2025年11月28日，中山大学，珠海

基于人工智能的原子核第一性原理研究

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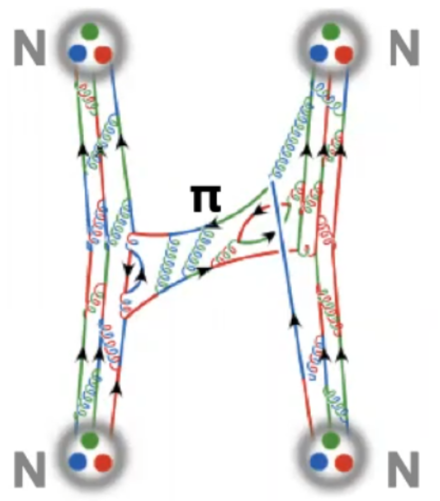
Outline

- 原子核第一性原理计算及其挑战
- 基于人工神经网络的量子多体波函数
- 基于人工智能的原子核第一性原理研究
- 总结与展望

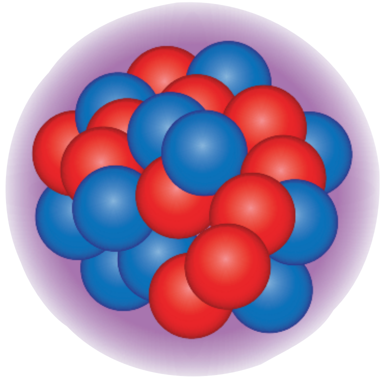
原子核的第一性原理研究

利用量子力学的基本原理，从核子间相互作用出发，理解原子核的各种性质。

- **通过核子散射数据确定核力**
  - 唯象模型, 介子交换模型
  - 有效场论 (EFT)



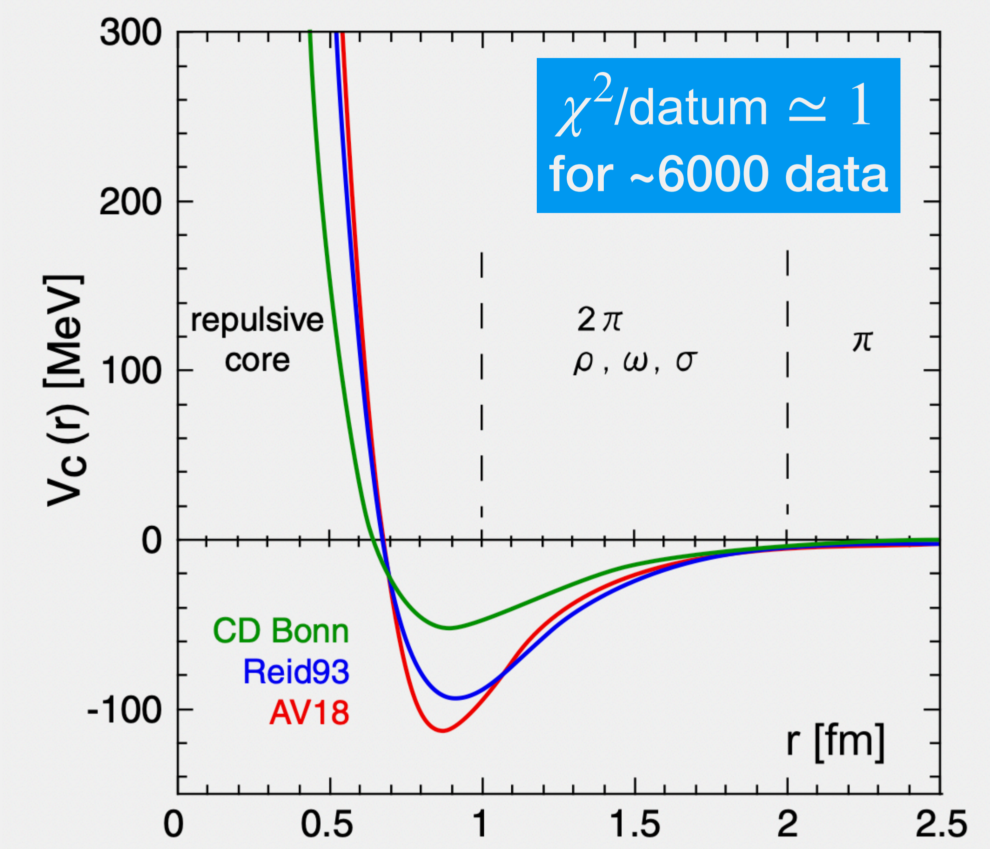
- **求解核多体问题**
  - 原子核粗块性质: 质量, 半径, …
  - 核谱学: 能级, 电磁跃迁, …
  - 核物质状态方程: 中子星, …
  - 新物理: 无中微子双贝塔衰变, …
  - …



Ab initio calculations with *NN* forces

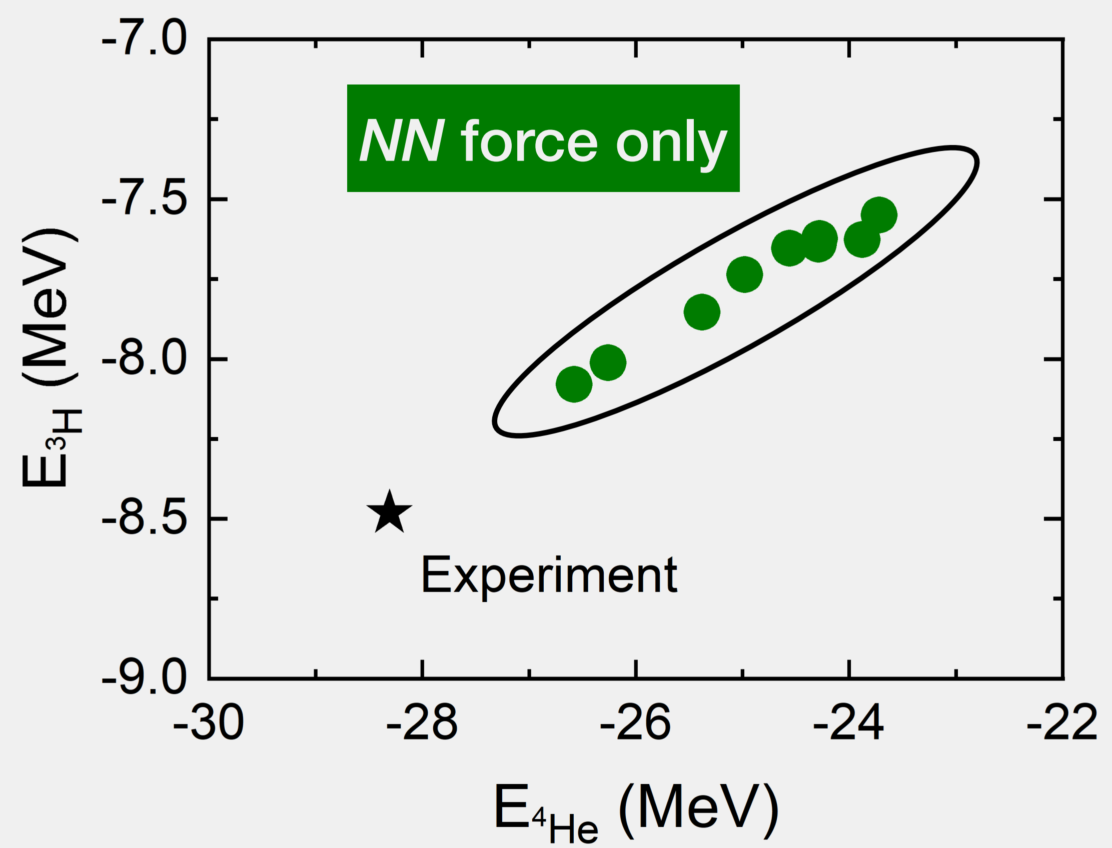
Many two-nucleon (*NN*) interactions, applied to nonrelativistic *ab initio* calculations, provide **insufficient binding** for light nuclei.

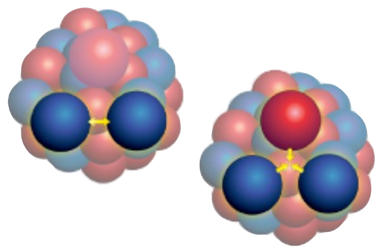
NN forces



Taken from Ishii et al., PRL 99, 022001 (2007)

^{3}H and ^{4}He

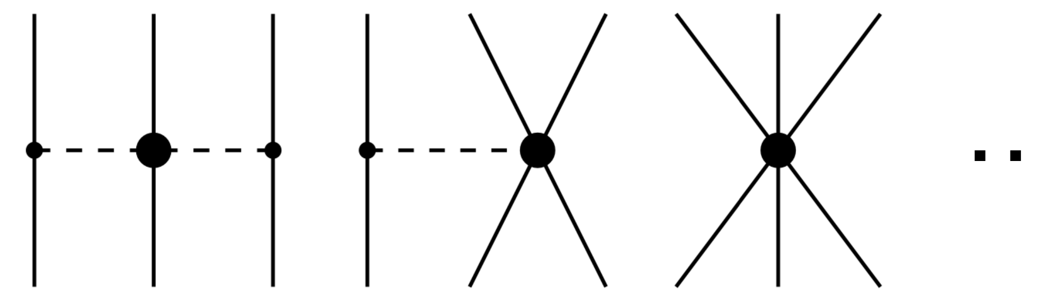




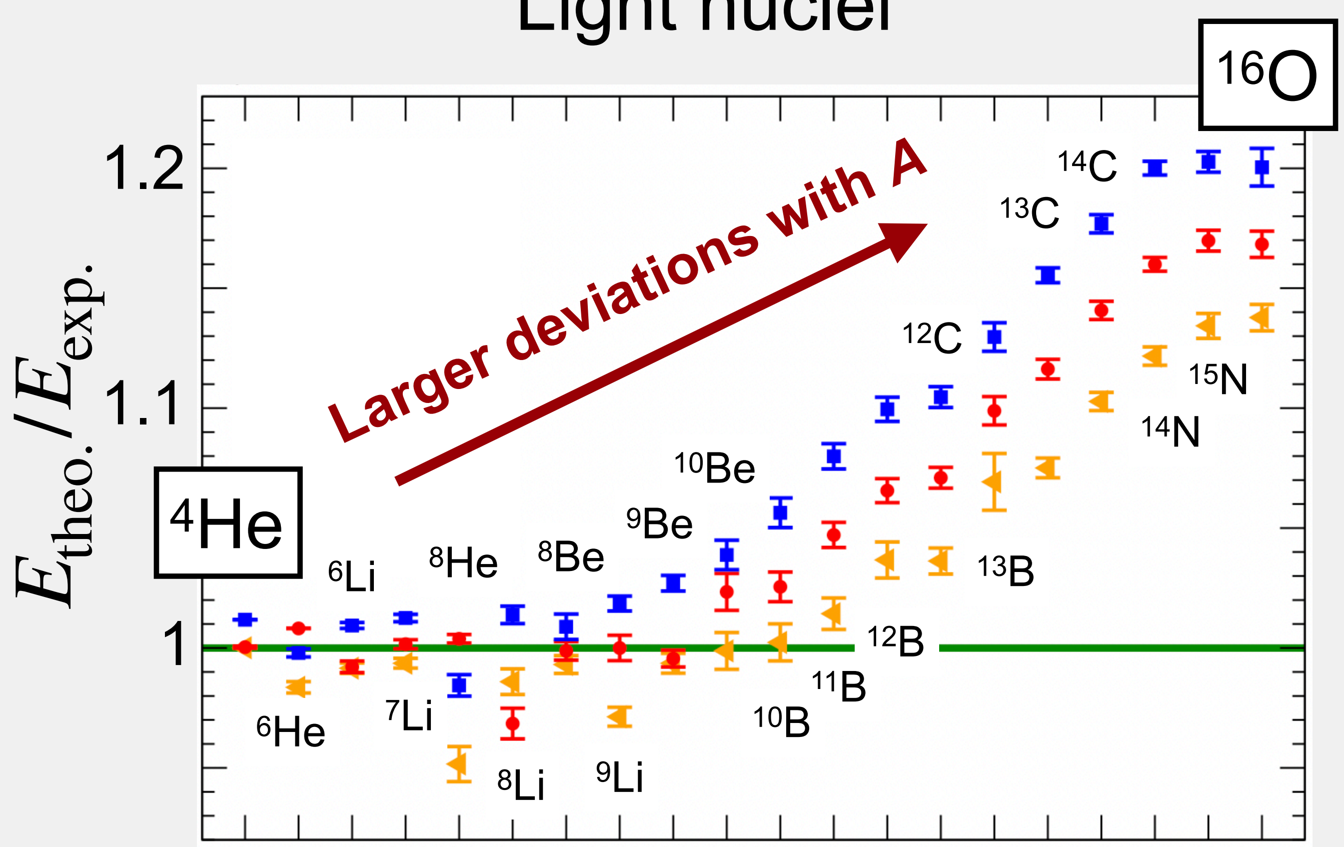
Three-nucleon forces are needed !

Ab initio calculations with *NN*+3*N* forces

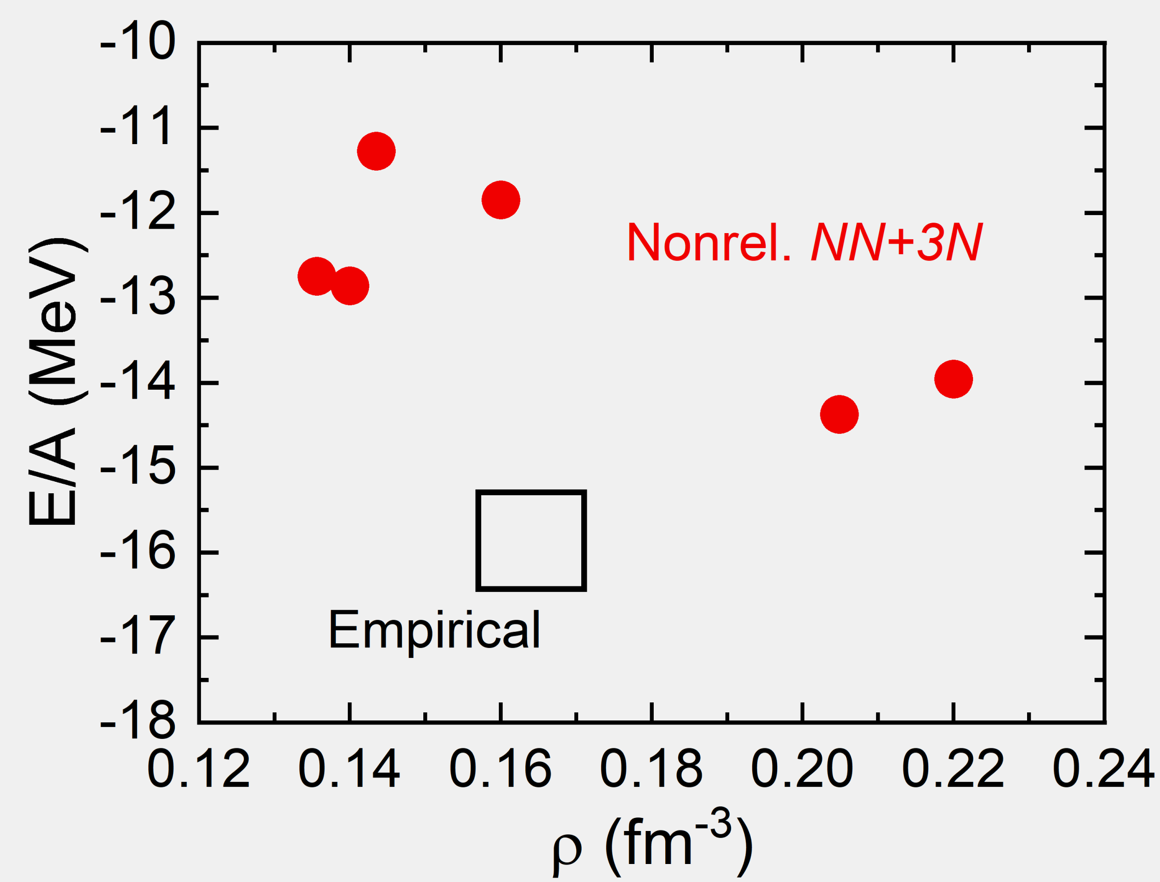
- **3*N*-force models fitting to**
  - A = 3 binding energy / beta decay
  - pd/nd scattering
  - …



Light nuclei



Nuclear matter



Lonardoni et al., PRL 120, 122502 (2018)
LENPIC Collaboration, PRC 103, 054001 (2021)

Drischler et al., PRL 122, 042501(2019)
Akmal et al., PRC 58, 1804 (1998); Sammarruca et al., PRC 91, 054311 (2015)
Lonardoni et al., Phys. Rev. Research 2, 022033(R) (2022)

Possible solutions …

Accurate *ab initio* explanations of medium-mass nuclei

—— an outstanding problem in nuclear physics!

- **Including many-body forces** **(*4N*-, *5N*-, …, density-dependent)**
  - fit to medium-mass and heavy nuclei
  - density functional theory

tractable
non-ab initio.

- **Adjust *3N* and/or *2N* forces to medium-mass nuclei**
  - may sacrifice the accuracy for free-space scattering data
  - possible inconsistent *3N/2N* forces

controversial.

- **Improving nuclear forces by going for higher order**
  - N4LO inducing new operator structures of *3N* forces
  - but **complicated** …

intractable
ab initio.

