FeynmanNet方法及其应用

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Outline

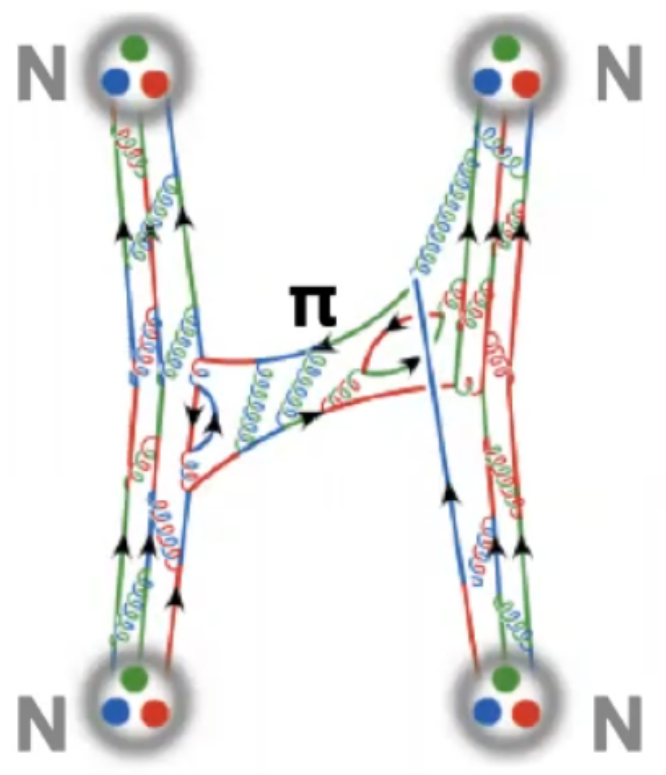
- 原子核第一性原理计算及其挑战
- 基于人工神经网络的量子多体波函数
- FeynmanNet方法及其应用
- 总结与展望

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。

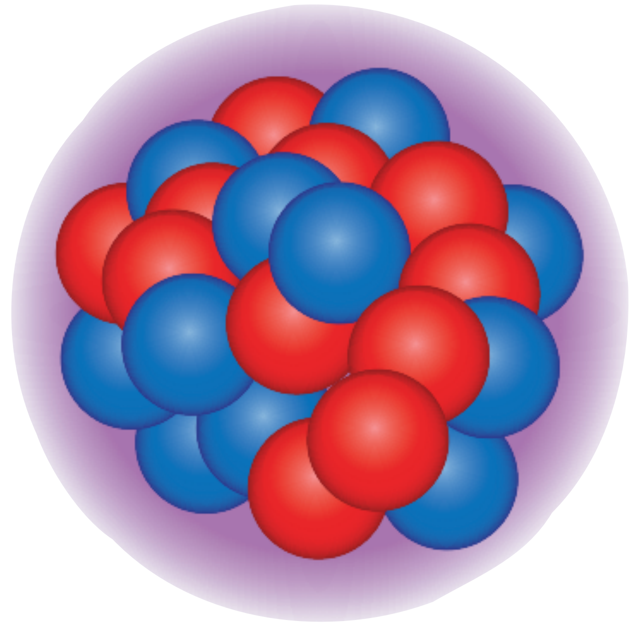
◉ 构建核力

- 唯象模型、介子交换模型
- 有效场论 (EFT)



◉ 求解核多体问题

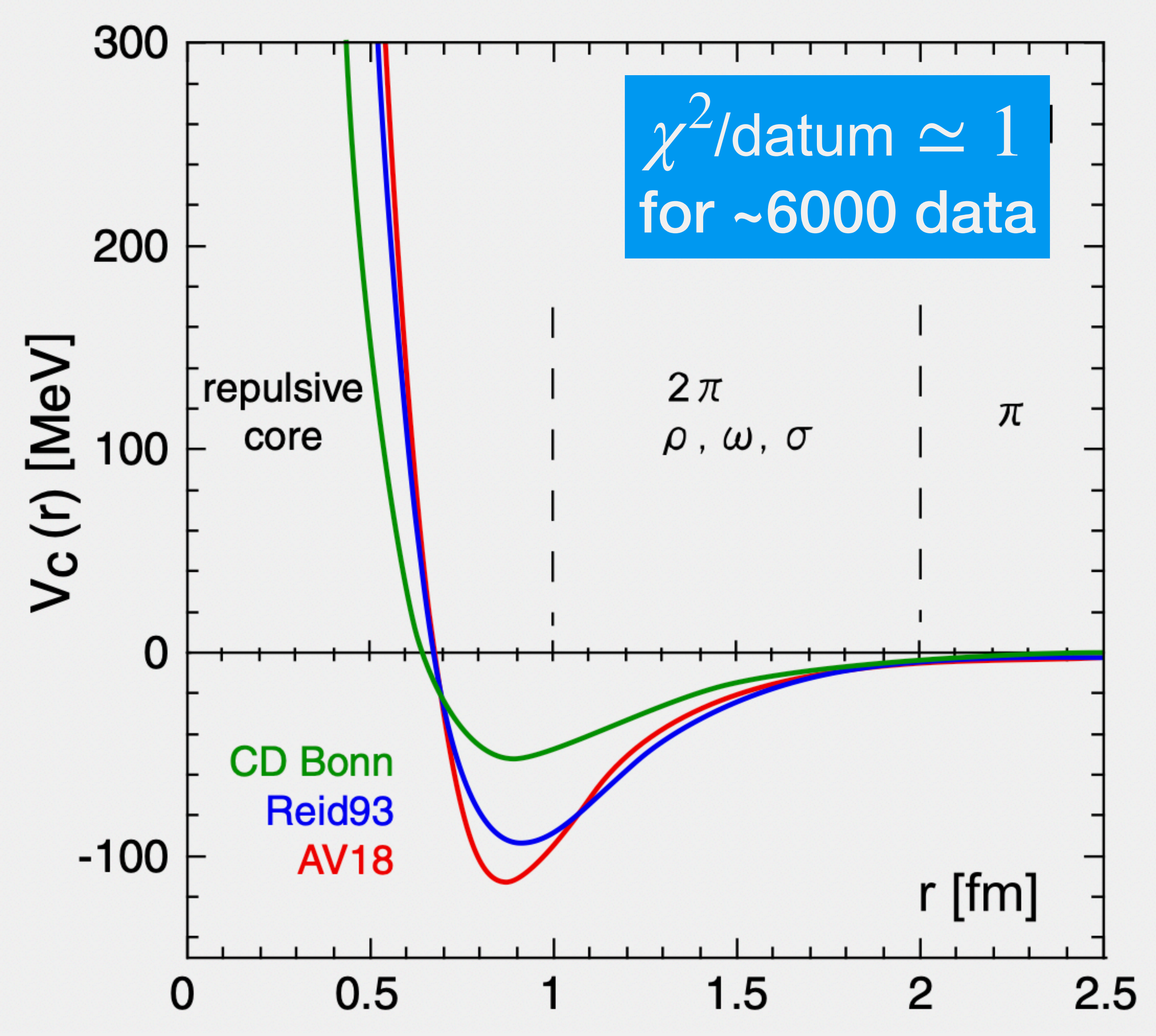
- 原子核粗块性质：质量、半径 …
- 核谱学：能级、电磁跃迁 …
- 核物质状态方程：中子星 …
- 新物理：无中微子双贝塔衰变 …
- …



Ab initio calculations with *NN* forces

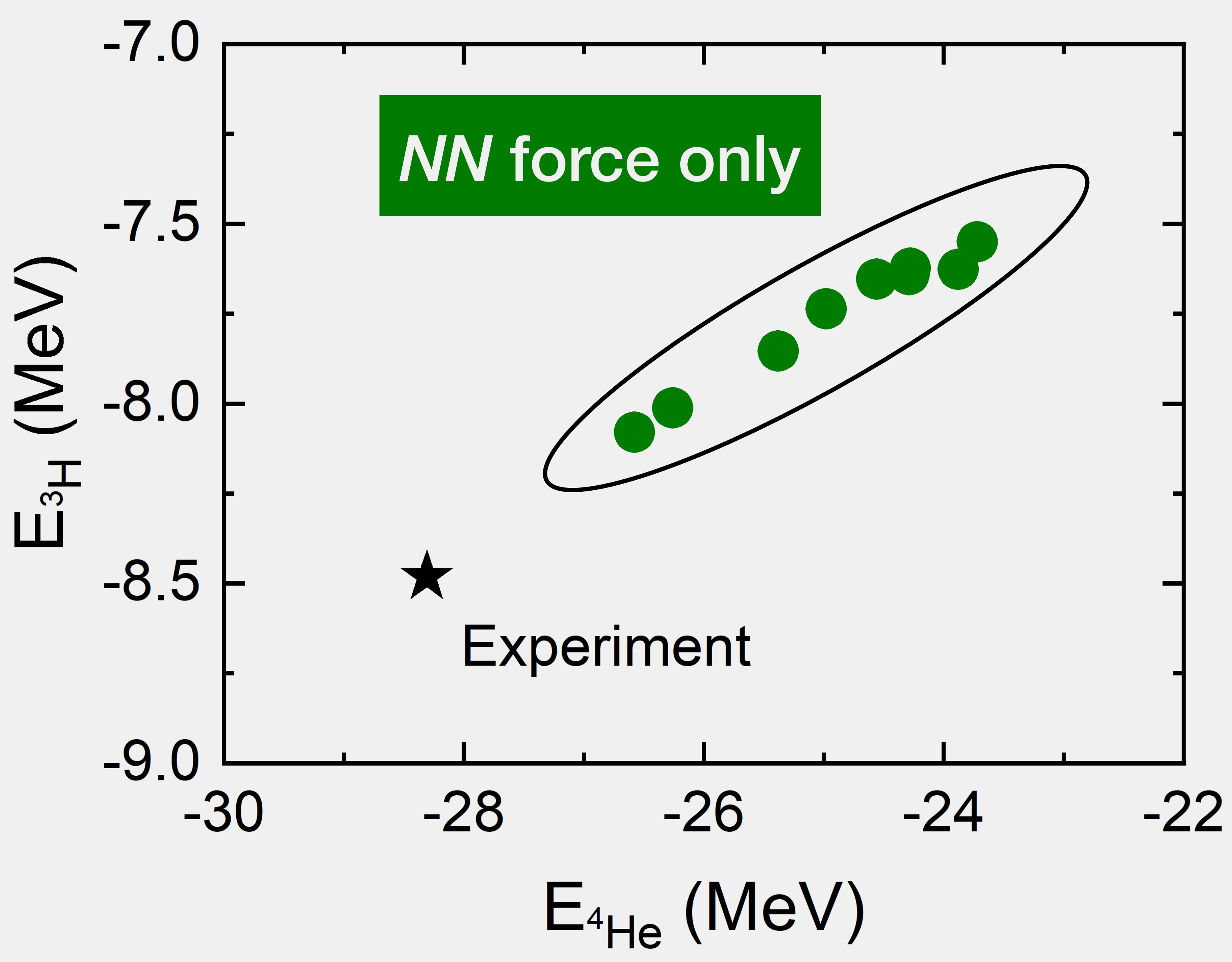
Many two-nucleon (NN) interactions, applied to nonrelativistic *ab initio* calculations, provide **insufficient binding** for light nuclei.

