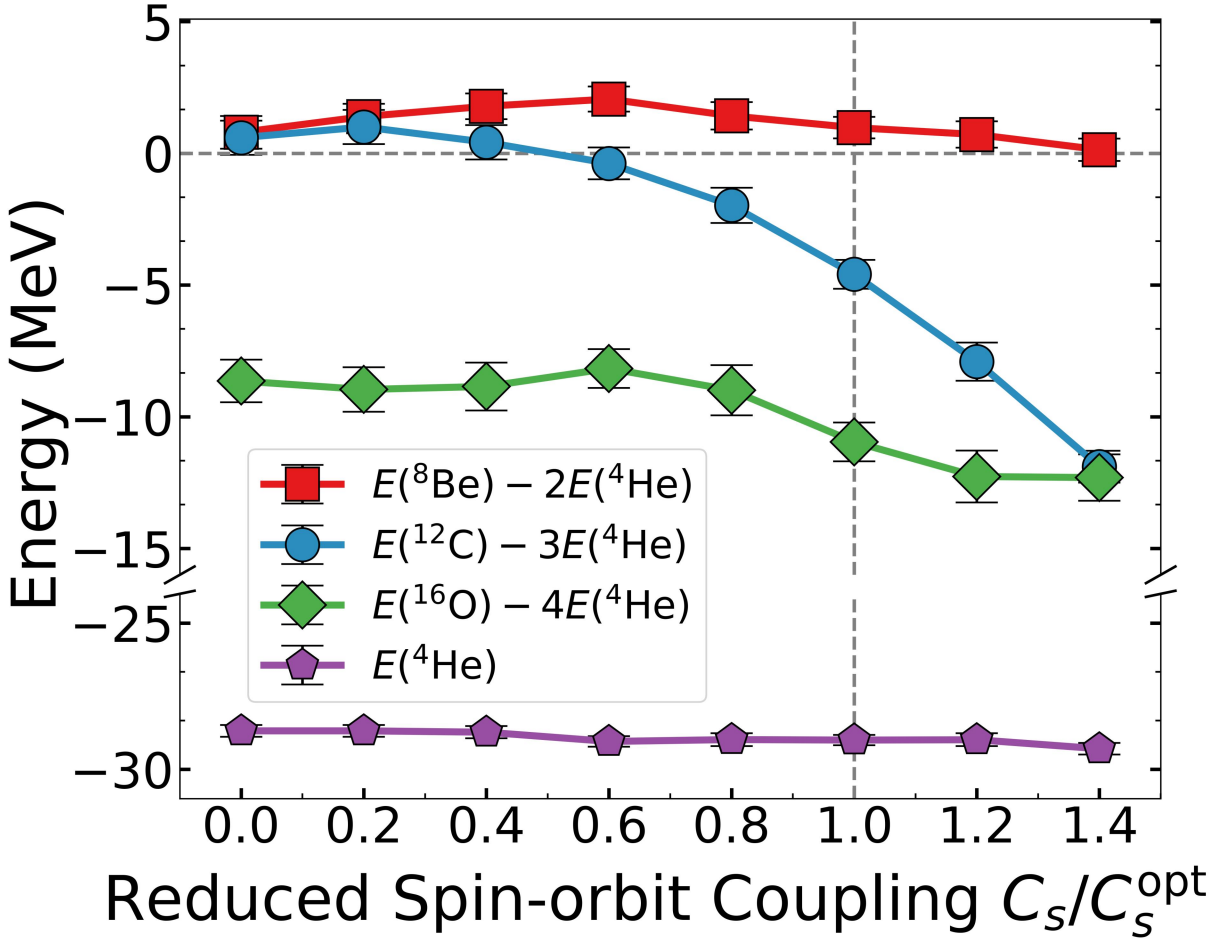




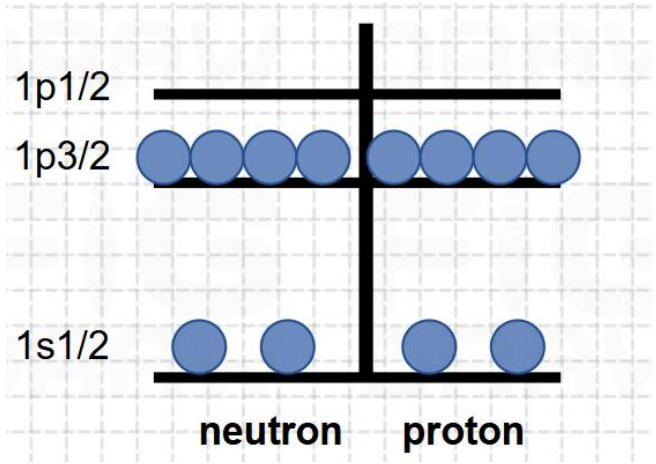
The orbital splitting is entirely attributed to the spin-orbit term $j(q \times k) \cdot (\sigma_1 + \sigma_2)/2$

The emergence of magic number 6

$$H = H_{\text{free}} + \frac{1}{2!}C_2\sum_{\vec{n}}\tilde{\rho}(\vec{n})^2 + \frac{1}{3!}C_3\sum_{\vec{n}}\tilde{\rho}(\vec{n})^3 + c * C_{sl}V_{\frac{1}{2}(\vec{q}\times\vec{S})\cdot\vec{k}}$$



As the spin-orbit coupling increases, ^{12}C transitions from three free alpha particles to a single nuclei.



This fact suggests the possibility of the existence of **magic number 6**.

Summary and Perspective

04

Summary and Perspective

01 We establish a **non-perturbative ab initio** calculation model that includes spin-orbit coupling and **without sign problem**.

02 **Accurate parameter derivatives** are obtained through Monte Carlo sampling, enabling gradient descent to determine the system parameters.

03 The optimized interaction reproduces binding energies for A<=56 with an accuracy comparable with the state-of-the-art mean field models.

Perspective: **Neutron rich** nuclei; **heavier nuclei** with A~100; **interactions optimized** with more constraints (radius, nuclear matter, etc.); applications in nuclear **structure** studies (clustering, halo nuclei, paring, nuclear shapes, spectroscopy, etc.)

Thanks for your attention

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中国工程物理研究院研究生院