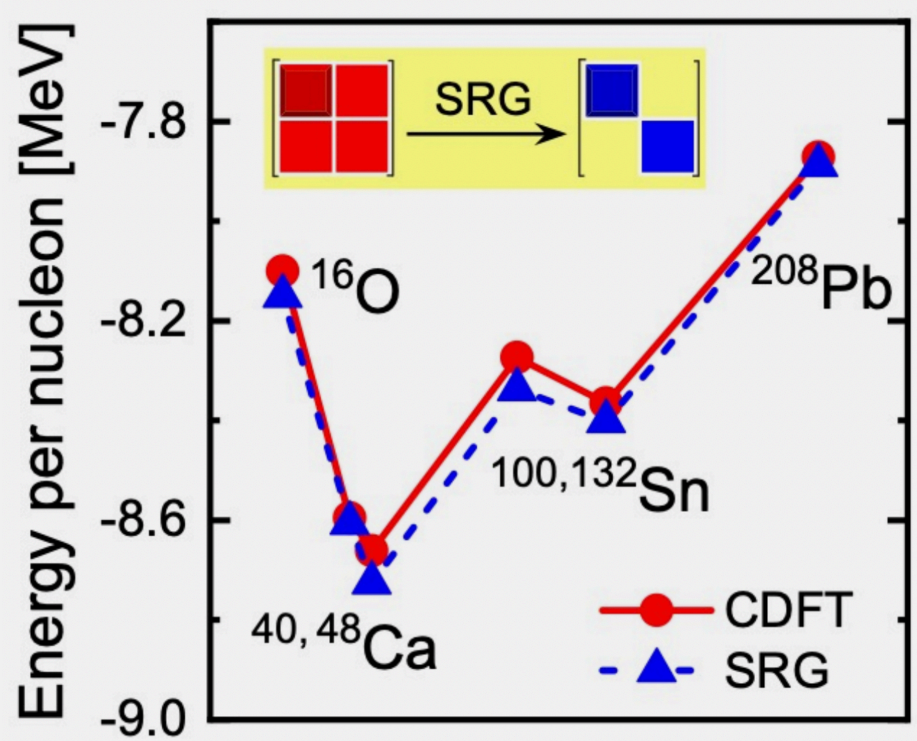
Our strategy: going for a relativistic *ab initio* framework

Relativistic effects

Bridge the Rel. and Nonrel. DFTs

$$4\pi r^2 \rho_v(r) = \rho_0 + \frac{d}{dr}\left[\frac{1}{4\tilde{M}^2}\frac{\kappa}{r}\rho_0\right] + \frac{d^2}{dr^2}\left[\frac{1}{8\tilde{M}^2}\rho_0\right] + O(\tilde{M}^{-3}),$$

Rel. Nonrel. (including high-order terms …)



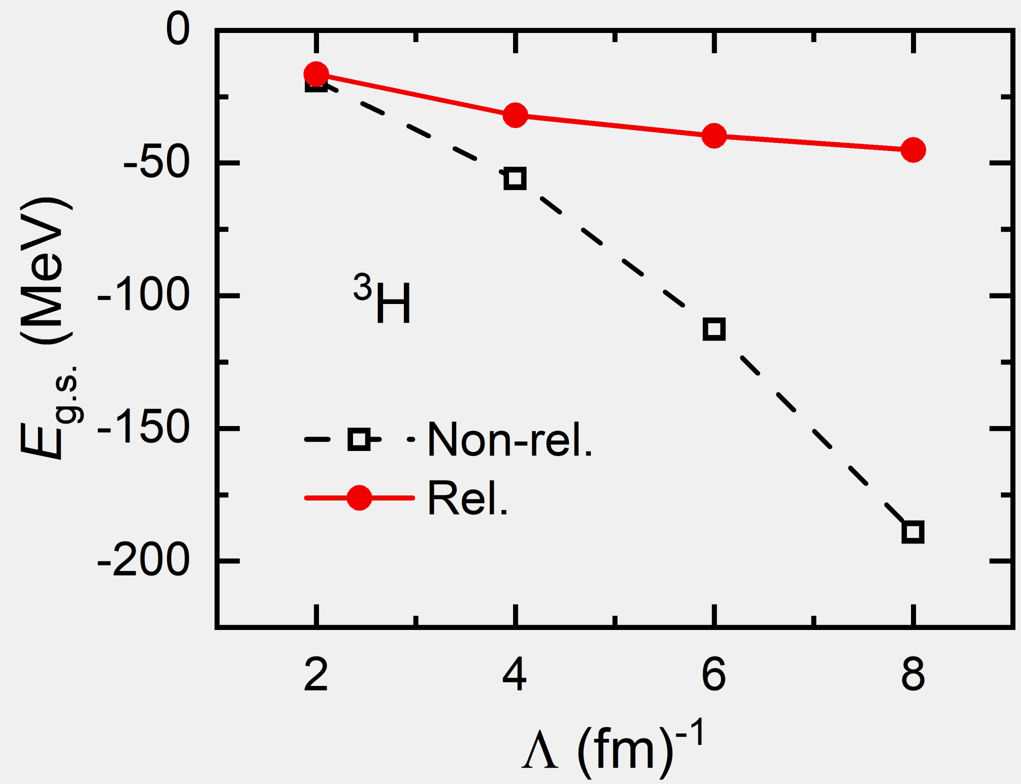
Ren and PWZ, PRC 102, 021301(R) (2020)
Editors' Suggestion

Rel. and Nonrel. VMC with LO forces

$$\left[\sum_{i=1}^{A} K_i + \sum_{i<} v(\boldsymbol{r}_{ij})\left(1 + v_t(\boldsymbol{r}_{ij}, \hat{\boldsymbol{p}}_{ij}^2) + v_b(\boldsymbol{r}_{ij}, \hat{\boldsymbol{P}}_{ij}^2)\right)\right]\Psi(\boldsymbol{R}) = E\Psi(\boldsymbol{R})$$

Nonrel Rel. corrections

Thomas collapse avoided !



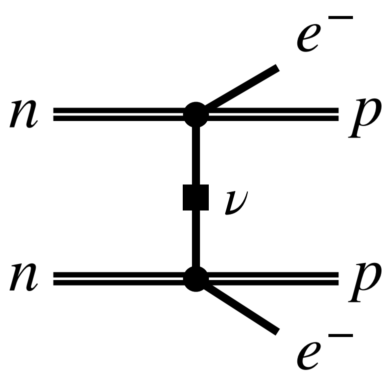
Yang and PWZ, PLB 835, 137587 (2022)

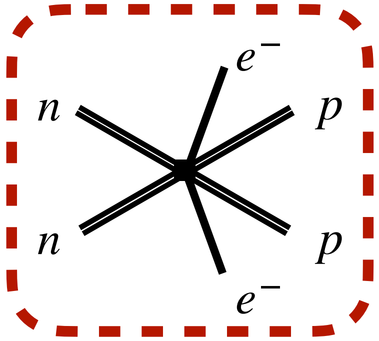
The relativity brings high-order effects …

Relativistic EFT for Neutrionless $\beta\beta$ decay

"Featured in Physics"

PRL 120, 202001 (2018); PRL 126, 172002 (2021)



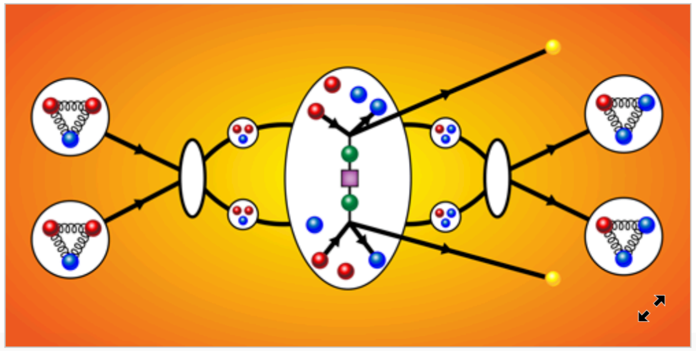


SYNOPSIS

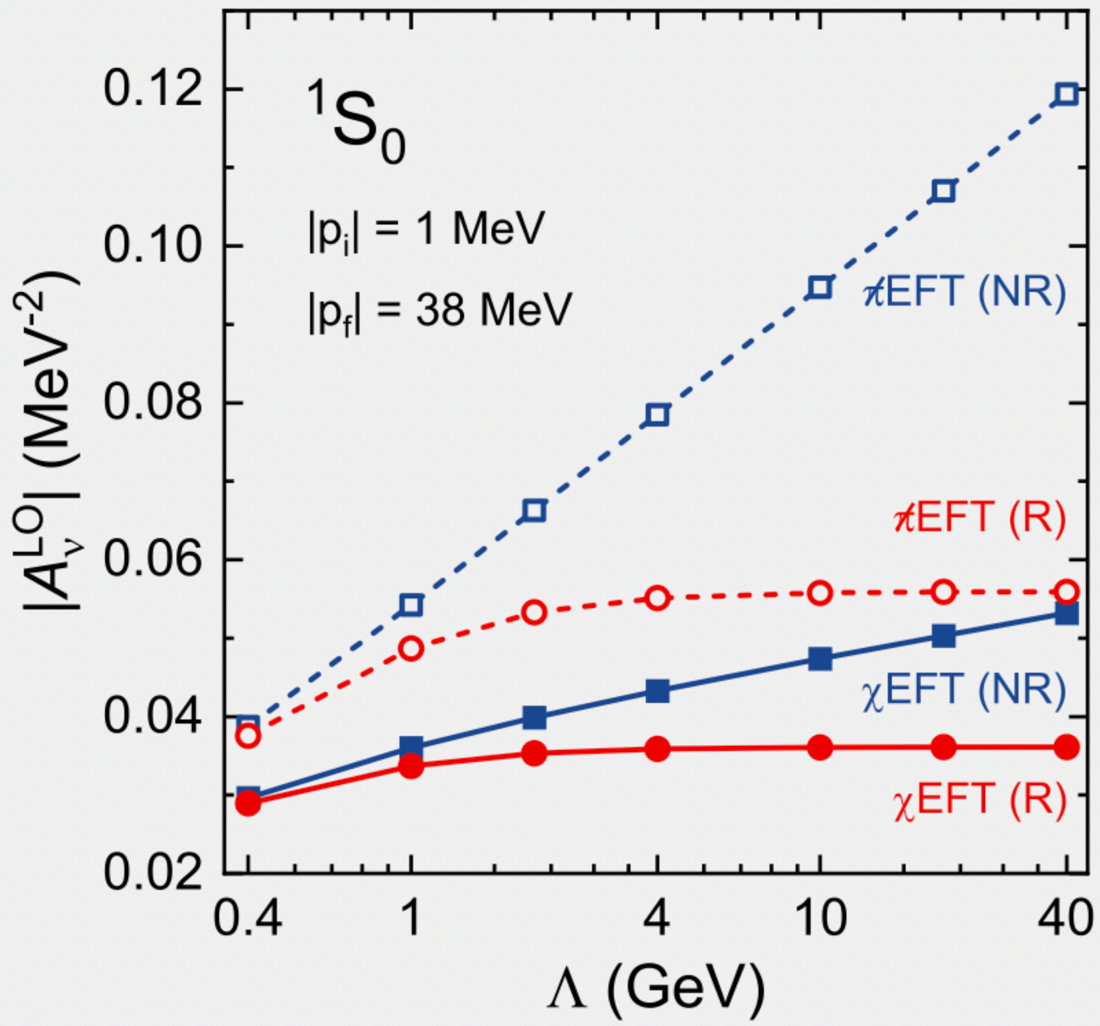
A Missing Piece in the Neutrinoless Beta-Decay Puzzle

May 16, 2018 • *Physics* 11, s58

The inclusion of short-range interactions in models of neutrinoless double-beta decay could impact the interpretation of experimental searches for the elusive decay.



Contrary to the nonrelativistic case, relativistic chiral EFT can be renormalized without promoting the N2LO contact term to LO.

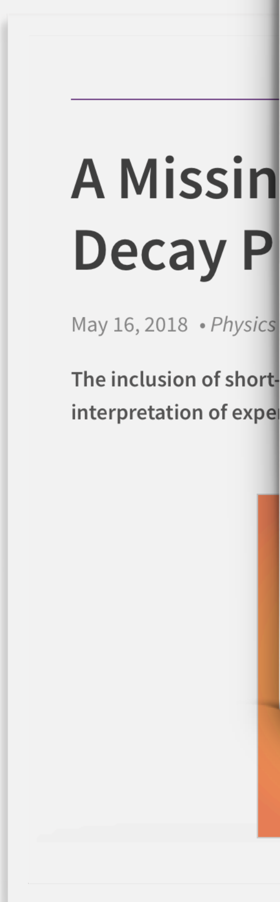


Yang and **PWZ**, PLB 855, 138782 (2024)
Yang and **PWZ**, PRL 134, 242502 (2025)

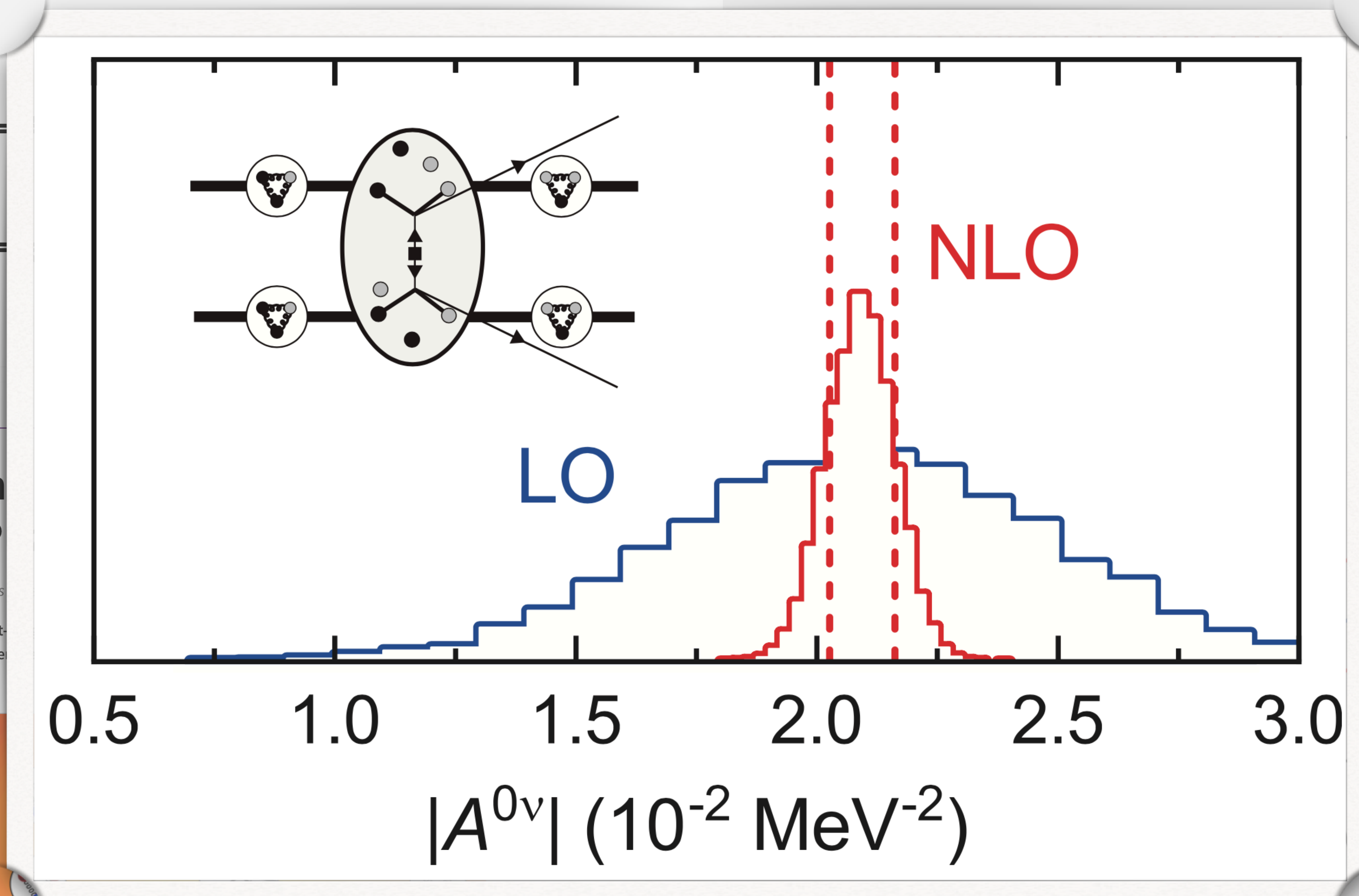
Relativistic EFT for Neutrionless $\beta\beta$ decay

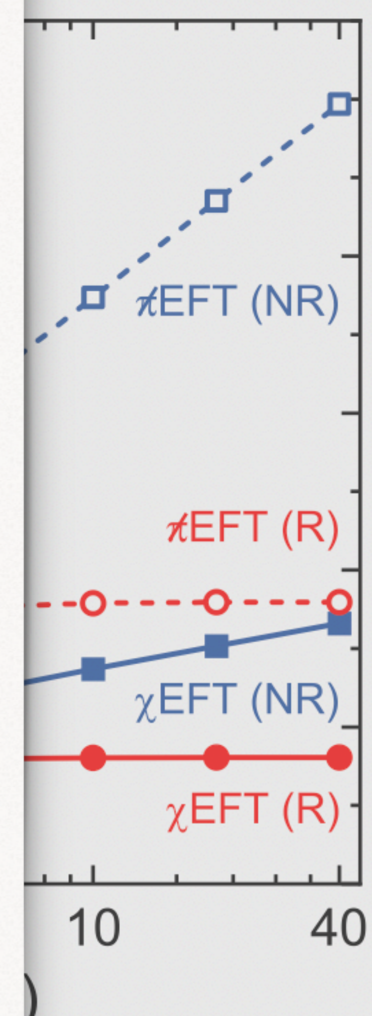
"Featured in Physics"

PRL 120, 202001 (2018); PRL 126, 172002 (2021)



Contrary to the nonrelativistic case, relativistic chiral EFT can be renormalized without promoting