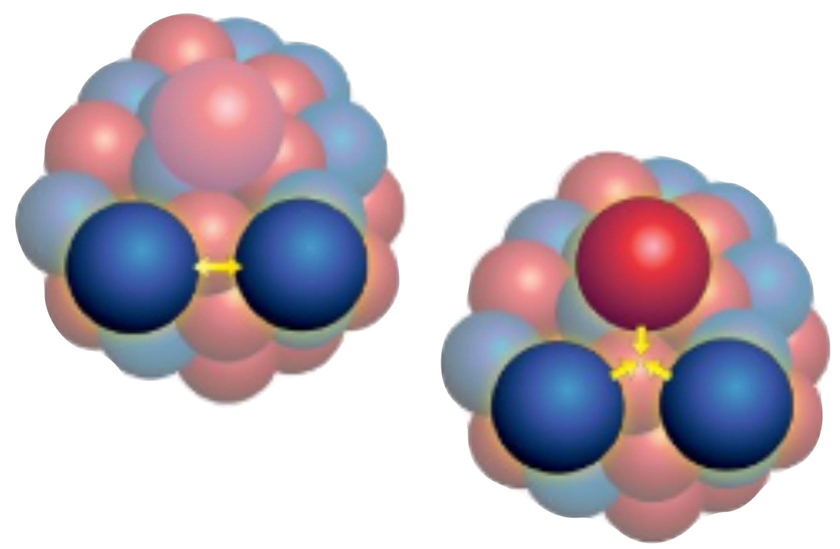
NN forces



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

^{3}H and ^{4}He

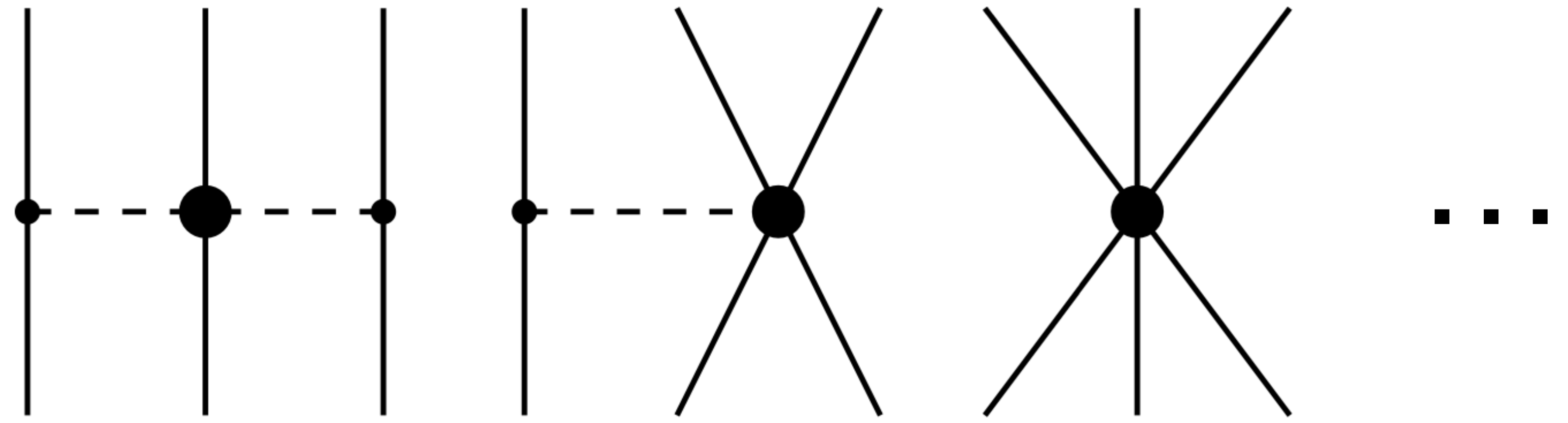


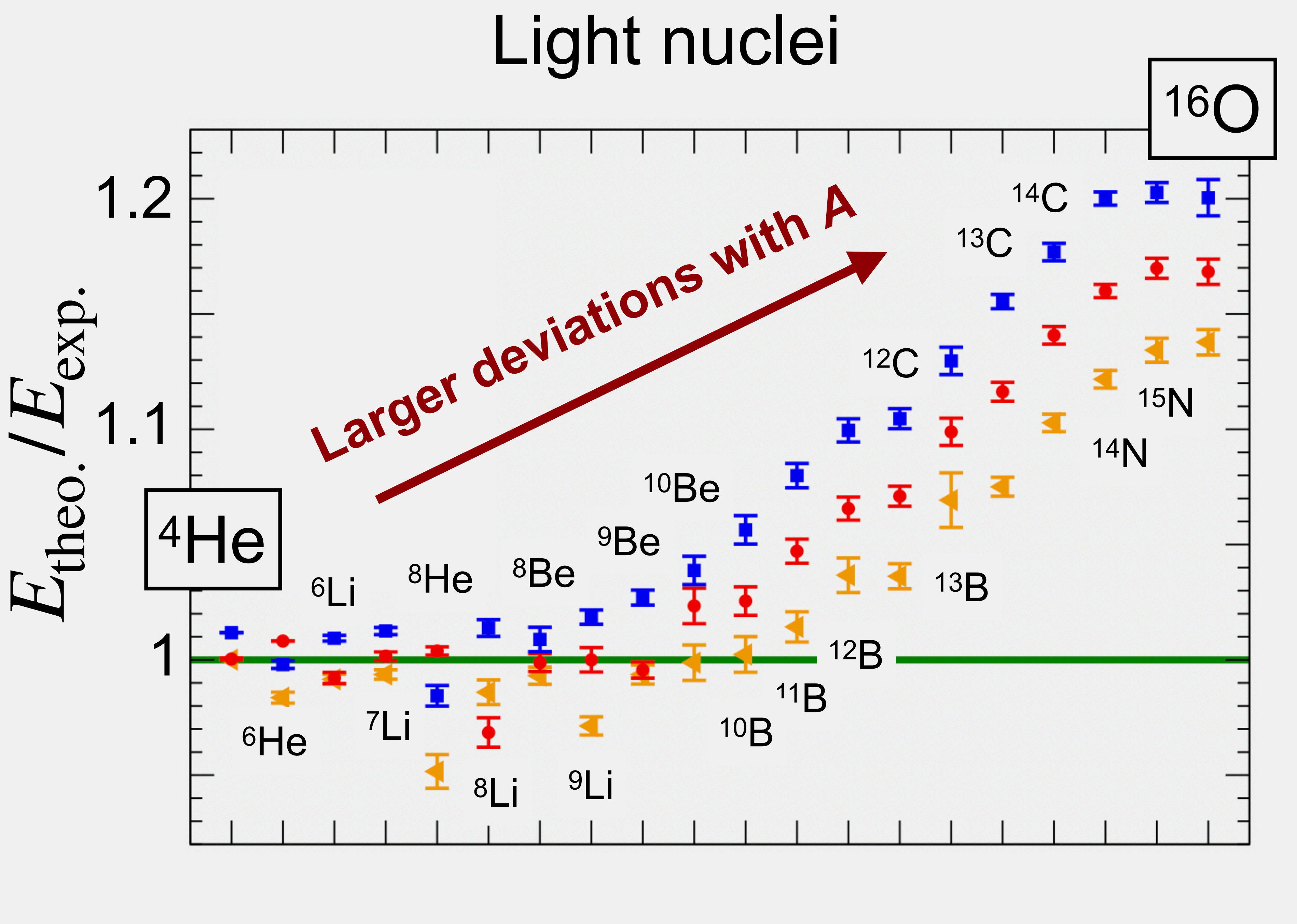


3N forces needed !