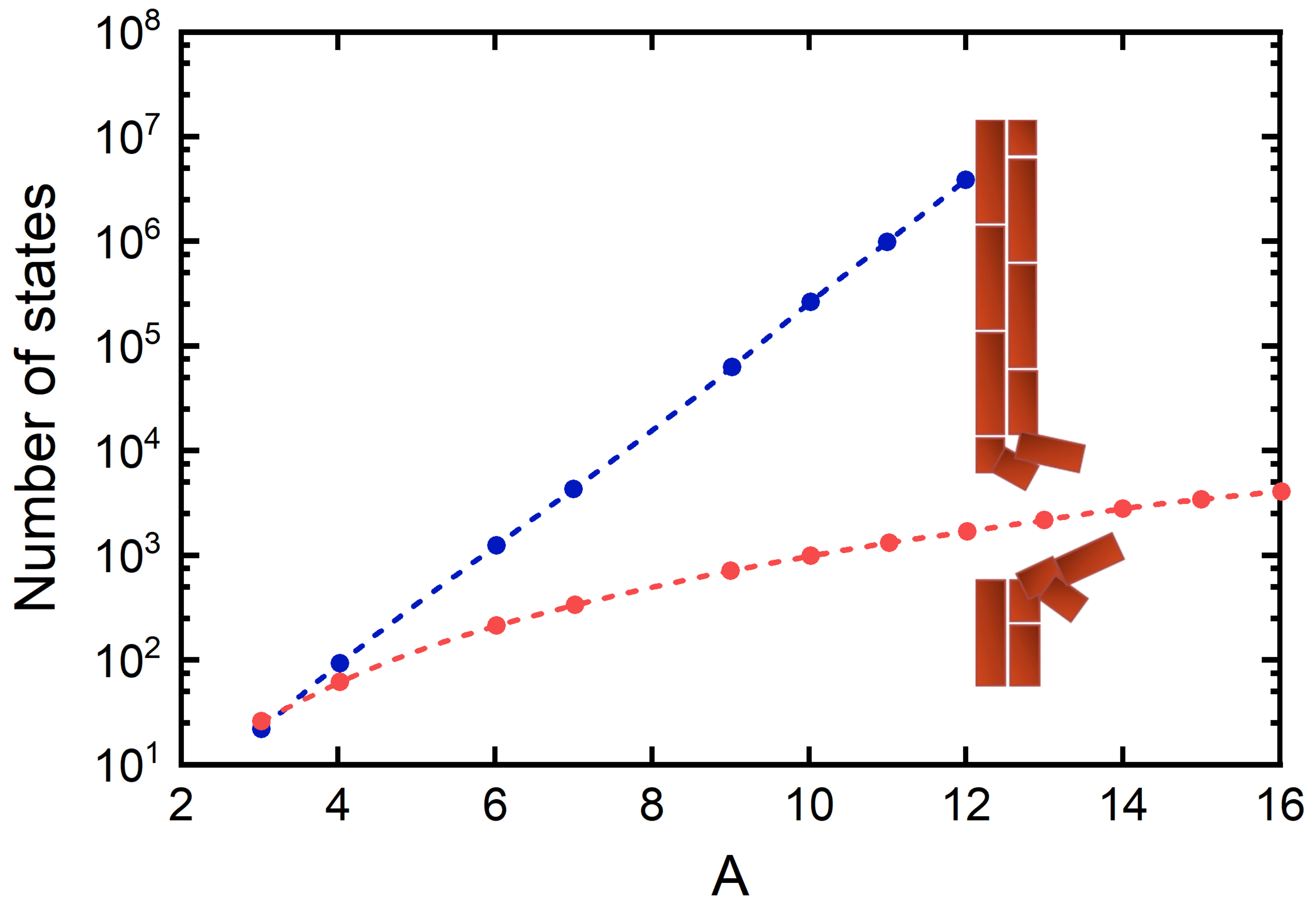


Yang and **PWZ**, PLB 855, 138782 (2024)
Yang and **PWZ**, PRL 134, 242502 (2025)

原子核第一性原理研究的挑战

维度灾难: 多体波函数维度随着核子数增加呈指数增长.

Carlson et al., Rev. Mod. Phys. 87, 1067 (2015)



Devising a polynomial scaling and accurate trial wave function ?

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Artificial Neural Networks

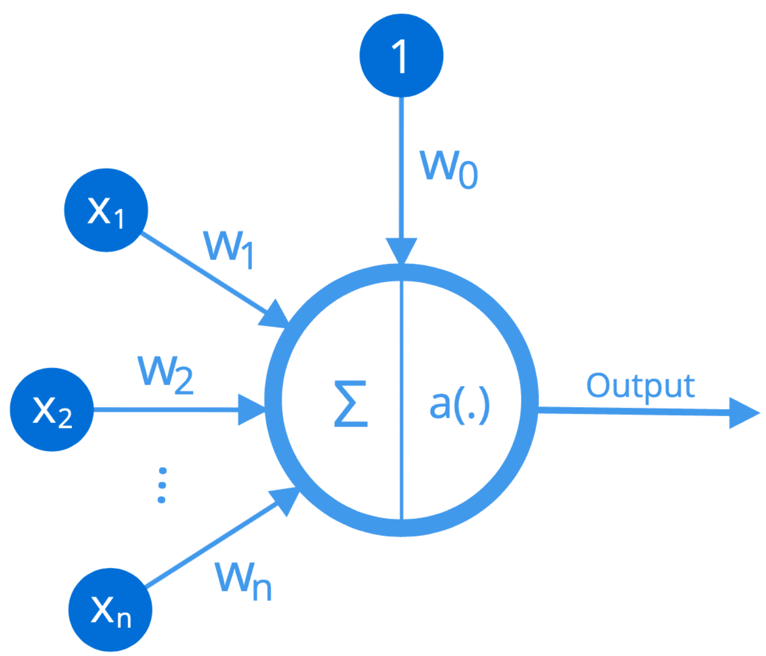
- ★ a model inspired by the human brain's neural structure.
- ★ a nested sequence of linear and non-linear functions with variable parameters.
- ★ approximate any continuous functional relationship between inputs and outputs.

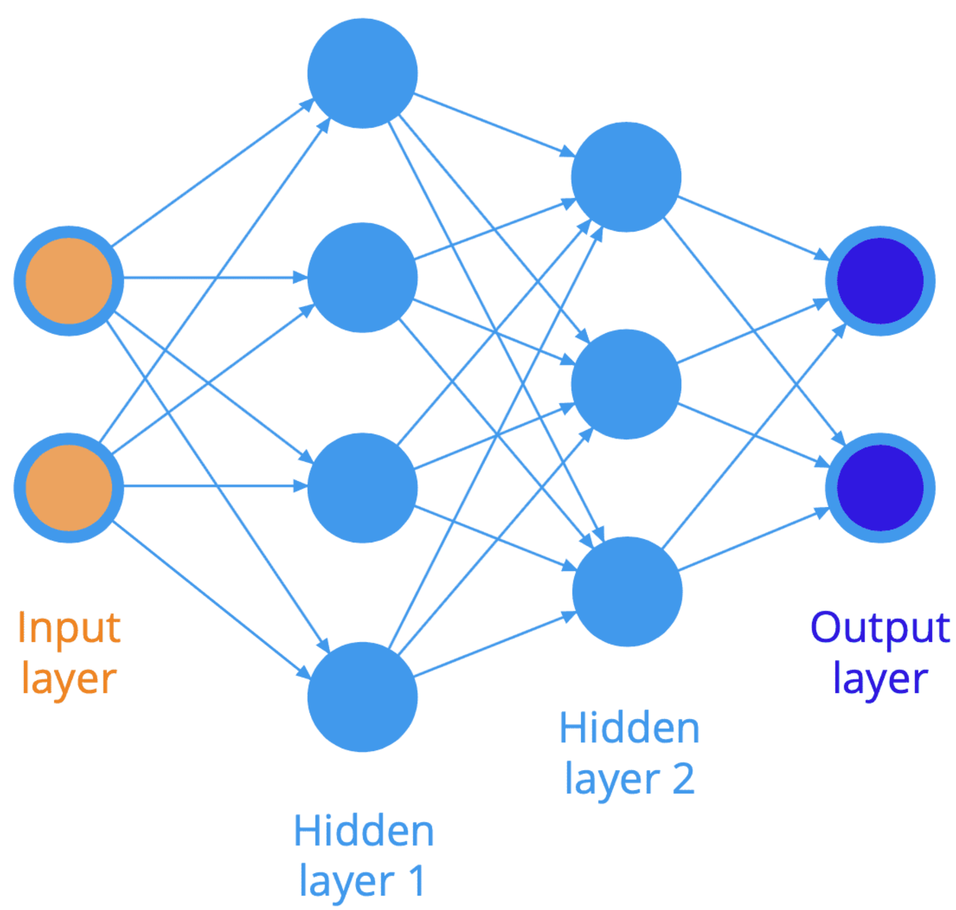
Universal Approximation Theorem: **existence / limit theorem**

a single-hidden-layer neural network can approximate any continuous function.

George Cybenko (1989); Kurt Hornik (1991)

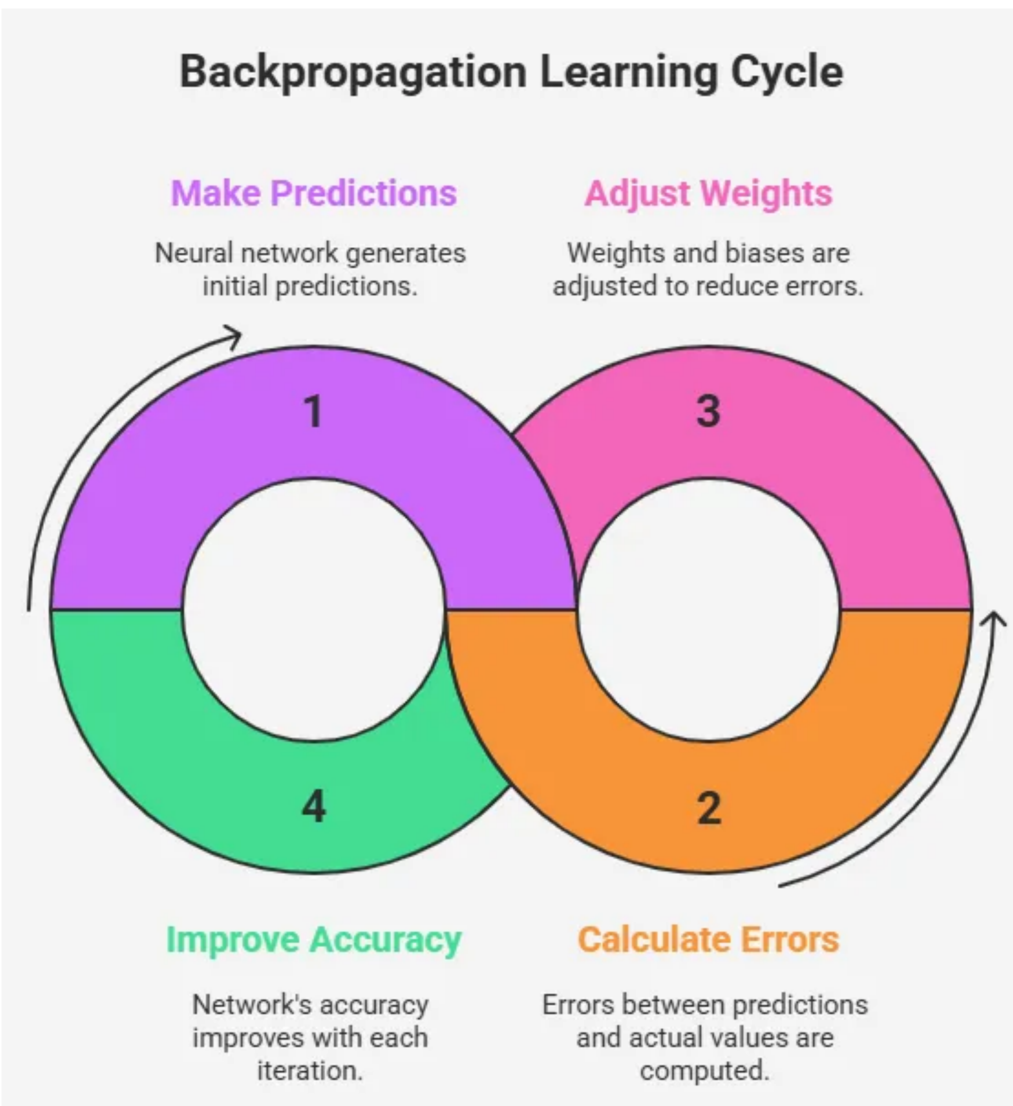
$$\text{output} = a(z) = a\left(\left(\sum_{i=1}^{n} x_i \times w_i\right) + b\right)$$

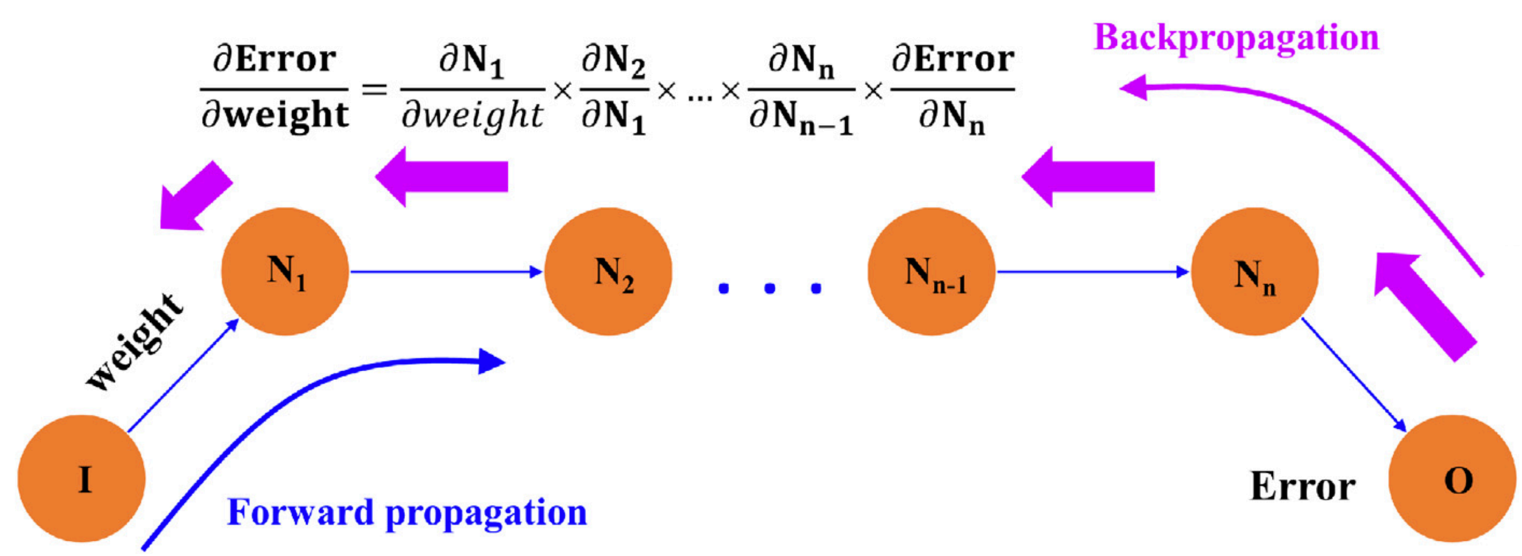




Backpropagation

- ★ To create a training mechanism for neural networks
- ★ A method minimizing the cost function by updating the weights with the gradient descent.
- ★ It's fast, simple, and easy to program

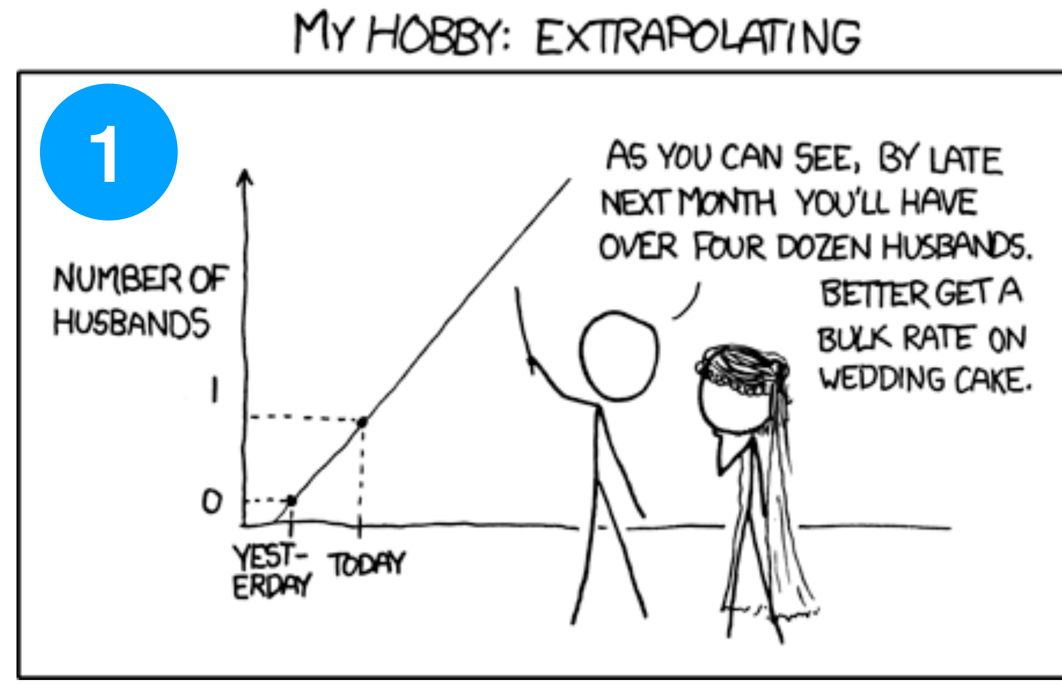


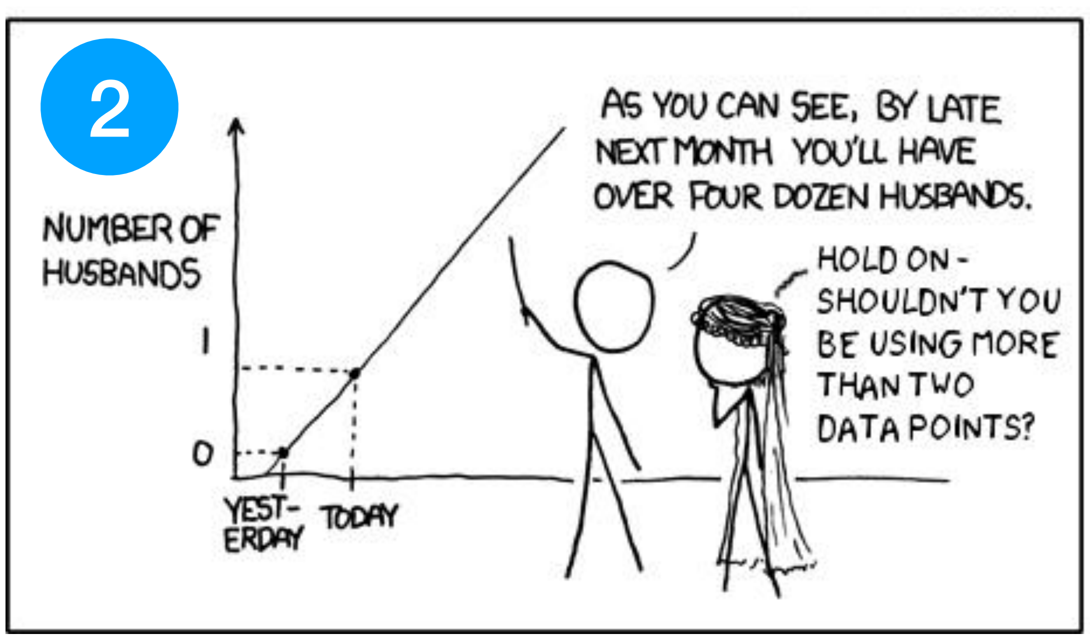


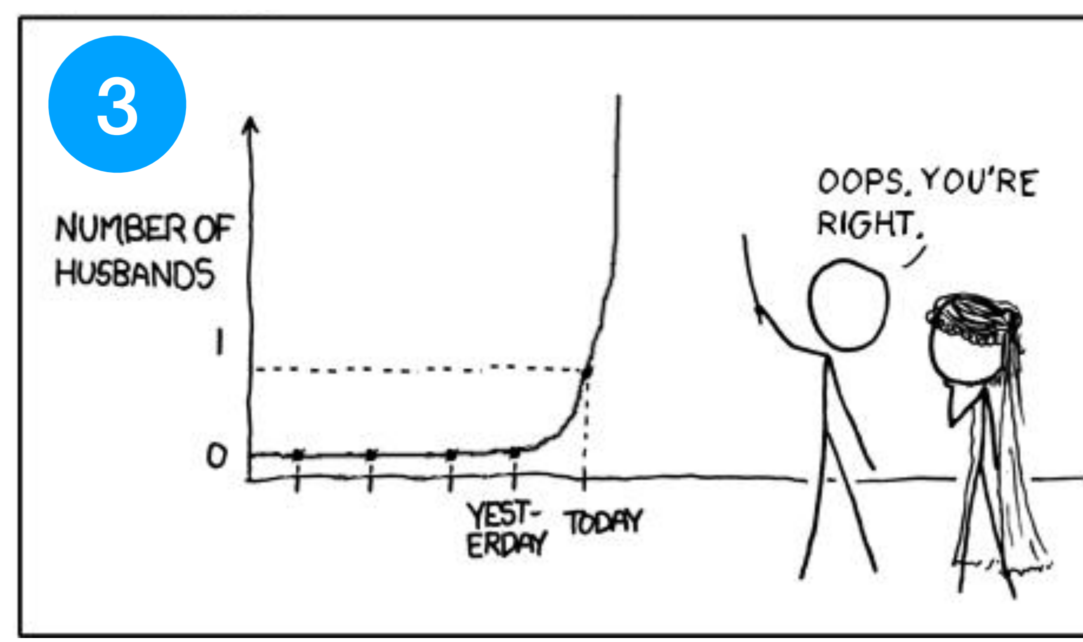
Artificial Intelligence / Idiot

★ In many cases, nuclear input requires the use of **extensive extrapolations** based on predicted quantities.

★ However, **extrapolations are not a viable option** in all instances.

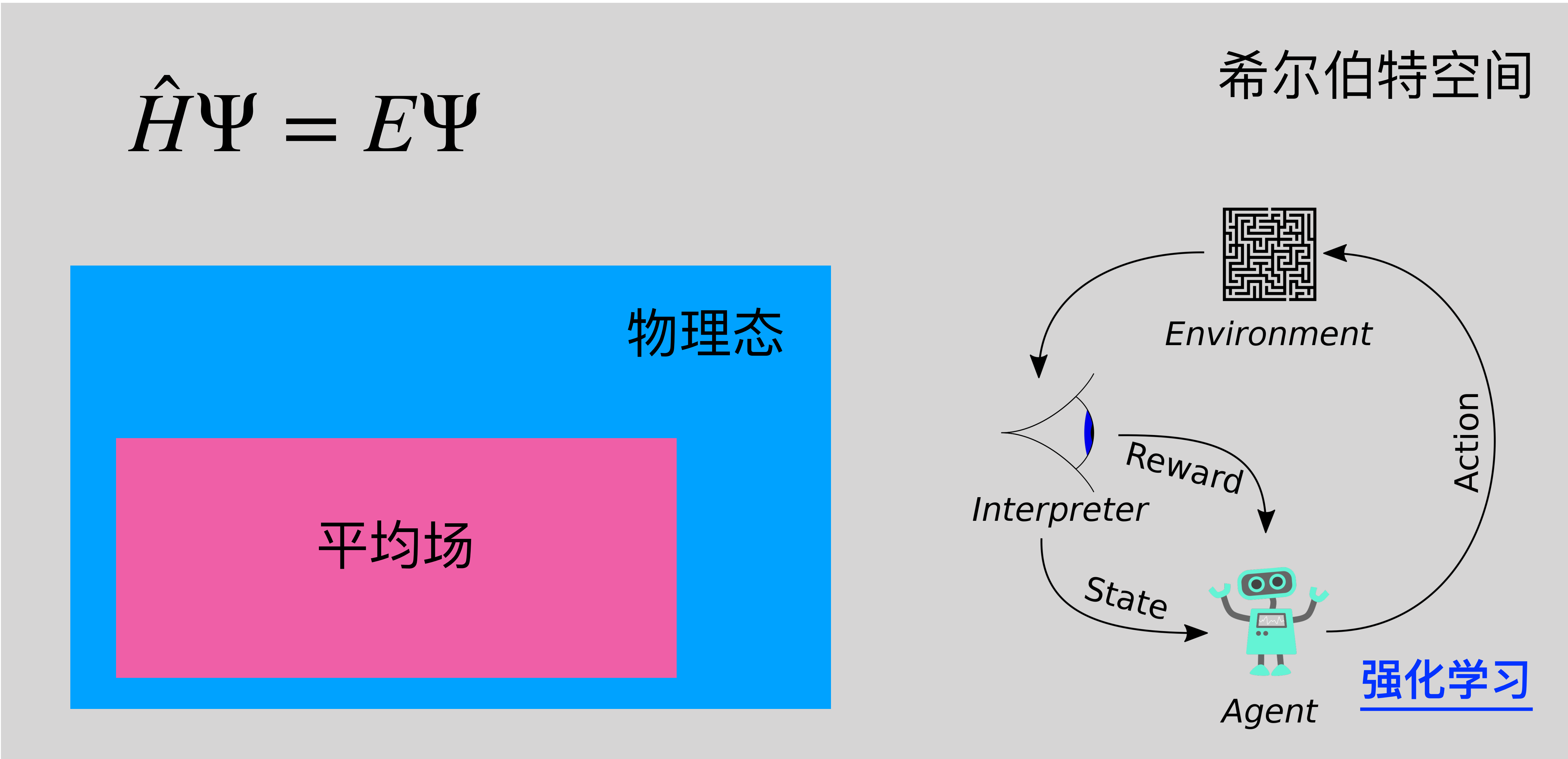






https://xkcd.com/

人工神经网络波函数



人工神经网络波函数：

以**更小代价**表示**更高精度**的薛定谔方程的解

ANN for quantum many-body problem

Carleo and Troyer, Science, **355**, 602 (2017)

RESEARCH

RESEARCH ARTICLE

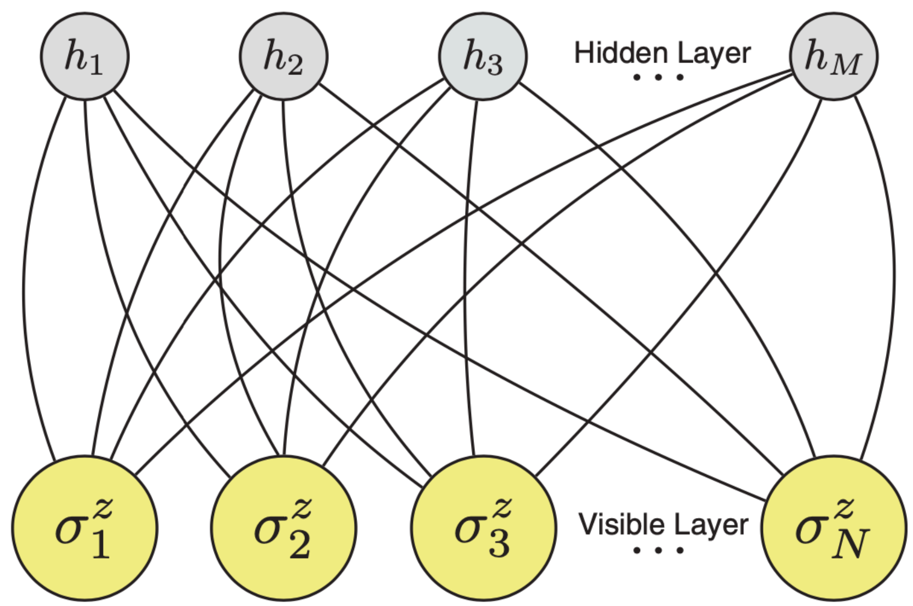
MANY-BODY PHYSICS

Solving the quantum many-body problem with artificial neural networks

Giuseppe Carleo[1*] and Matthias Troyer[1,2]

The challenge posed by the many-body problem in quantum physics originates from the difficulty of describing the nontrivial correlations encoded in the exponential complexity of the many-body wave function. Here we demonstrate that systematic machine learning of the wave function can reduce this complexity to a tractable computational form for some notable cases of physical interest. We introduce a variational representation of quantum states based on artificial neural networks with a variable number of hidden neurons. A reinforcement-learning scheme we demonstrate is capable of both finding the ground state and describing the unitary time evolution of complex interacting quantum systems. Our approach achieves high accuracy in describing prototypical interacting spins models in one and two dimensions.

$$\Psi_M(\mathcal{S};\mathcal{W}) = \sum_{\{h_i\}} e^{\sum_j a_j\sigma_j^z + \sum_i b_i h_i + \sum_{ij} W_{ij} h_i \sigma_j^z}$$



For electron systems

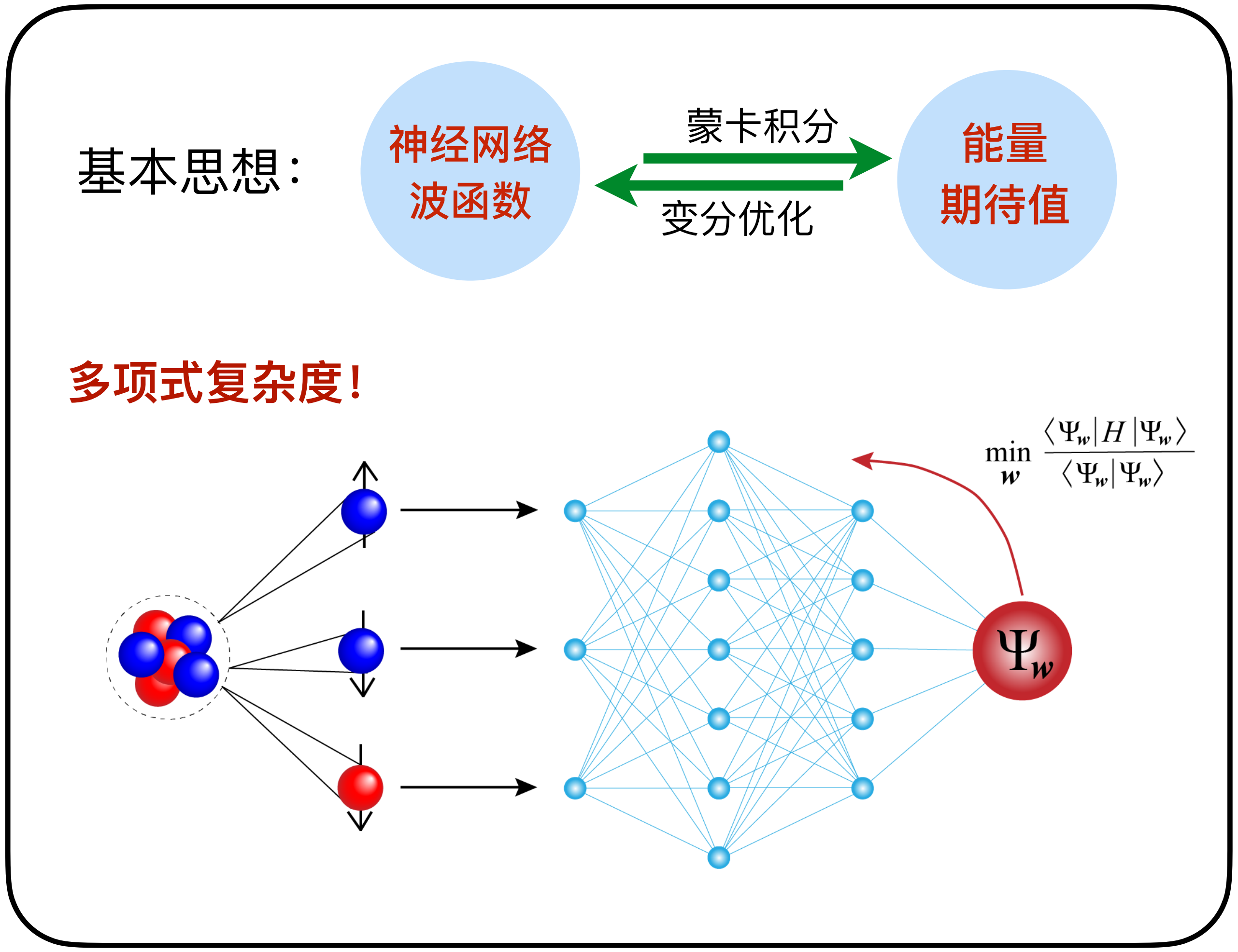
FermiNet **PauliNet**

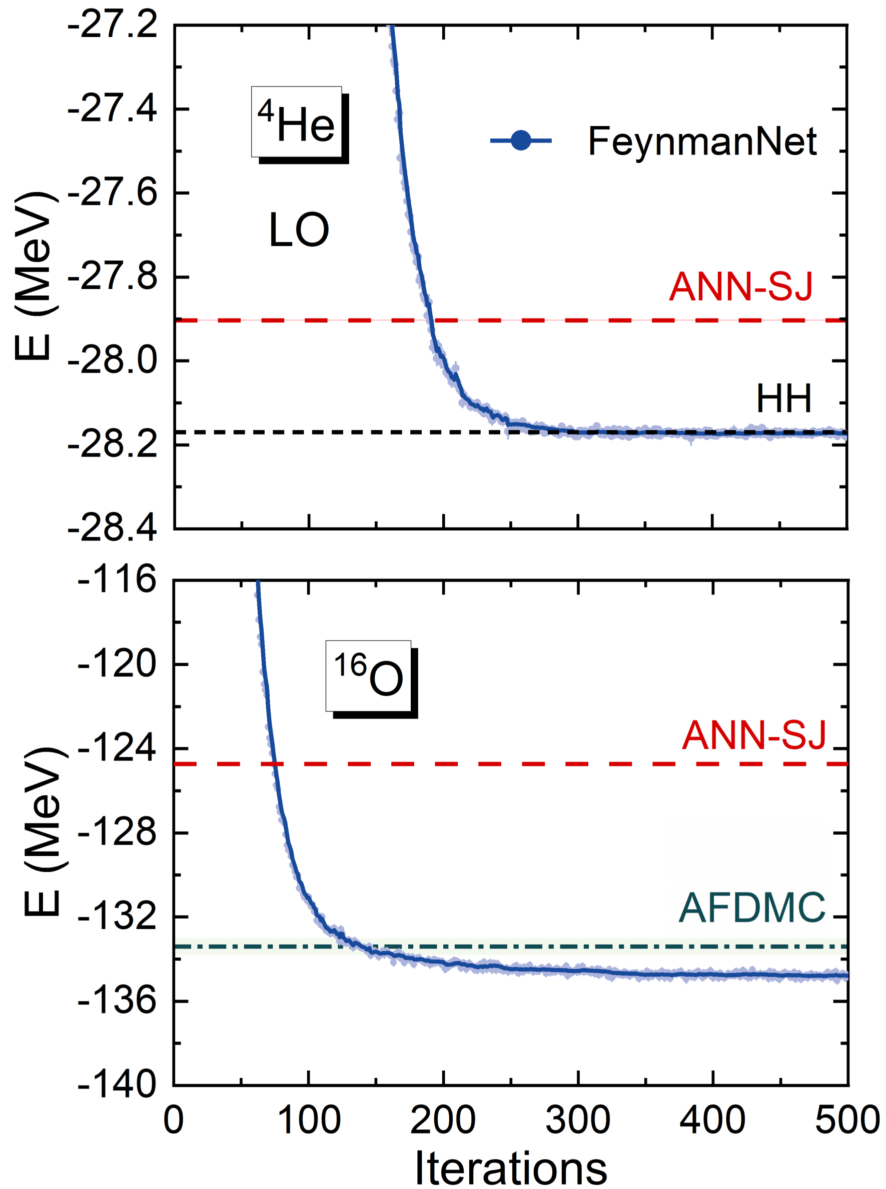
Hermann et al., Nat. Chem. 12, 891 (2020)