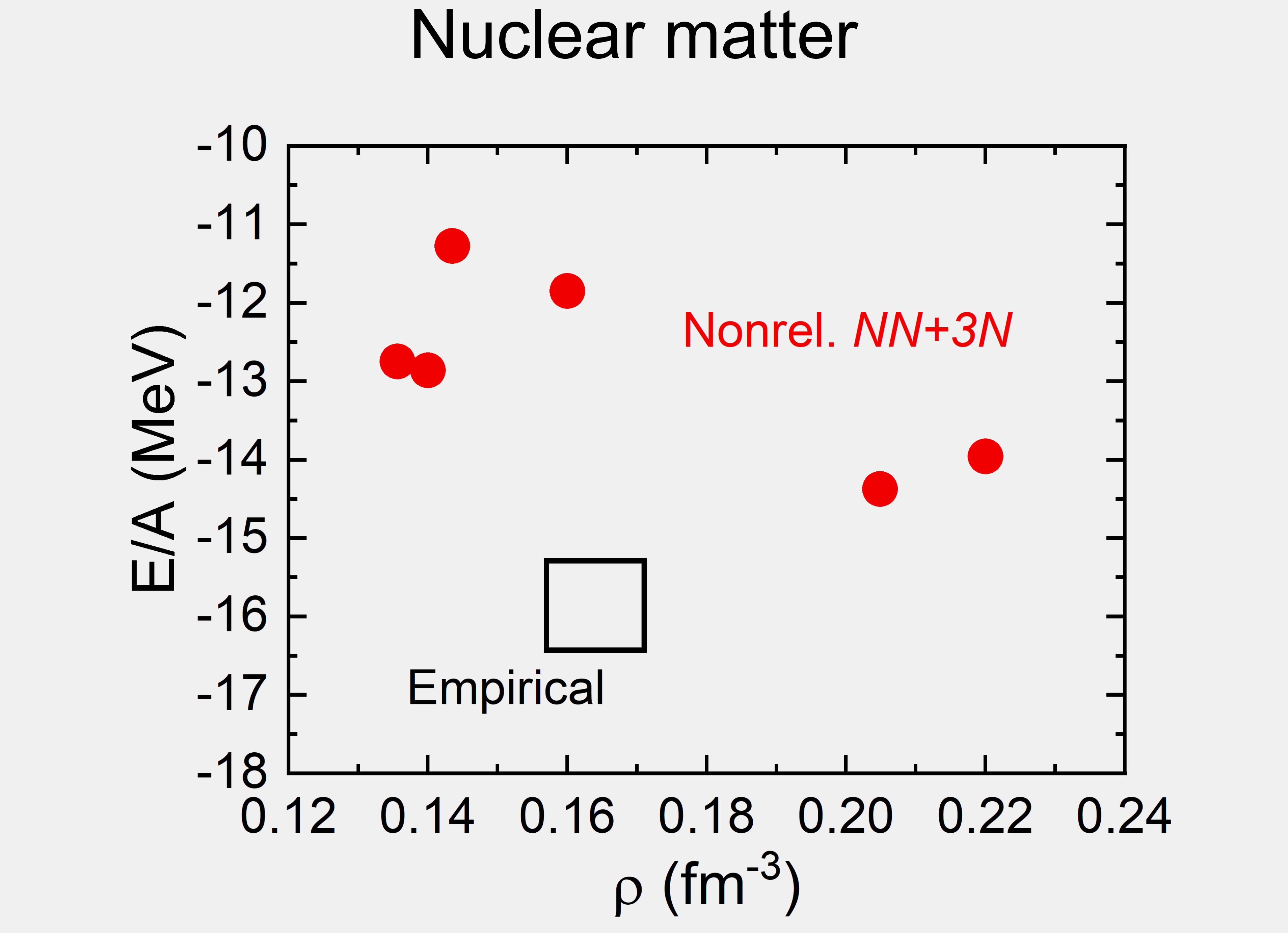
Ab initio calculations with *NN*+3*N* forces

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





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 ?

- **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

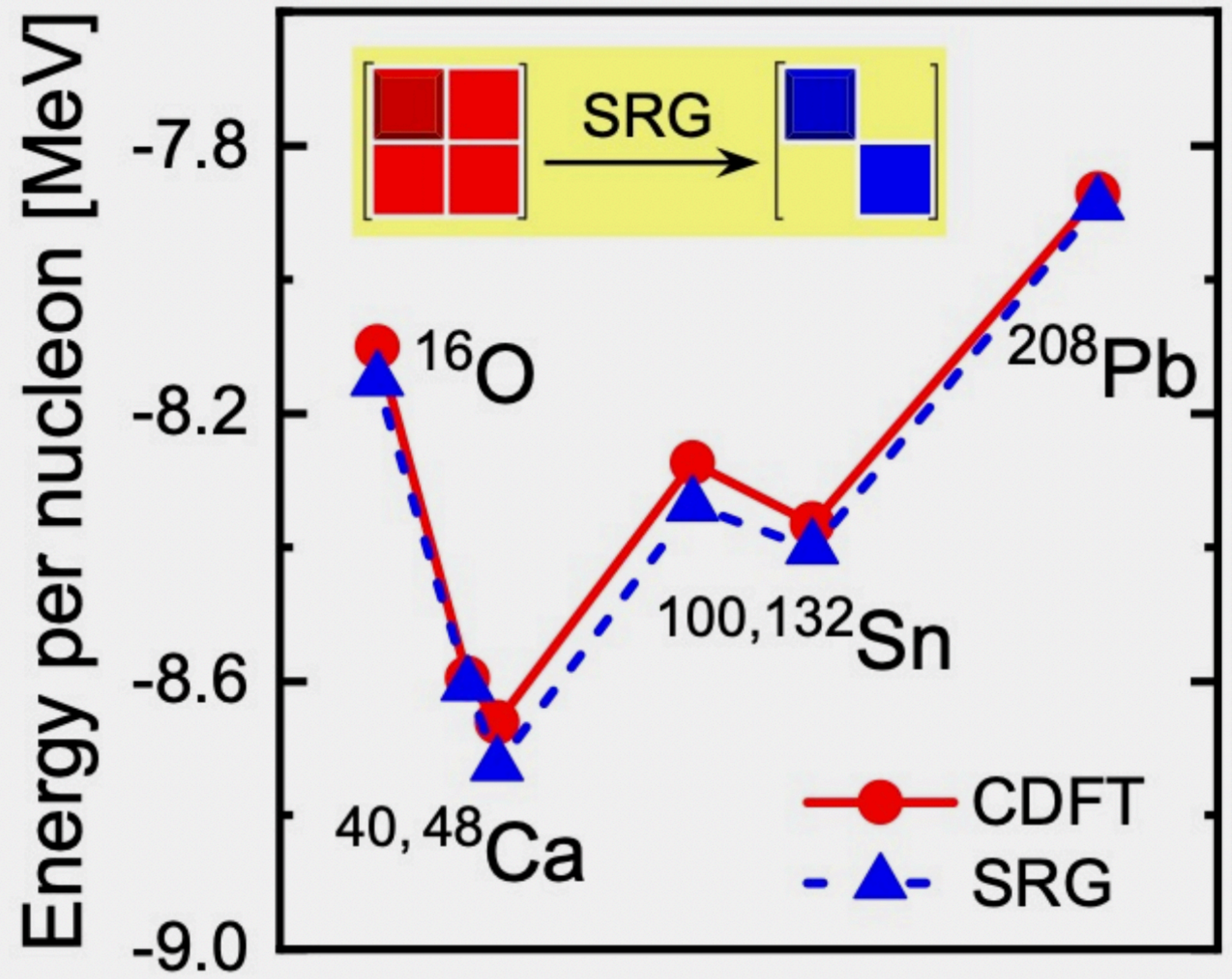
Relativistic effects

The relativity brings high-order effects …

Bridge the Rel. and Nonrel. DFTs

$$\underbrace{4\pi r^2 \rho_v(r)}_{\text{Rel.}} = \underbrace{\rho_0 + \frac{d}{dr}\left[\frac{1}{4\tilde{M}^2}\frac{\kappa}{r}\rho_0\right] + \frac{d^2}{dr^2}\left[\frac{1}{8\tilde{M}^2}\rho_0\right] + O(\tilde{M}^{-3})}_{\text{Nonrel. (including high-order terms …)}}$$

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



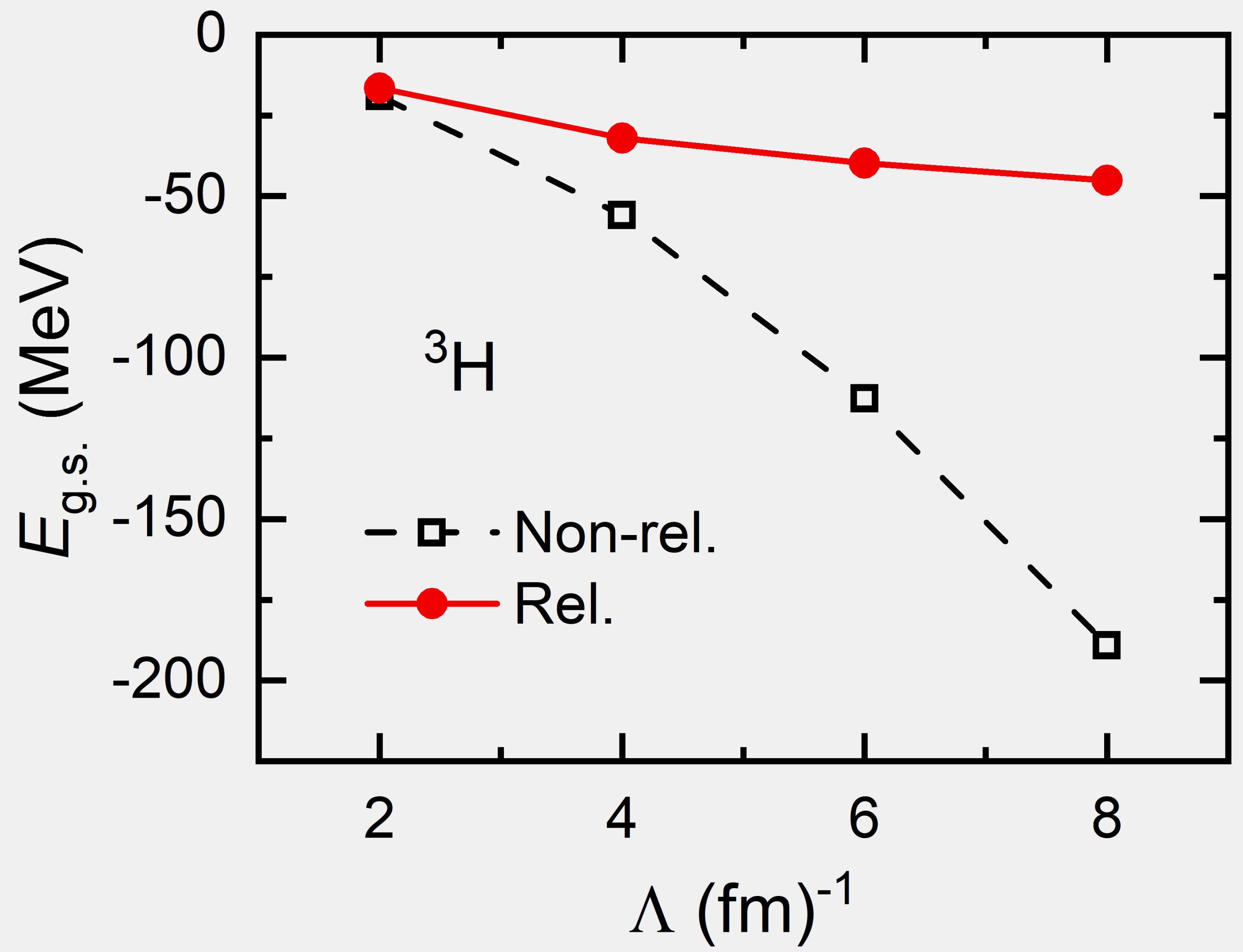
Ren and PWZ, PRC 102, 021301(R) (2020)
Editors' Suggestion

Rel. and Nonrel. VMC with LO forces

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

Nonrel Rel. corrections

Thomas collapse avoided !