Pfau et al., Phys. Rev. Research 2, 033429 (2020)

基于人工神经网络求解原子核

- **FeymanNet:** 基于深度学习的原子核第一性原理计算方案。
- **FeymanNet** 提供了目前最精确的原子核神经网络波函数。





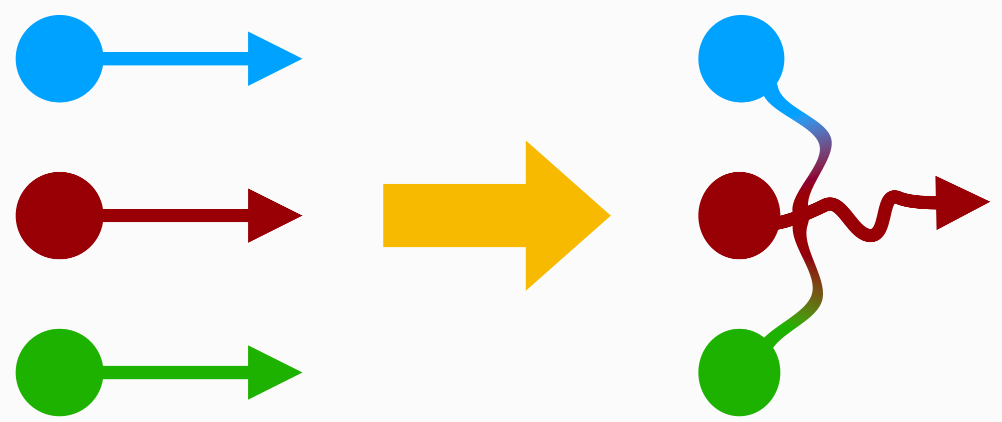
Yang and **PWZ**, PLB 835, 137587 (2022)

Yang and **PWZ**, PRC 107, 034320 (2023)

Yang, Epelbaum, Meng, Meng, **PWZ**, PRL135, 172502 (2025)

Yang and **PWZ**, PRC 107, 034320 (2023)

FeynmanNet的构造：Backflow transformation



Feynman and Cohen, Phys. Rev. 102, 1189 (1956)

$$\Psi_{\mathrm{SD}}(\boldsymbol{x}_1,\ldots,\boldsymbol{x}_N) = \det[\varphi_\mu(\boldsymbol{x}_i)]$$

★ 满足费米子交换对称性

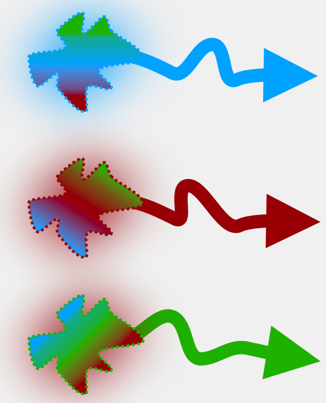
★ 坐标 $\boldsymbol{x}_i$ 为粒子 i 的位置

★ 粒子的动量只与其自身相关

★ **每个粒子的动量是“独立的”！**

$$\nabla_j \det[\varphi_\mu(\boldsymbol{x}_i)] = \det[\ldots, \nabla_j\varphi_\mu(\boldsymbol{x}_j), \ldots]$$

$$\Psi_{\mathrm{BF}}(\boldsymbol{x}_1,\ldots,\boldsymbol{x}_N) = \det[\varphi_\mu(\tilde{\boldsymbol{x}}_i)]$$



有效坐标 $\tilde{\boldsymbol{x}}_i = f(\boldsymbol{x}_i;\{\boldsymbol{x}_{/i}\})$

★ 有效坐标 $\tilde{\boldsymbol{x}}_i$ 依赖于所有粒子的位置 $\{\boldsymbol{x}_i\}$

★ **粒子的动量与所有粒子相关**

★ 当一个粒子移动时，会像液体流动一样，拖动周围的粒子“概率流”；**Backflow**

★ BF波函数包含复杂的多体关联

★ BF变换可改善波函数的 nodal surface

★ BF波函数满足费米子交换对称性

$$\nabla_j \det[\varphi_\mu(\tilde{\boldsymbol{x}}_i)] = \sum_k \det\left[\ldots, \nabla_j\varphi_\mu(\tilde{\boldsymbol{x}}_k), \ldots\right]$$

Backflow 波函数的人工神经网络表达

$\det[\varphi_\mu(\boldsymbol{x}_i)] \to \det[\varphi_\mu(\tilde{\boldsymbol{x}}_i)]$

费米子交换反对称性

- 交换任意两个粒子 $i \leftrightarrow j$，其有效坐标 $\tilde{\boldsymbol{x}}_i, \tilde{\boldsymbol{x}}_i$ 也被交换
- 要求每个 $\tilde{\boldsymbol{x}}_i$ 都以完全对称的方式依赖于所有其他粒子 **label-symmetric**
- 例如：

$$\tilde{\boldsymbol{x}}_i = \boldsymbol{x}_i + \sum_{j\neq i} \eta(x_{ji})(\boldsymbol{x}_j - \boldsymbol{x}_i)$$

神经网络波函数

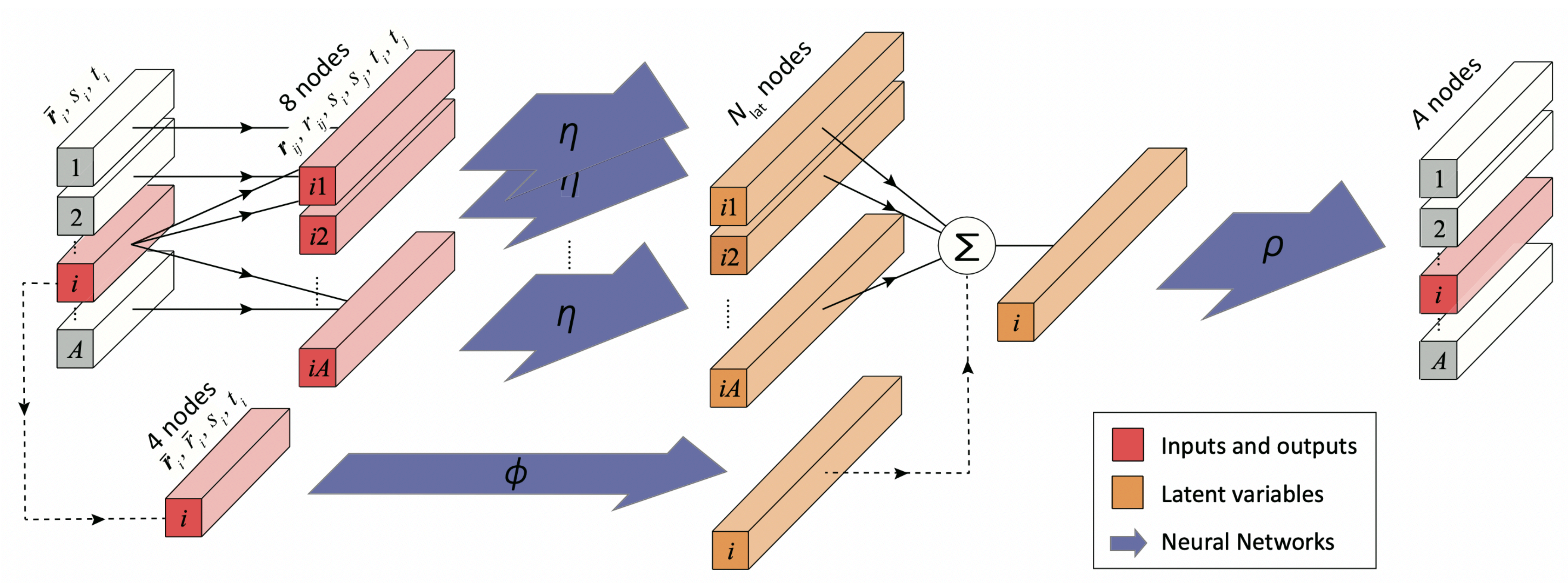
- 考虑坐标、自旋、同位旋 $\boldsymbol{x}_i = (\bar{\boldsymbol{r}}_i, s_i, t_i)$
- 用隐变量表示有效坐标：

$$\mathbf{M}_{i\mu}(\boldsymbol{x}_1, \ldots, \boldsymbol{x}_A) = \rho_\mu\left(\phi(\boldsymbol{x}_i) + \sum_{j\neq i} \eta(\boldsymbol{x}_{ij})\mathrm{e}^{-r_{ij}^2/R^2}\right), \quad \mu = 1, \ldots, A$$

Yang and PWZ, PRC, 107, 034320 (2023)

Architecture

$$\Psi_{\mathrm{BF}} = \det[\varphi_\mu(\tilde{\boldsymbol{x}}_i)] = \det[\mathbf{f}_{i\mu}] \qquad \mathbf{f}_{i\mu}(\boldsymbol{x}_1, \ldots, \boldsymbol{x}_A) = \rho_\mu\left(\phi(\boldsymbol{x}_{ii}) + \sum_{j\neq i} \eta(\boldsymbol{x}_{ij}) e^{-r_{ij}^2/R^2}\right), \quad \mu = 1, \ldots, A$$



$(1+\hat{P})\ [(1+\hat{T})]$ Spatial- [Time-] reversal symmetry

Yang and PWZ, PRC, 107, 034320 (2023)

FeynmanNet

★ **Jastrow 关联**：调整波函数在节点之间的形状，不改节点面；**振幅修正**

★ **Backflow 关联**：连续坐标变换，平滑扭曲节点面，不改节点面拓扑结构；**几何修正**

★ **多行列式叠加**：节点面之间的干涉叠加，节点重组，改变节点面拓扑结构；**拓扑修正**

$$\Psi^{(\alpha)}(\boldsymbol{x}_1,\ldots,\boldsymbol{x}_A) = \mathrm{e}^{\mathscr{U}^{(\alpha)}(\boldsymbol{x}_1,\ldots,\boldsymbol{x}_A)} \sum_n w_n \det \boldsymbol{\Phi}^{(\alpha,n)}(\boldsymbol{x}_1,\ldots,\boldsymbol{x}_A), \quad \alpha = \mathrm{R}, \mathrm{I}.$$

$$[\boldsymbol{\Phi}^{(\alpha,n)}]_{i\mu} = \mathbf{f}_{i\mu}^{(\alpha,n)}(\boldsymbol{x}_1,\ldots,\boldsymbol{x}_A)\varphi_\mu(\boldsymbol{x}_i),$$

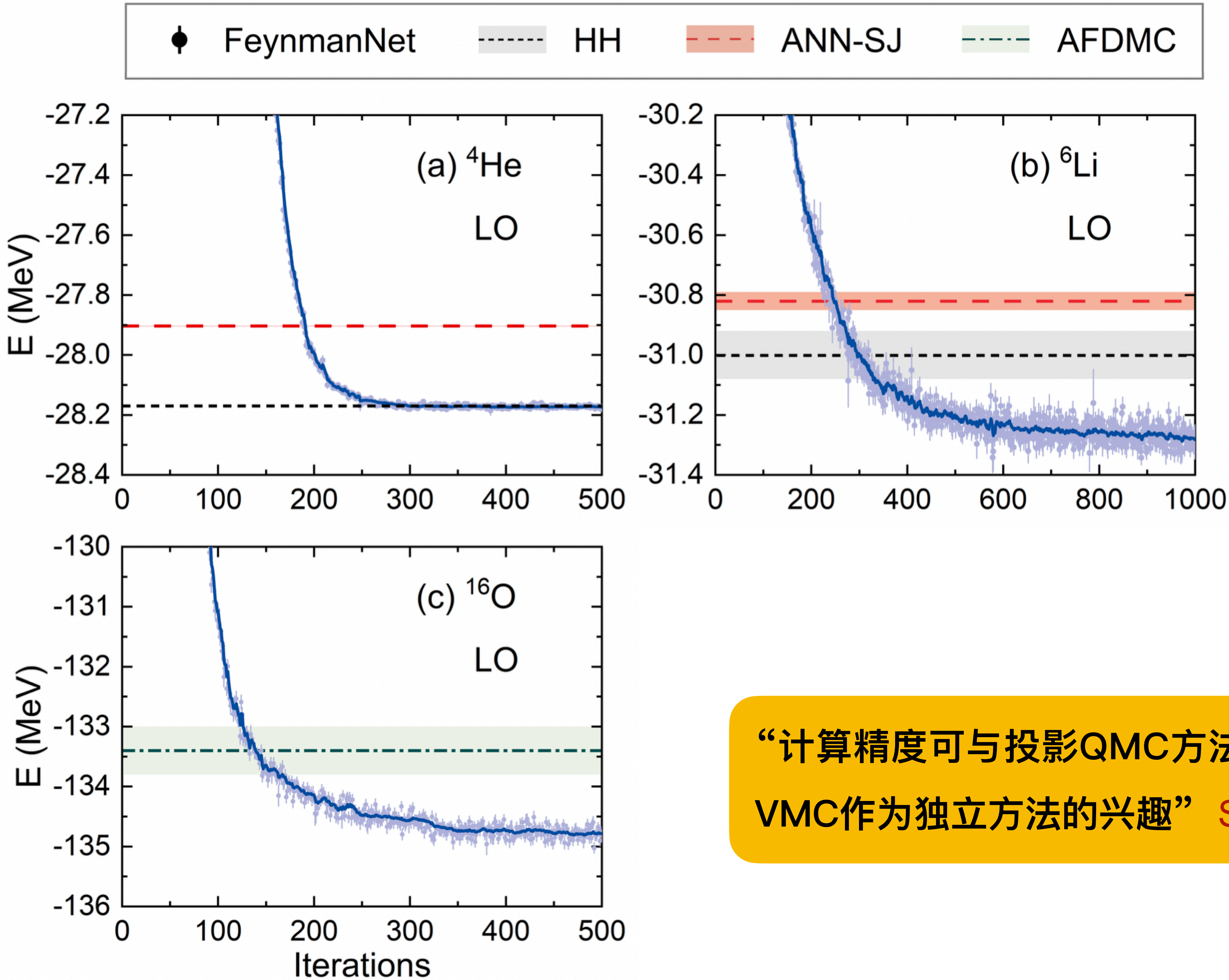
Slater 行列式：$\det \phi_{i\mu} = \det \varphi_\mu(\boldsymbol{x}_i)$

$$\Psi(\boldsymbol{x}_1,\ldots,\boldsymbol{x}_A) = \boxed{\Psi^{(\mathrm{R})}}(\boldsymbol{x}_1,\ldots,\boldsymbol{x}_A) + \mathrm{i}\boxed{\Psi^{(\mathrm{I})}}(\boldsymbol{x}_1,\ldots,\boldsymbol{x}_A)$$

<u>**Complexed valued network!**</u>

Yang and PWZ, PRC, 107, 034320 (2023)

From ^{4}He to ^{16}O



“计算精度可与投影QMC方法相媲美，重新激发了将VMC作为独立方法的兴趣” Science, **385**, 846 (2024)

FeynmanNet: Yang and PWZ, PRC, 107, 034320 (2023)

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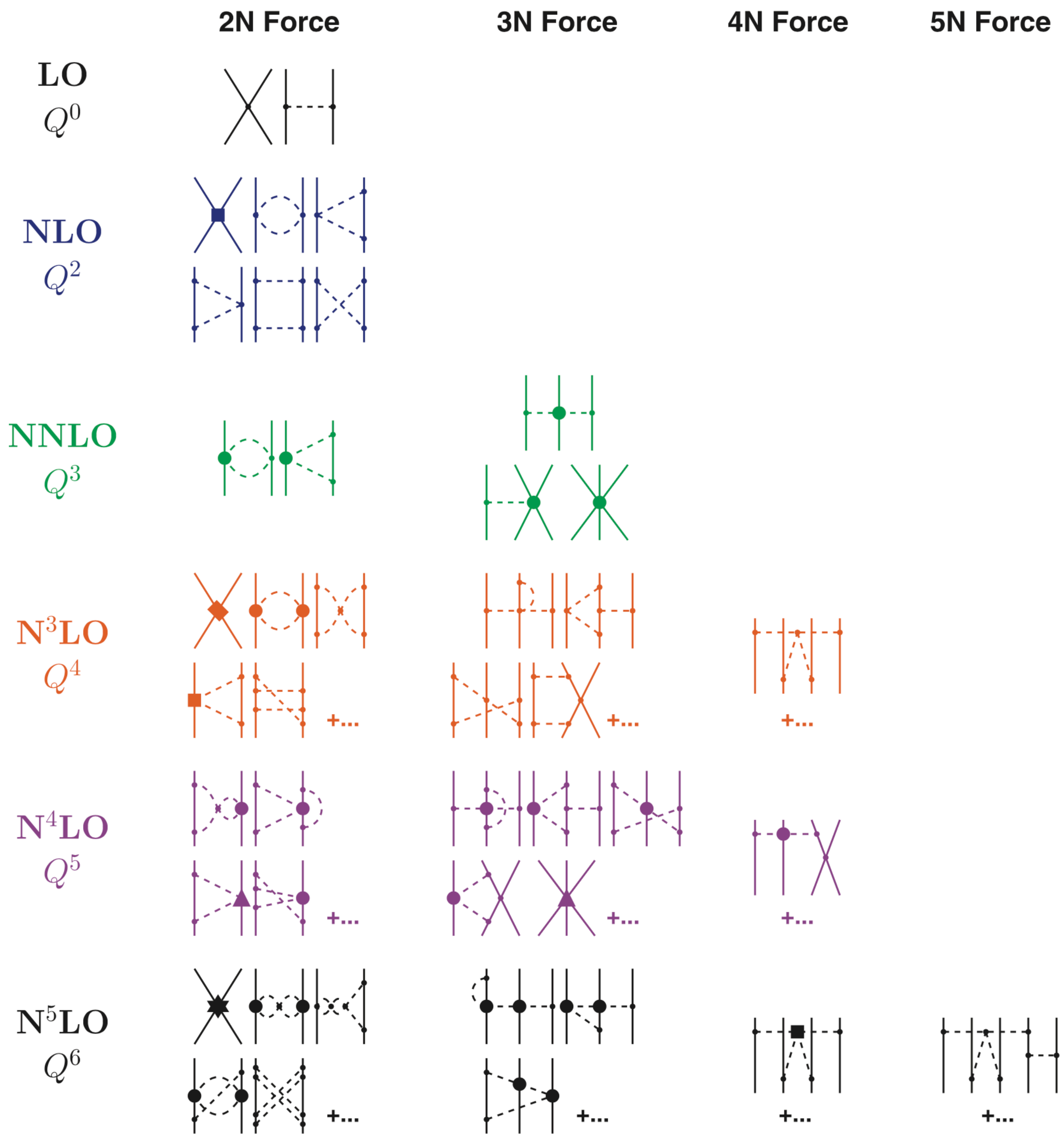
Nuclear forces based on Chiral EFT



- ✓ Attempts to connect with underlying theory (QCD)
- ✓ Systematic low-momentum expansion
- ✓ Consistent many-body forces
- ✓ Low-energy constants from experiment or lattice QCD
- ✓ Power counting's relation to renormalization still an open question

Machleidt and Sammarruca, PPNP, 137 (2024) 104117

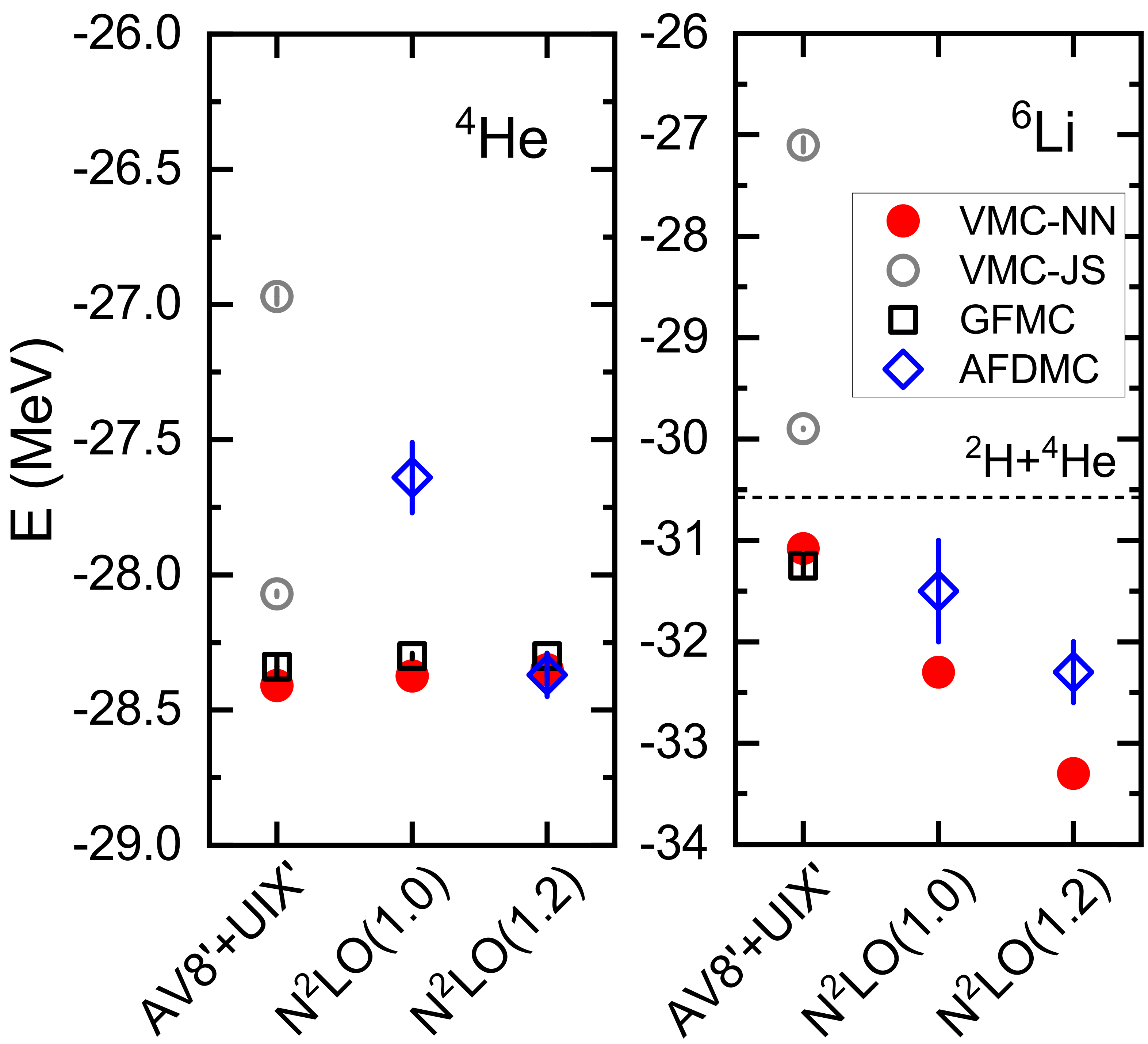
Nuclear forces based on Chiral EFT

Table 3.2
χ^2/datum for the fit of the 2016 NN data base by NN potentials at various orders of chiral EFT ($\Lambda = 500$ MeV in all cases).
Source: From Ref. [95].

T_{lab} bin (MeV)	No. of data	LO	NLO	NNLO	N^{3}LO	N^{4}LO
proton–proton						
0–100	795	520	18.9	2.28	1.18	1.09
0–190	1206	430	43.6	4.64	1.69	1.12
0–290	2132	360	70.8	7.60	2.09	1.21
neutron–proton						
0–100	1180	114	7.2	1.38	0.93	0.94
0–190	1697	96	23.1	2.29	1.10	1.06
0–290	2721	94	36.7	5.28	1.27	1.10
pp **plus** *np*						
0–100	1975	283	11.9	1.74	1.03	1.00
0–190	2903	235	31.6	3.27	1.35	1.08
0–290	4853	206	51.5	6.30	1.63	1.15

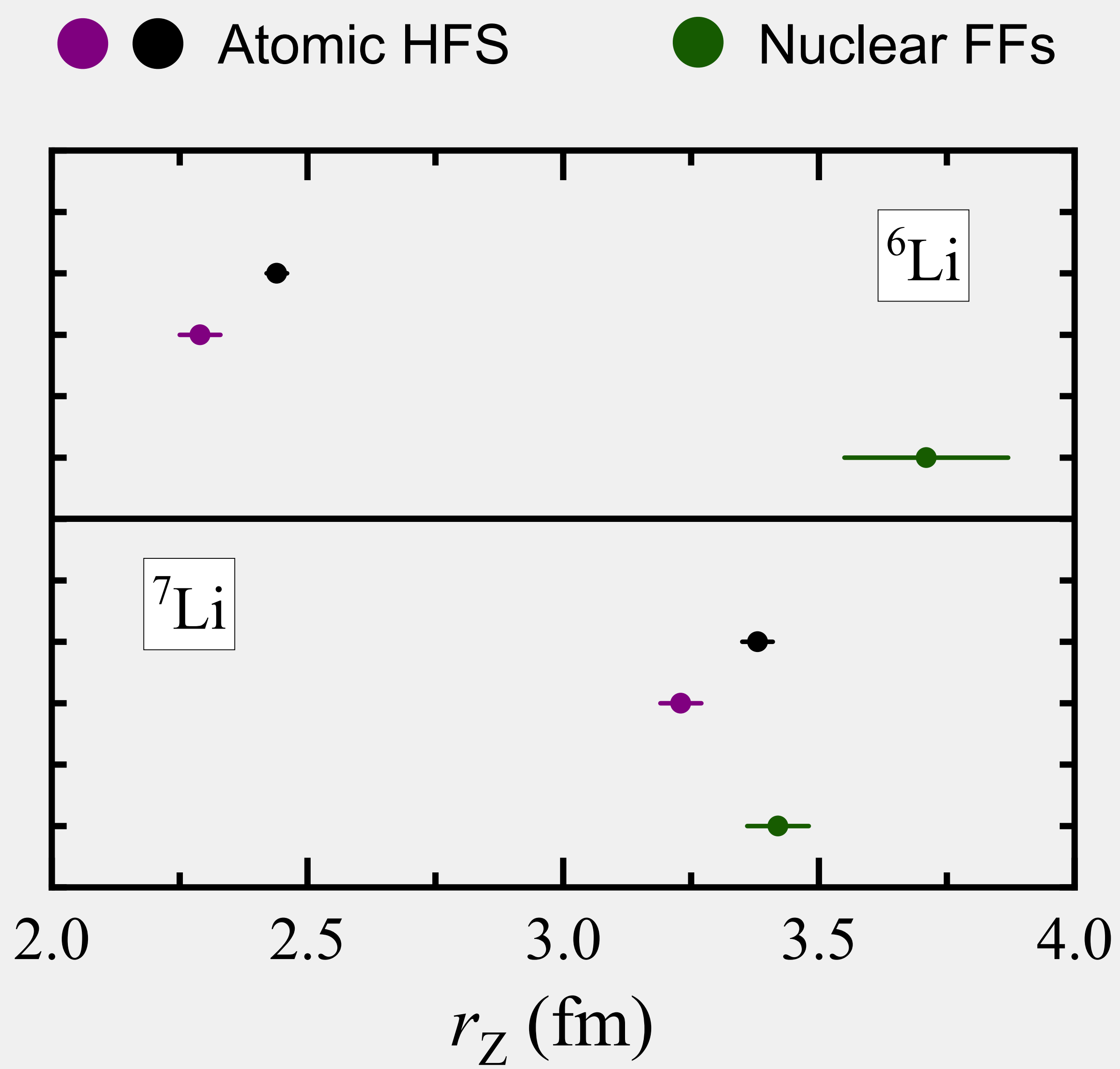
Machleidt and Sammarruca, PPNP, 137 (2024) 104117

Calculations with high-precision nuclear forces

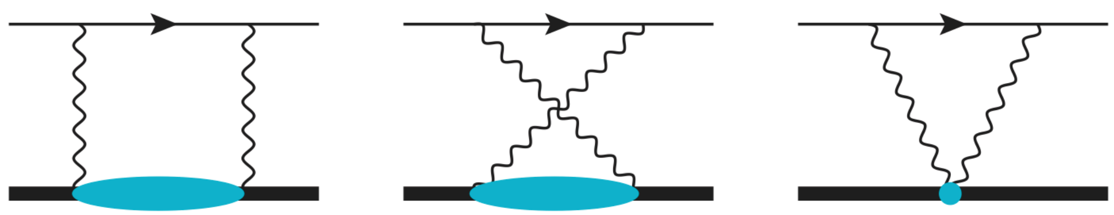


Yang, Epelbaum, Ji, **PWZ**, submitted

The puzzle of Lithium Zemach radii



$$r_Z = \int d^3r\, d^3r' \rho_E(\boldsymbol{r})\rho_M(\boldsymbol{r}')|\boldsymbol{r}' - \boldsymbol{r}|.$$



$$\delta r_{\text{pol}}(\bar{\omega}) = -\frac{1}{\mu Z}\sum_{i=1}^{A}\langle 0\,|\,\mu_i \delta r_i(\bar{\omega})\sigma_{zi}\,|\,0\rangle$$

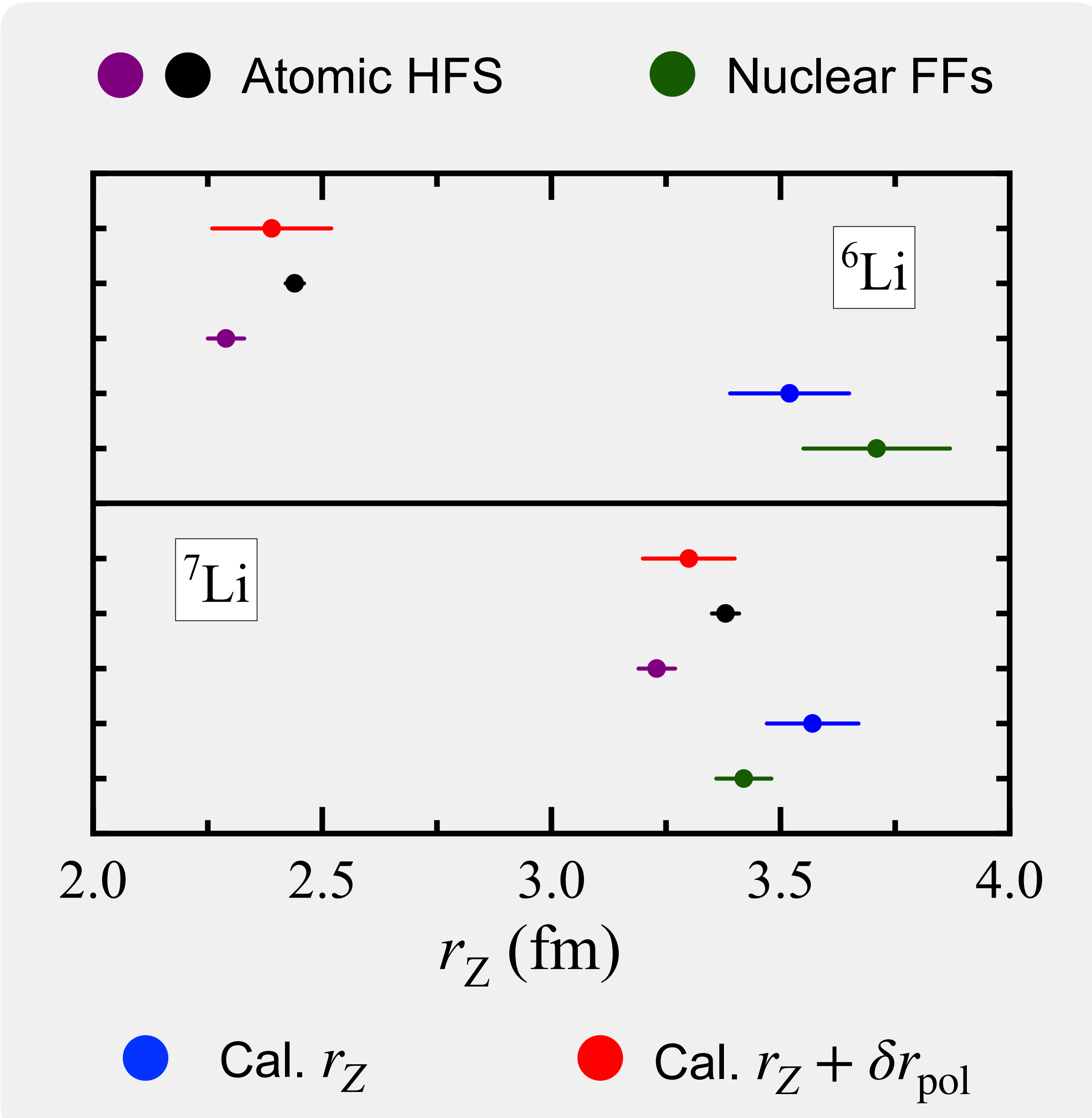
$$\simeq \begin{cases} -\dfrac{1}{Z}\dfrac{\mu_p}{\mu_p+\mu_n}\delta r_p(\bar{\omega}) & \text{odd-odd} \\ -\dfrac{1}{Z}\delta r_p(\bar{\omega}) & \text{odd-even} \\ 0 & \text{even-odd} \end{cases}$$

$\mu_p = 2.793\mu_N \quad \mu_n = -1.913\mu_N$

Nuclear polarizability: the dominant source for solving the puzzle

Yang, Epelbaum, Ji, **PWZ**, submitted

The puzzle of Lithium Zemach radii



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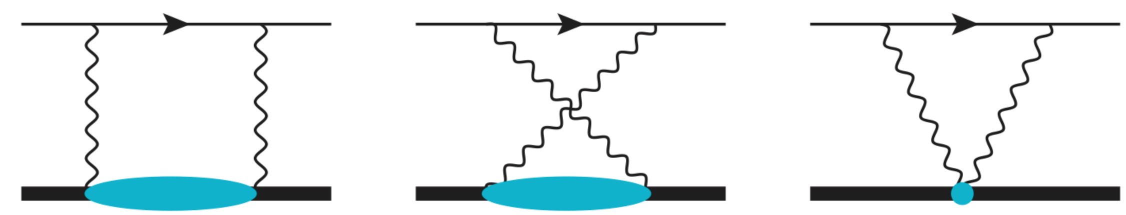