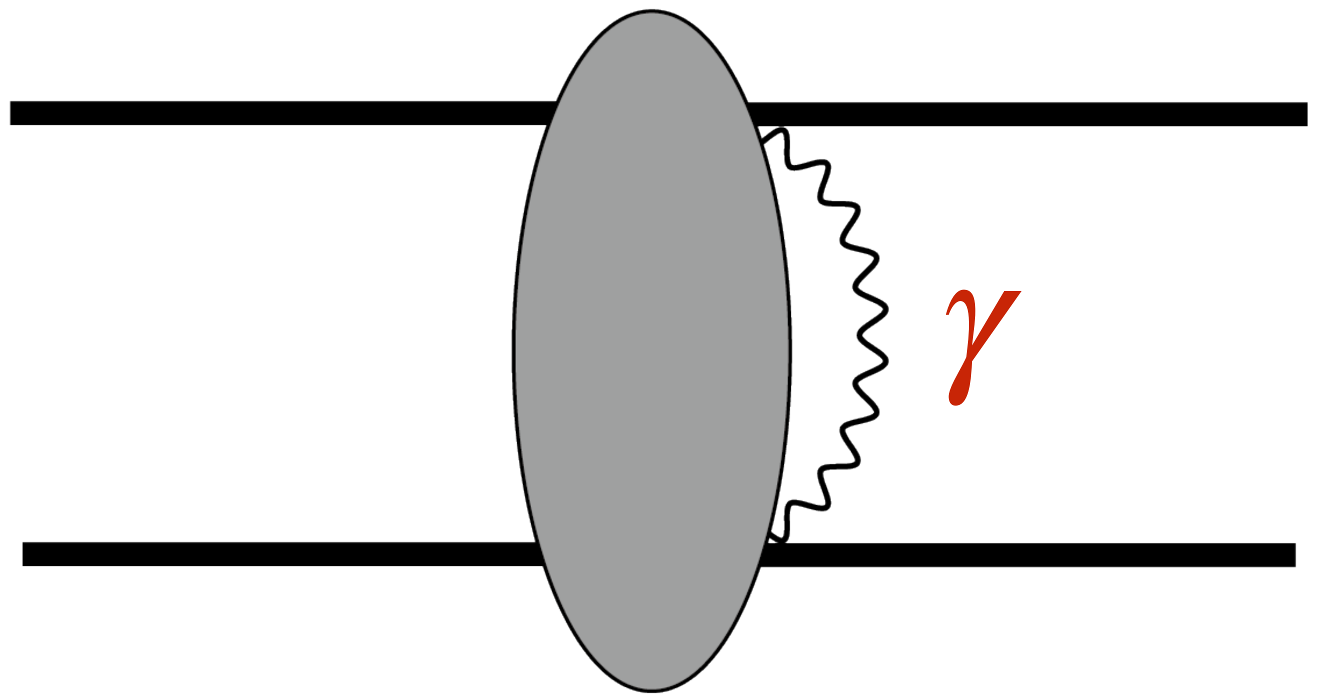


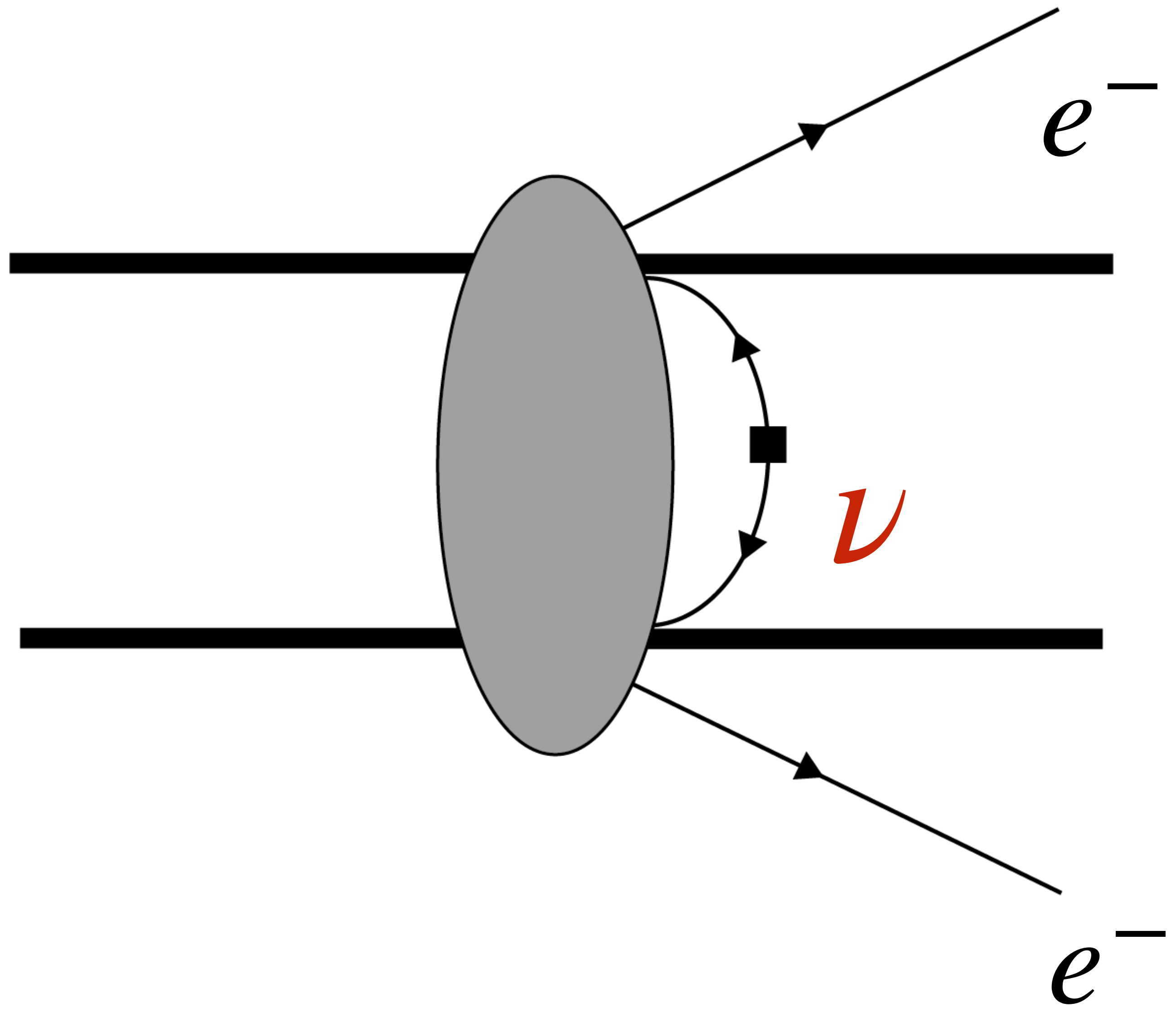
Yang and PWZ, PLB 835, 137587 (2022)

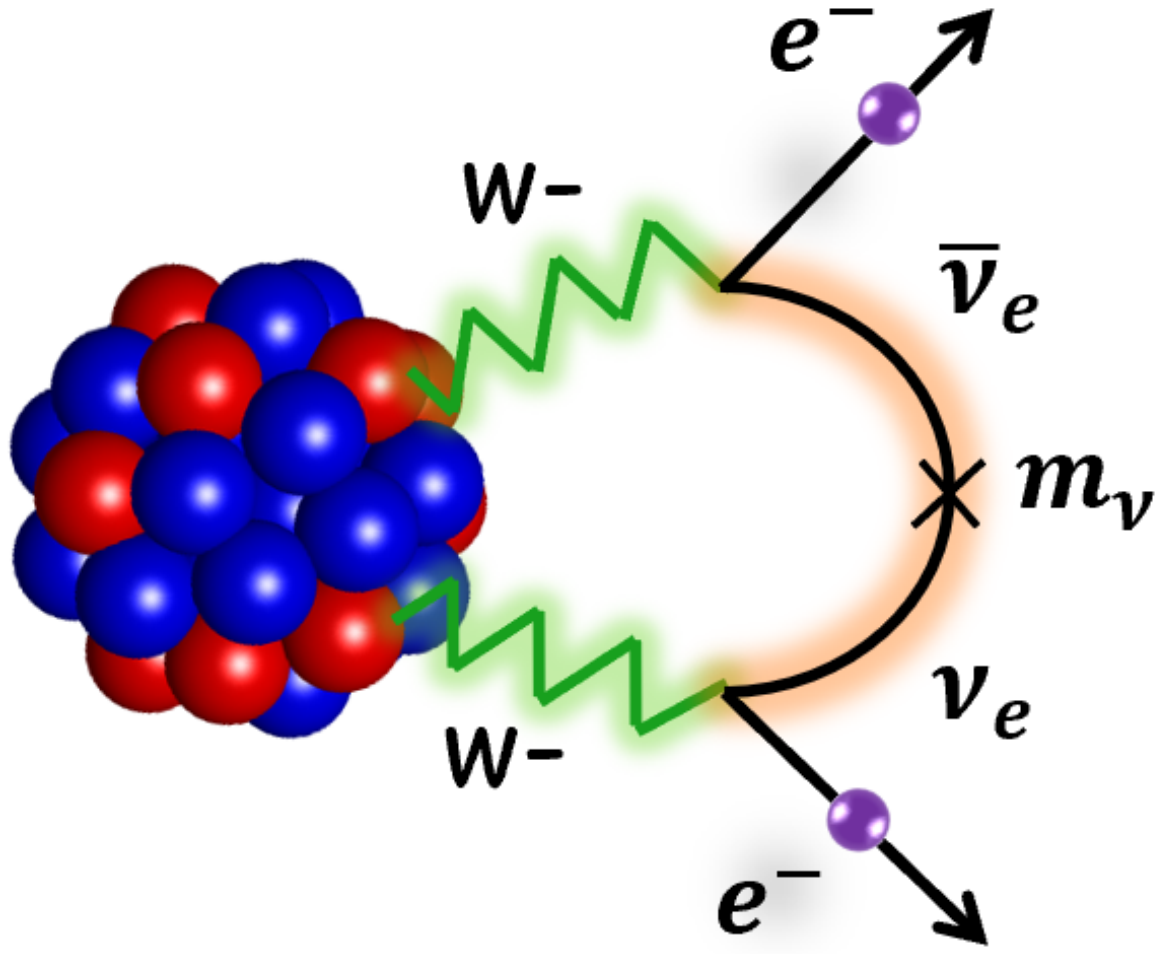
CSB and CIB of NN scattering

$$NN \to NN$$

$$nn \to ppee$$





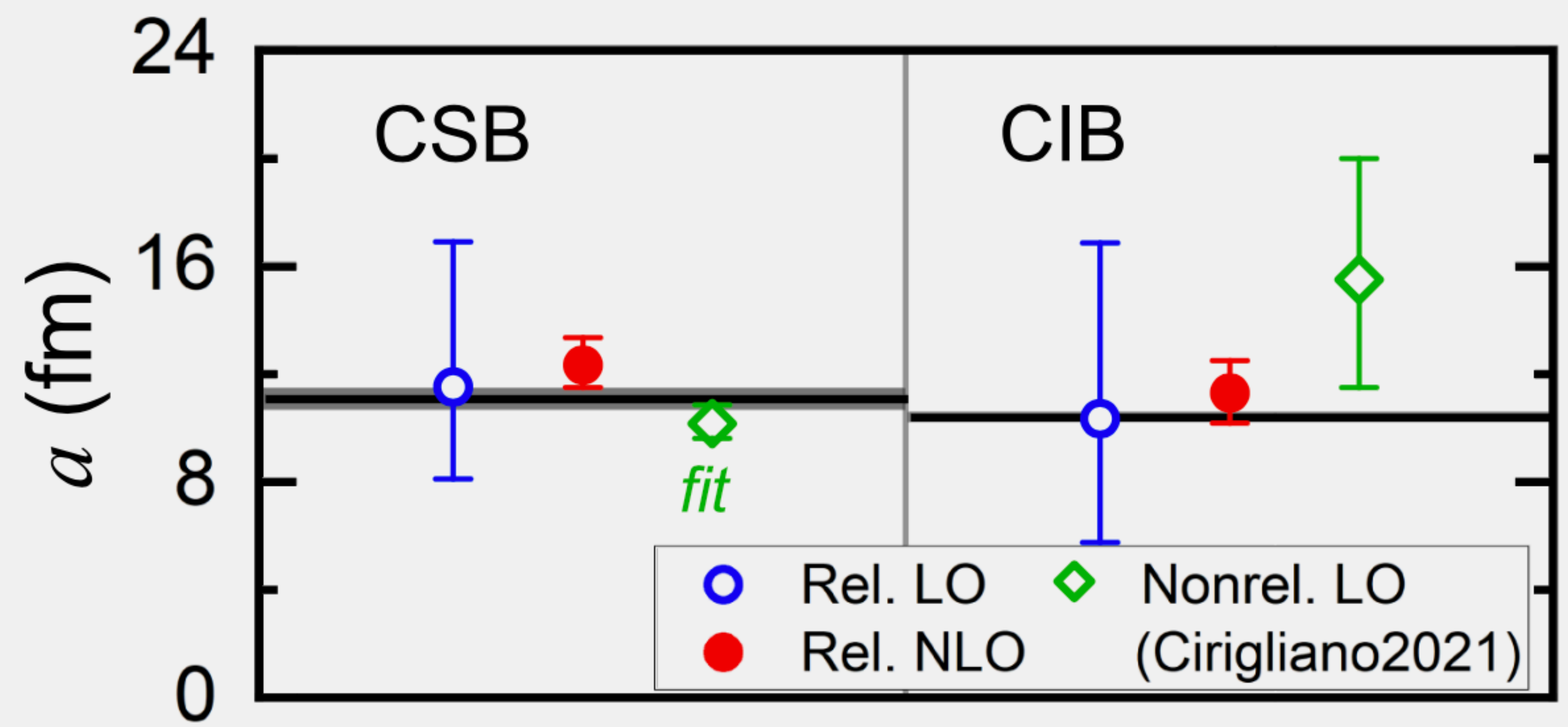


$$a_{nn} \neq a_{pp} \neq a_{np}$$

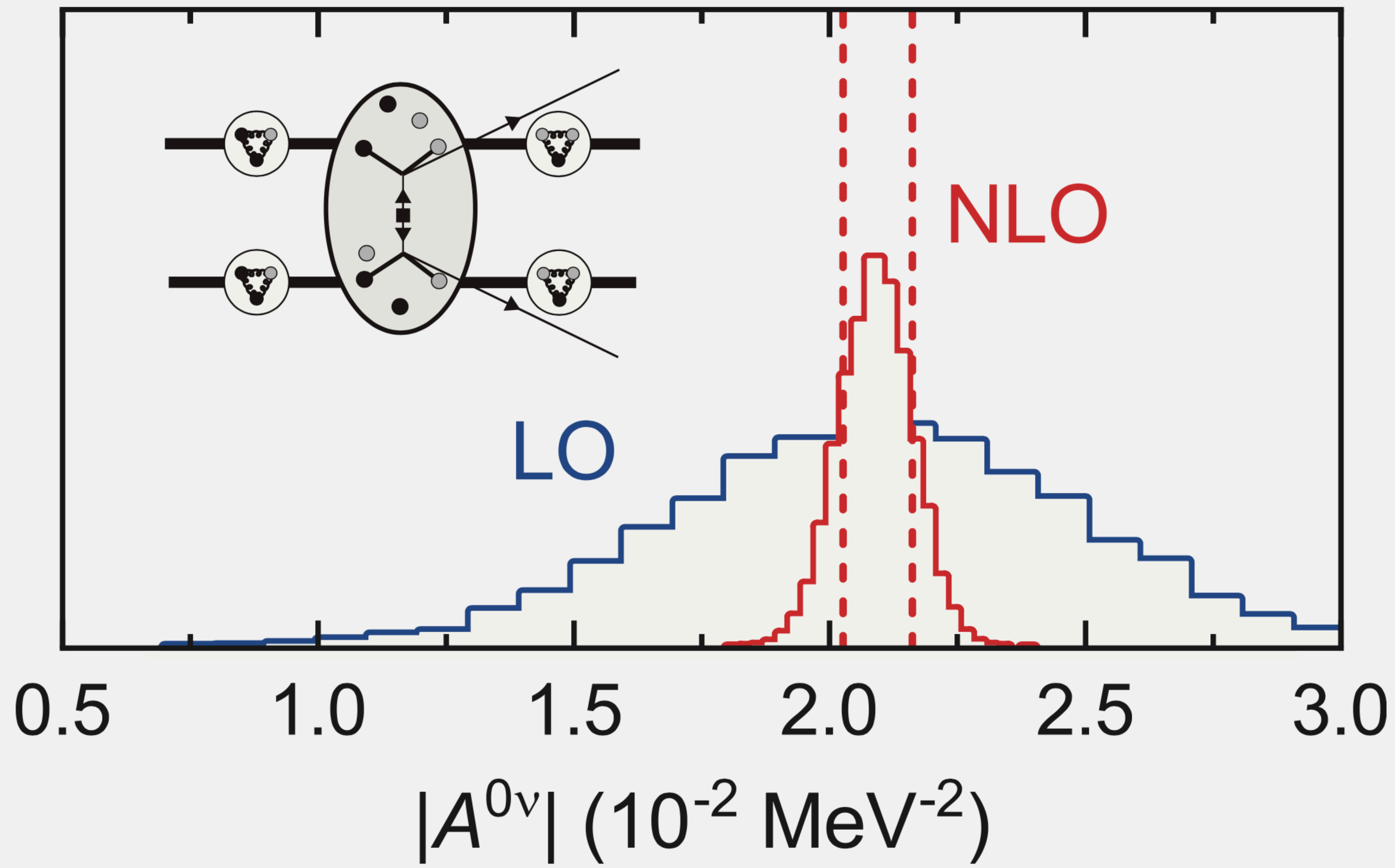
Cirigliano, Dekens, de Vries, Hoferichter, and Mereghetti, PRL 126, 172002 (2021)

Relativistic EFT for neutrinonless $\beta\beta$ decay

迄今**最精确的**两中子 $0\nu\beta\beta$ 衰变振幅



$a_{\mathrm{CSB}} = a_{pp} - a_{nn}$ $\quad a_{\mathrm{CIB}} = \dfrac{a_{nn} + a_{pp}}{2} - a_{np}$