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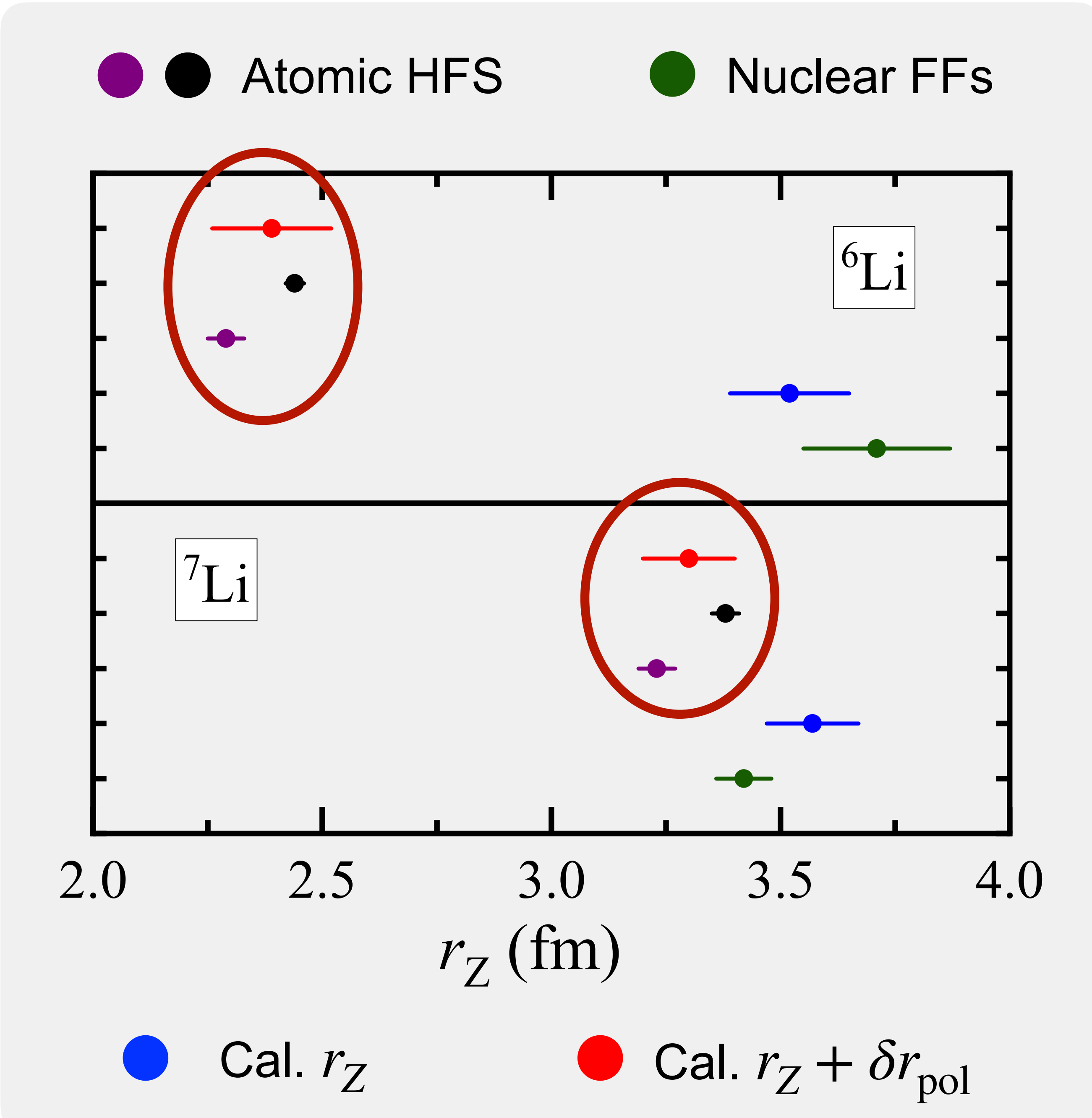

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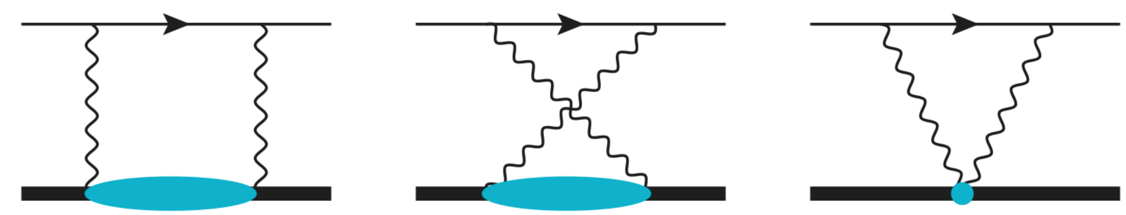

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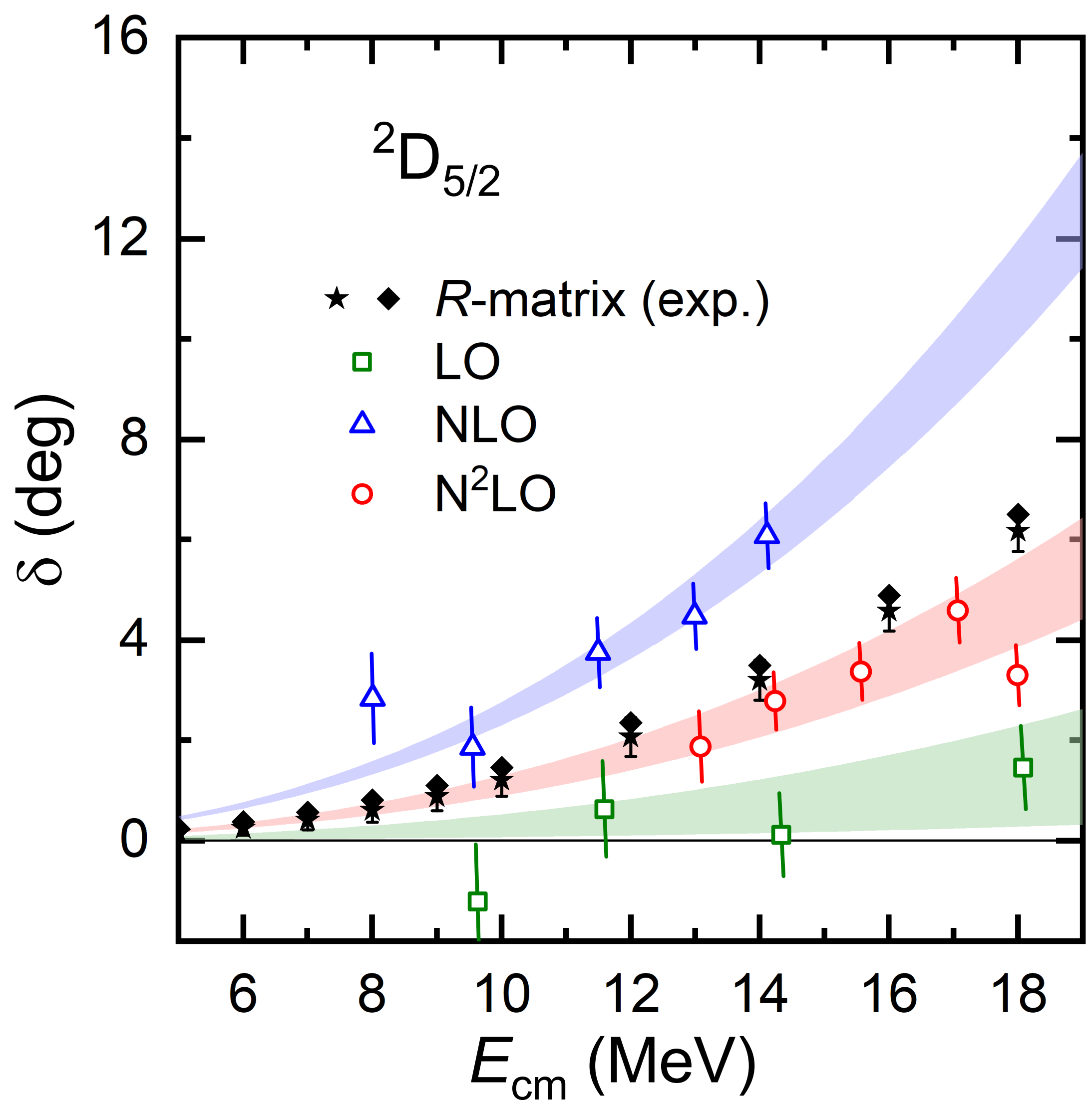
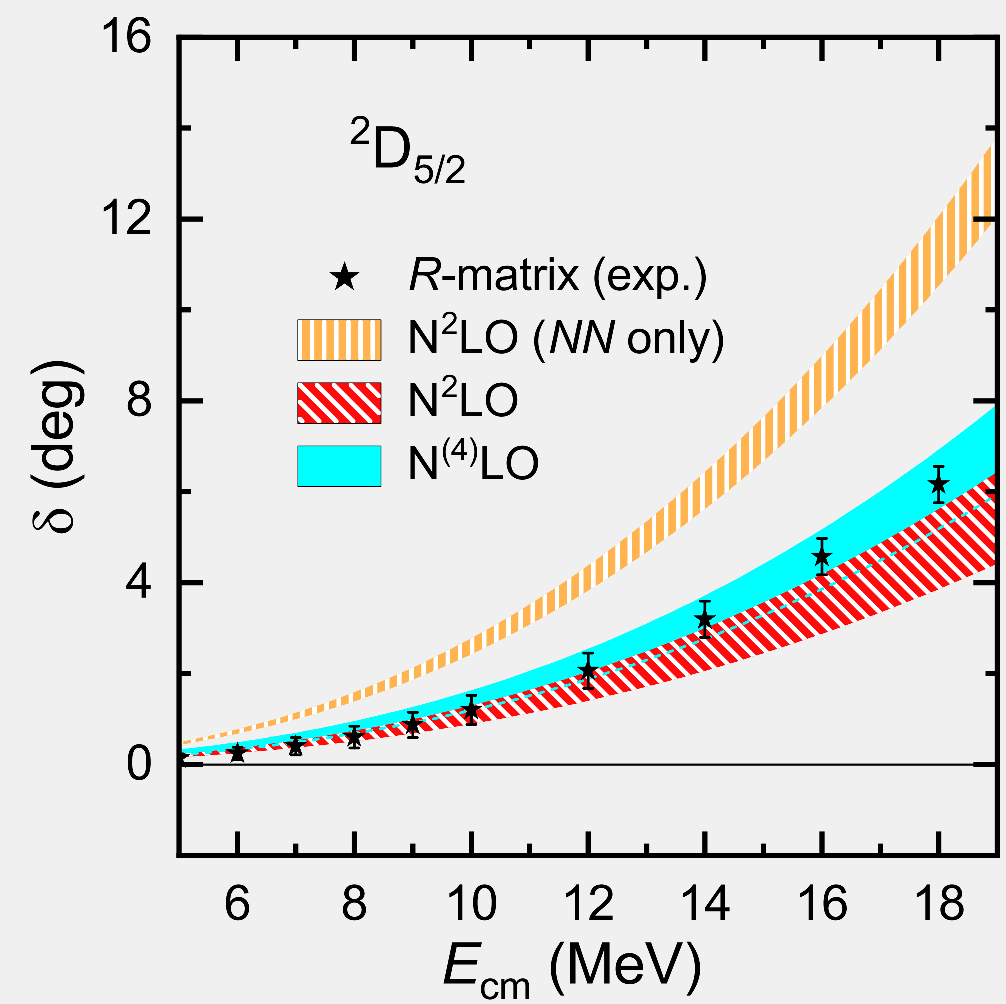
Peripheral neutron-alpha scattering

Experimentally probe the large-distance behavior of the **3N forces** governed by the chiral symmetry of QCD ?





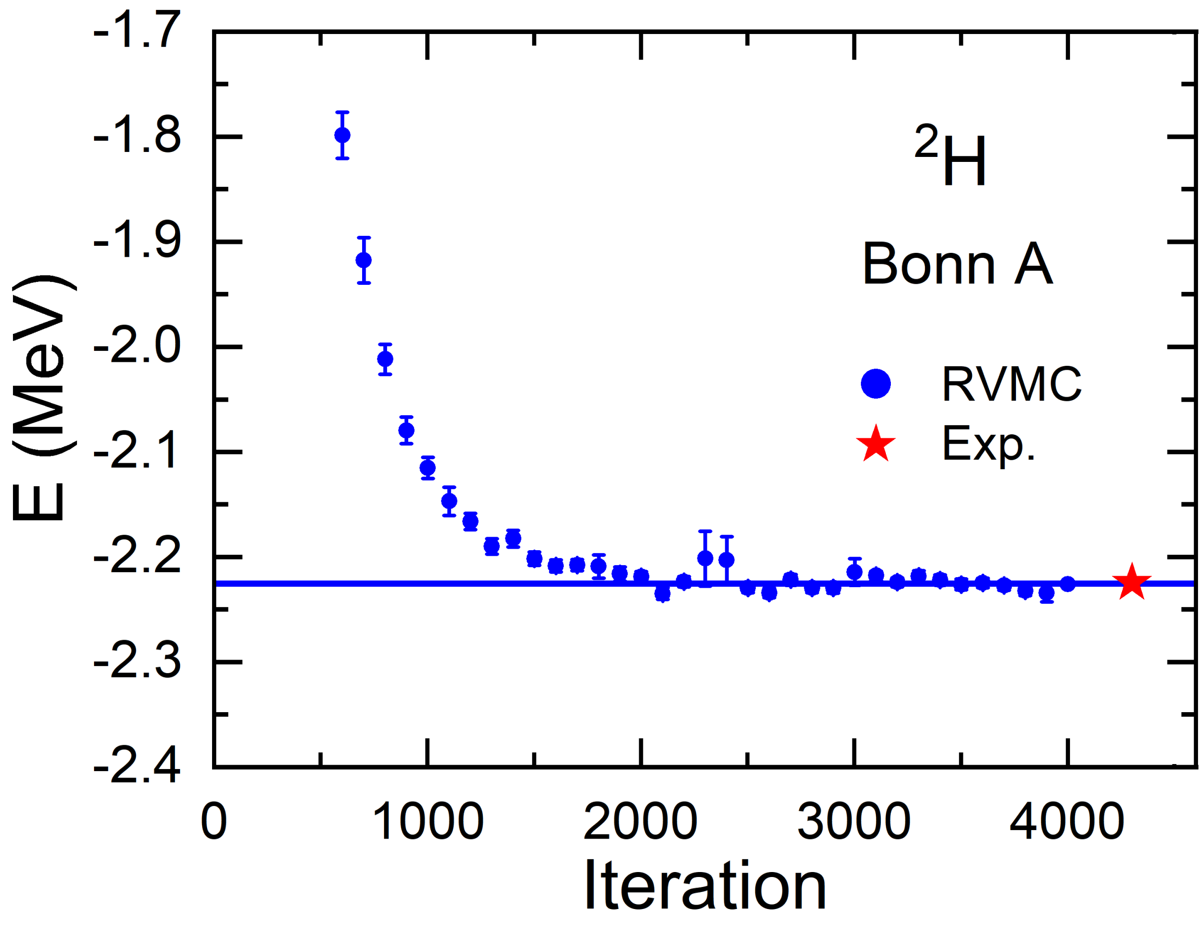
Yang, Epelbaum, Meng, Meng, **PWZ**, PRL135(2025)172502

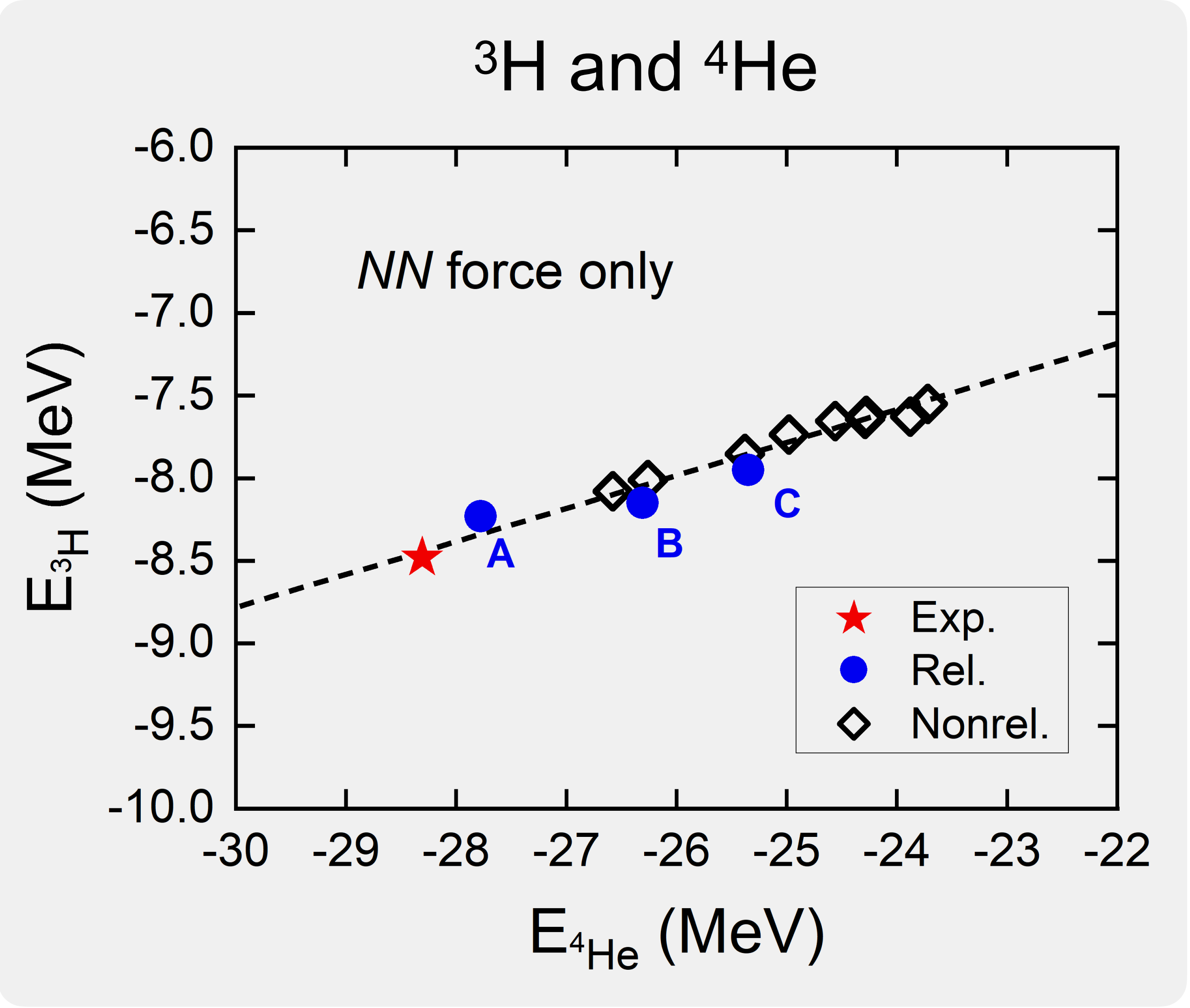
✓ A **sensitive and clean probe** of the long-range 3N forces!

✓ A **highly nontrivial test** of chiral EFT in the few-nucleon sector!

Relativistic calculations with realistic forces

Relativistic results **improve the underbinding** of light nuclei without 3N forces.



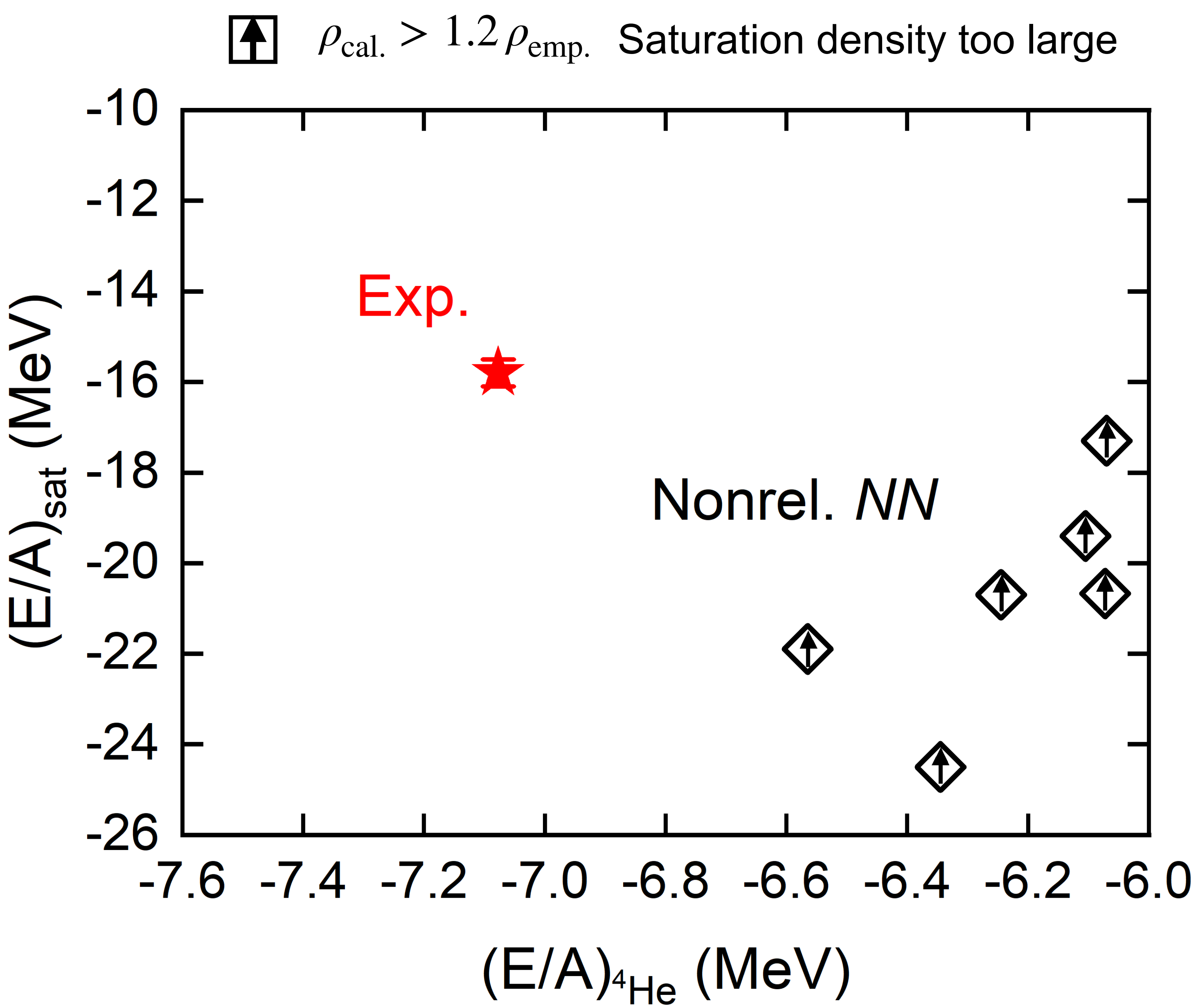


Yang and **PWZ**, CPL, 42 051201 (2025) "Express Letter"

Nonrel. calculations with AV18, CD-Bonn, Nijmegen I, II, Chiral forces

From light nuclei to nuclear matter

Yang, **PWZ**, CPL, 42 051201 (2025) “Express Letter”



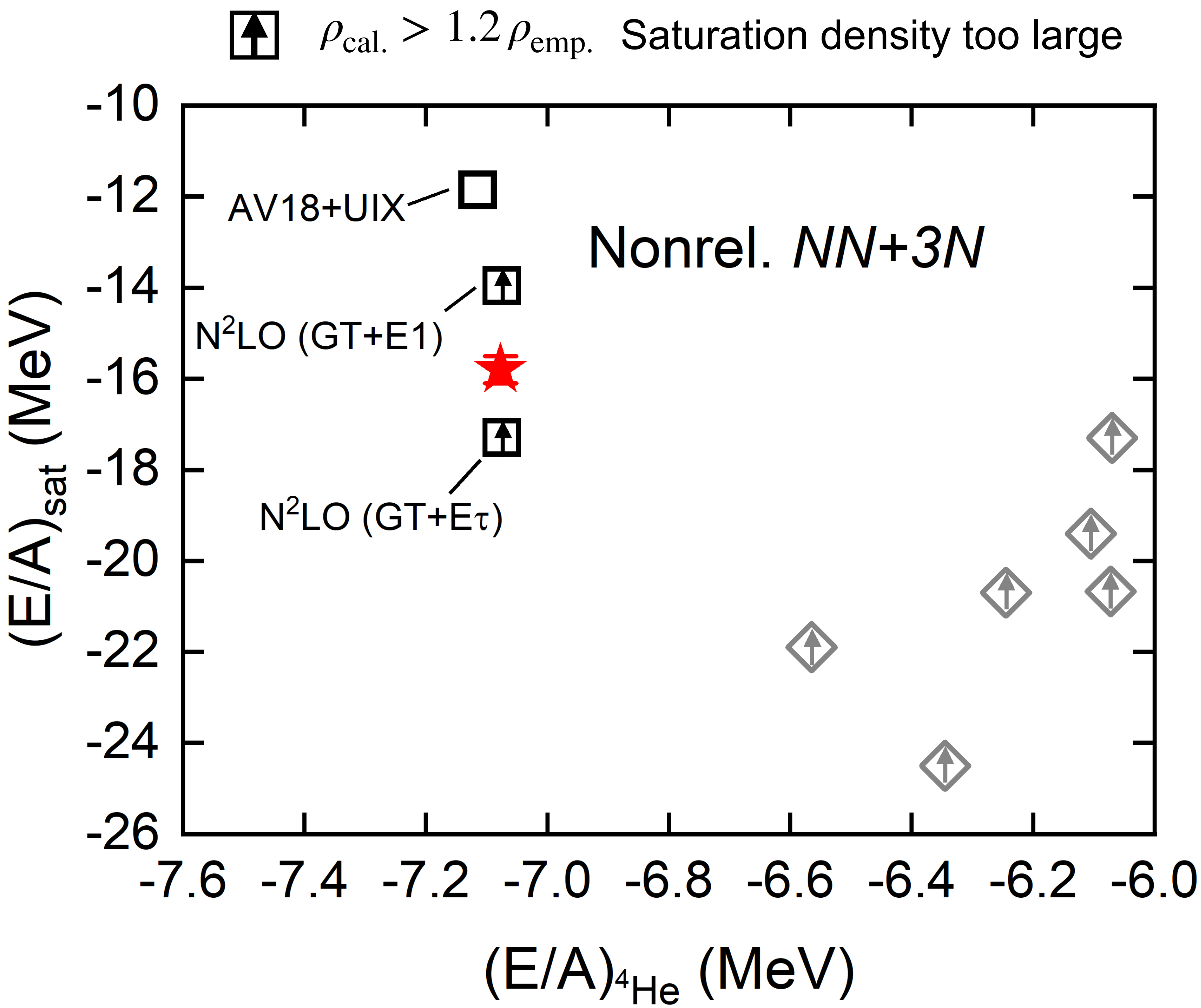
^{4}He	Nucl. Matt.

NN	Underbind	Overbind

RBHF nuclear matter: from Wang, Zhao, Ring, Meng, PRC 103, 054319 (2021)

From light nuclei to nuclear matter

Yang, **PWZ**, CPL, 42 051201 (2025) "Express Letter"



	^{4}He	Nucl. Matt.
NN	Underbind	Overbind
NN/3N	Fit	Diverse

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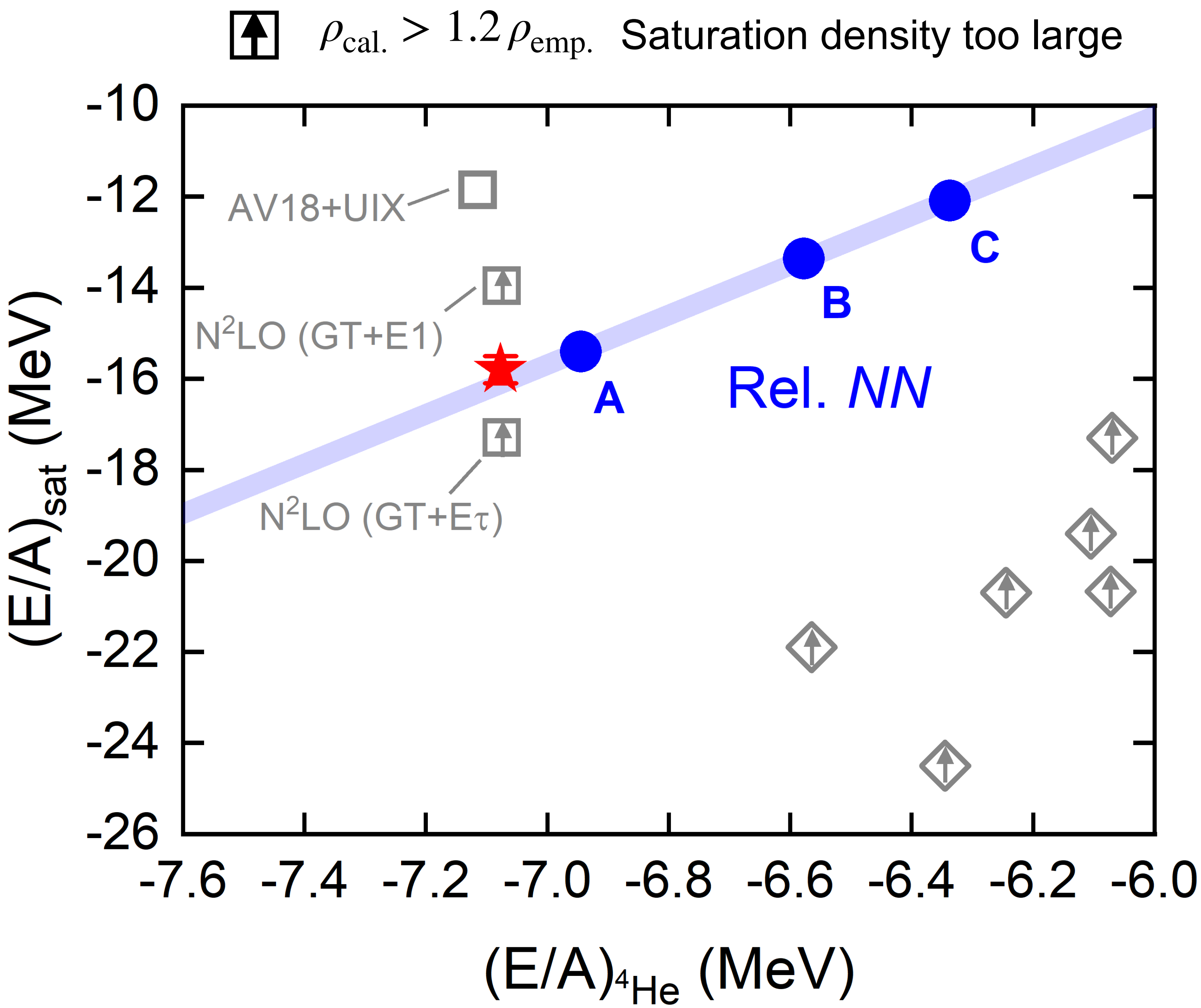


	^{4}He	Nucl. Matt.
NN	Underbind	Overbind
NN/3N	Fit	Diverse
Rel.	**Consistent !**	

RBHF nuclear matter: from Wang, Zhao, Ring, Meng, PRC 103, 054319 (2021)

Outline

- 原子核第一性原理计算及其挑战
- 基于人工神经网络的量子多体波函数
- 基于人工智能的原子核第一性原理研究
- 总结与展望

Summary

Machine learning has been applied to solve the *ab initio* nuclear many-body problem.

- **FeynmanNet** Deep neural-network representation of variational wave functions

  Among the most accurate; polynomial scaling with A

- The puzzle of Lithium Zemach radii

  Nuclear polarizability is the dominant source for solving the puzzle

- Peripheral neutron-alpha scattering

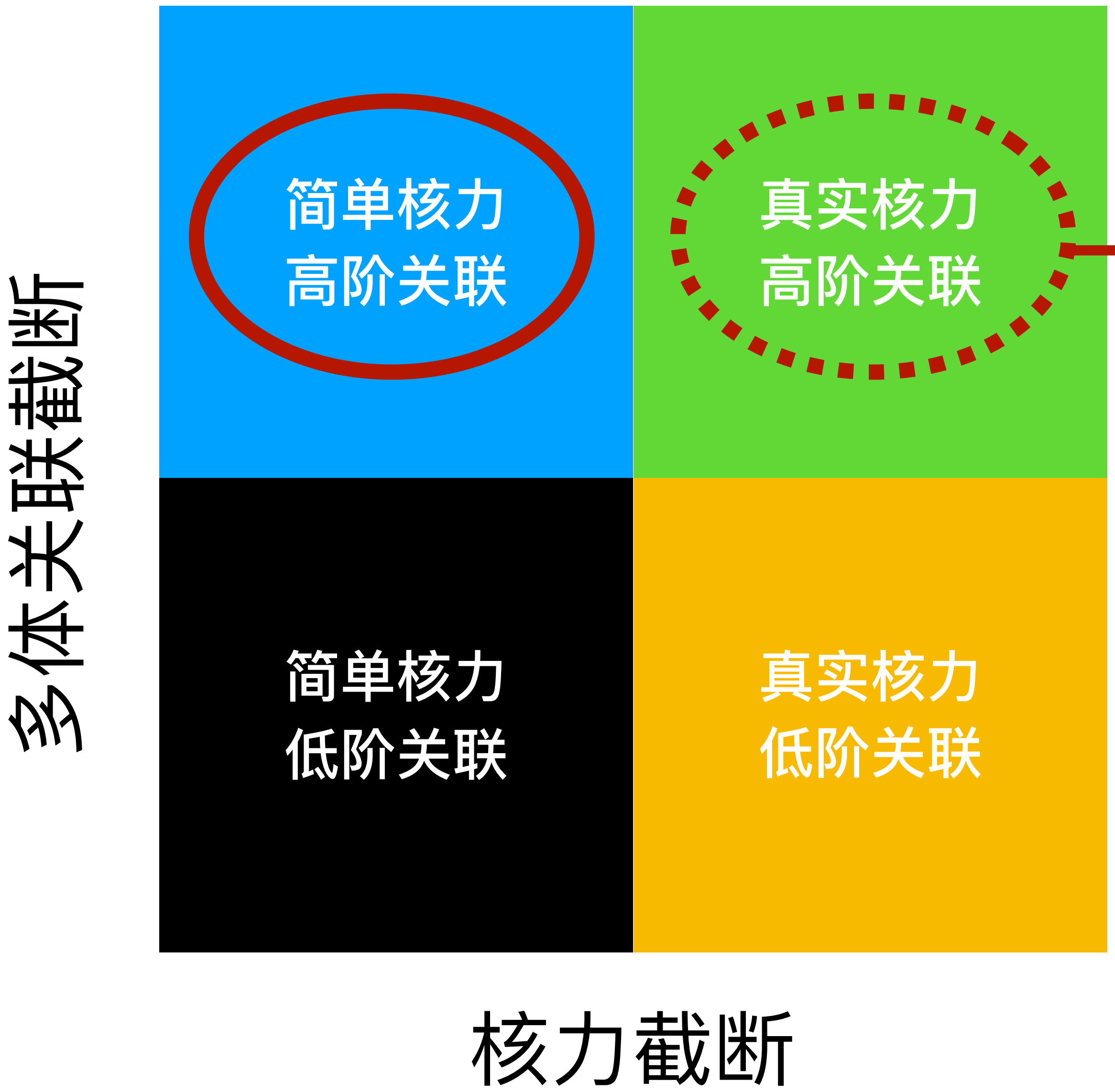
  A sensitive and clean probe of the long-range 3N forces!

- Relativistic calculations for $A \leq 4$ nuclei with the Bonn potential

  Ground-state energies nicely reproduced

  Consistency between the light nuclei and nuclear matter achieved

未来愿景



中等及重质量核结构
核物质状态方程
实时间动力学演化

先进的计算方向：

神经网络波函数是利用 **异构CPU/GPU**超级计算机的理想选择


Thank you.