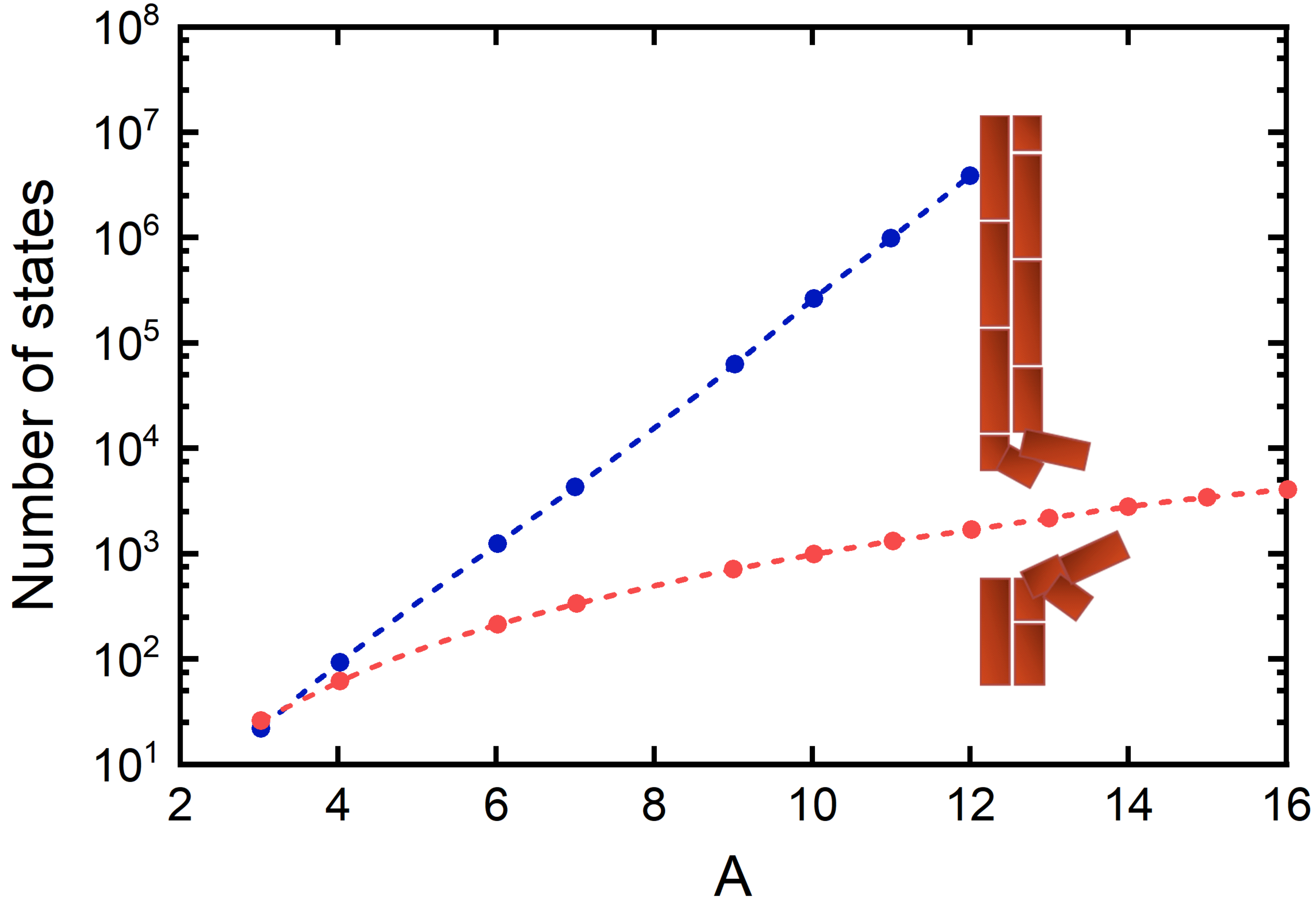


Yang and **PWZ***, PRL 134, 242502 (2025)

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)



效率 / 精度

Devising a **polynomial scaling** and **accurate** trial wave function ?

Artificial Neural Networks

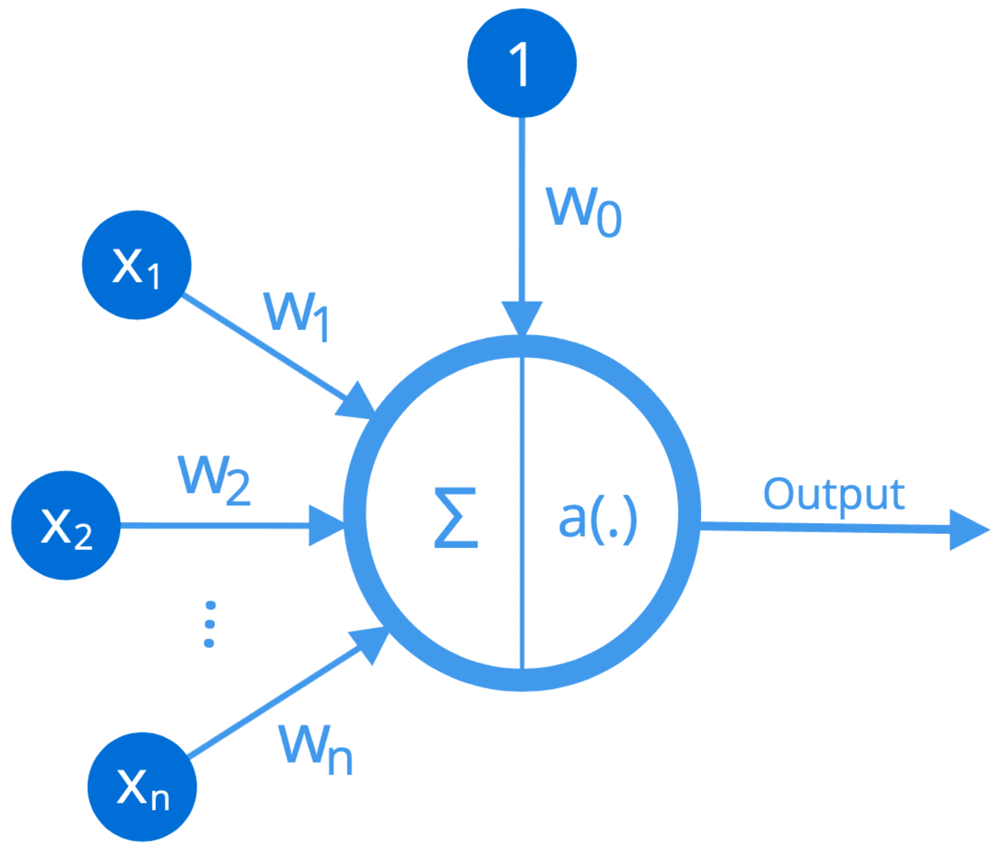
- ★ 一种受人脑神经结构启发的模型
- ★ 由带有可变参数的线性与非线性函数**嵌套**构成
- ★ 能够逼近输入与输出之间的任意连续函数关系

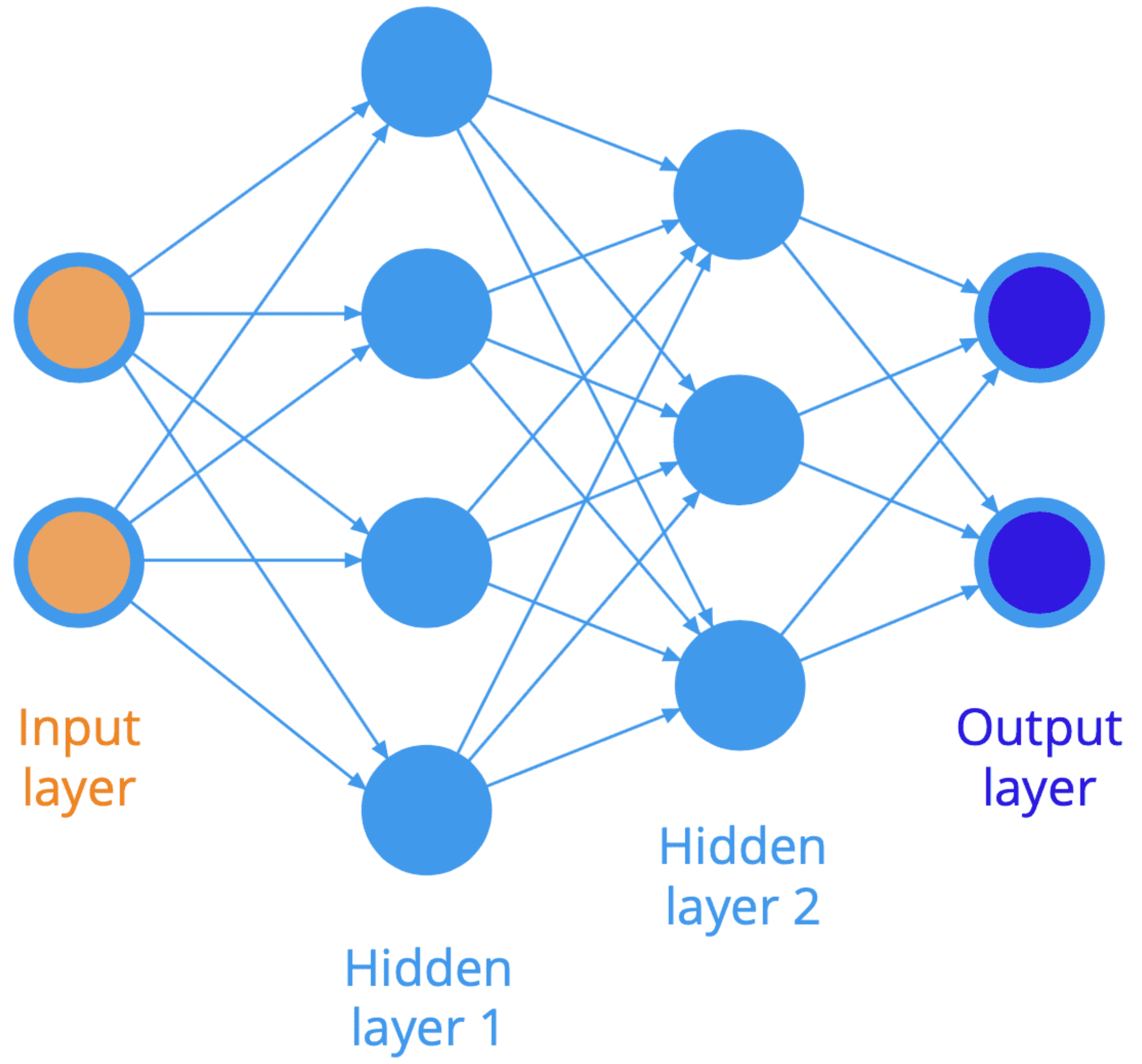
Universal Approximation Theorem: **existence / limit theorem**

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

George Cybenko (1989); Kurt Hornik (1991)

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





ANN for quantum many-body problem

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

RESEARCH

RESEARCH ARTICLE

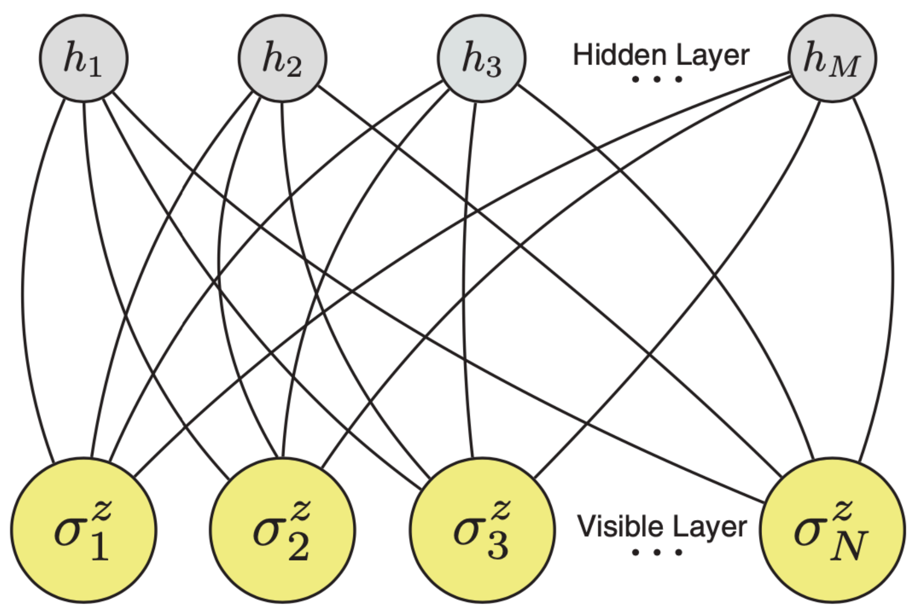
MANY-BODY PHYSICS

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.

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



原子核系统：

- ✓ **核力的复杂性**

  张量力、自旋–轨道耦合、多体力 …

- ✓ **更多自由度**

  空间、自旋、同位旋 …

- ✓ **强关联体系**

  短程关联、结团关联 …

- ✓ **自束缚体系**

  需要处理平移不变性 …

- ✓ ……

电子系统：

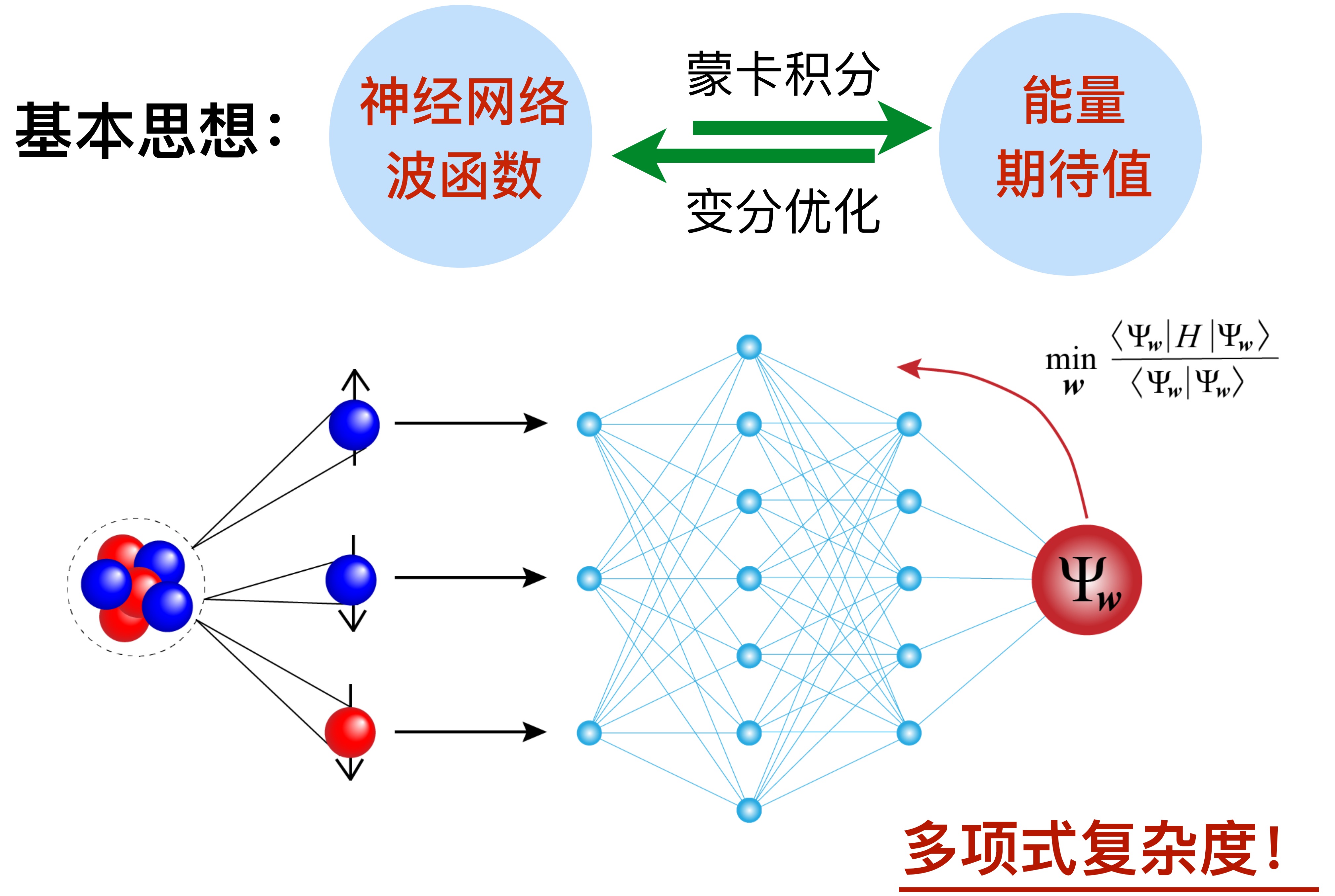
FermiNet PauliNet

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

Pfau et al., PRR 2, 033429 (2020)

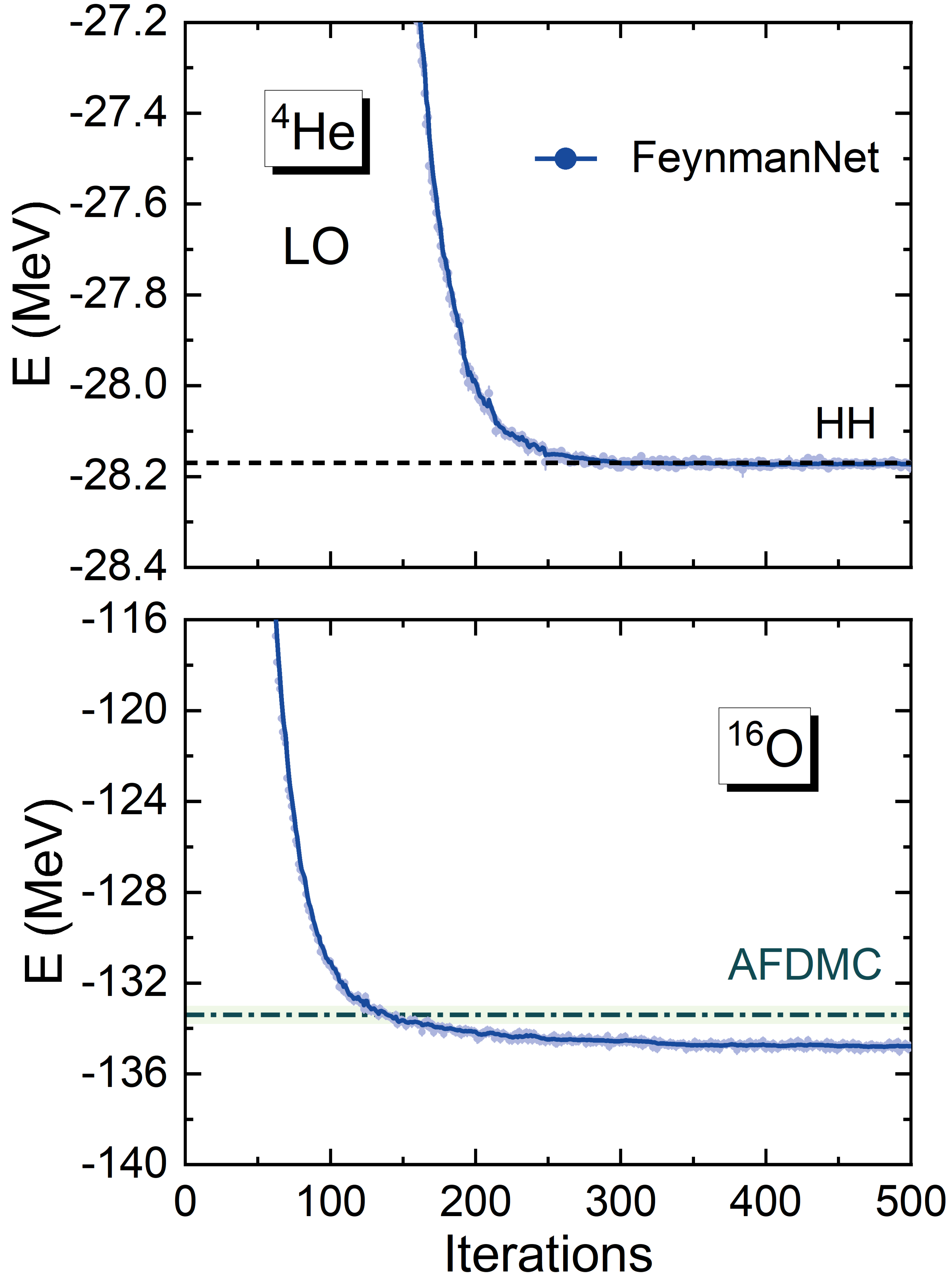
基于人工神经网络求解原子核

FeynmanNet: 深度学习驱动的原子核第一性原理计算方法，突破传统方法的精度与效率瓶颈

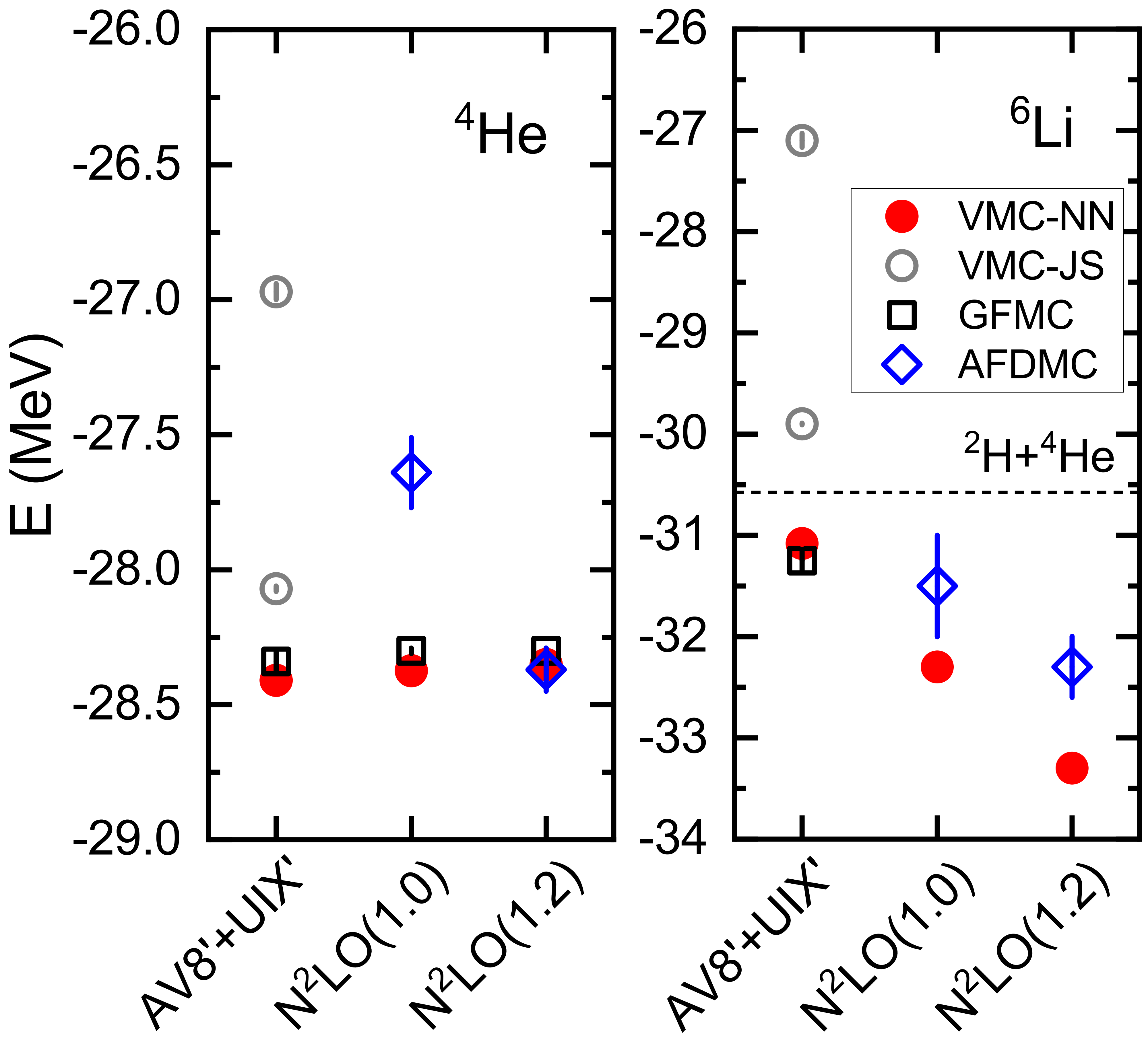


Yang and **PWZ***, PLB 835, 137587 (2022)

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



FeynmanNet的应用：高精度核力下的原子核基态



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

FeynmanNet的特点：

- ✓ 不存在费米子符号问题
- ✓ 无需软化核力
- ✓ 多项式复杂度
- ✓ 显式表达波函数
- ✓ ……

"*FeynmanNet achieves **high accuracy** while remaining **robust and efficient** "*

— Lovato, Carleo et al. arXiv: 2602.13826

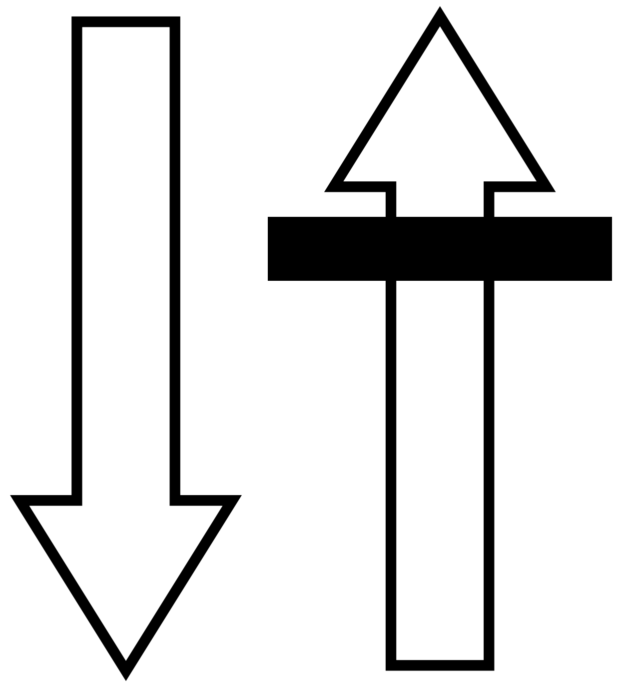
"计算精度可与投影QMC方法相媲美，重新激发了将VMC作为独立方法的兴趣"

Science, **385**, 846 (2024)

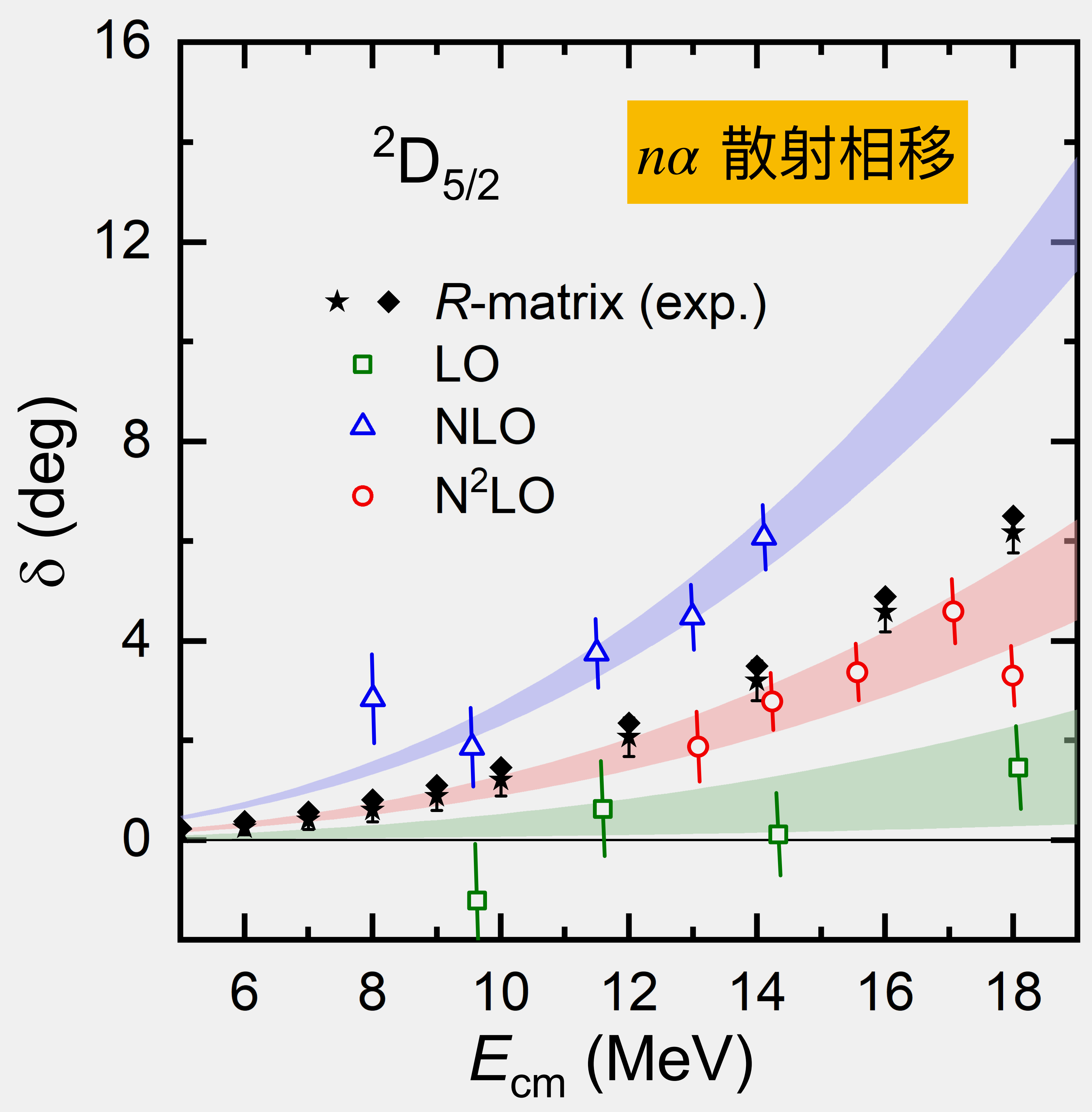
FeynmanNet的应用：少体散射

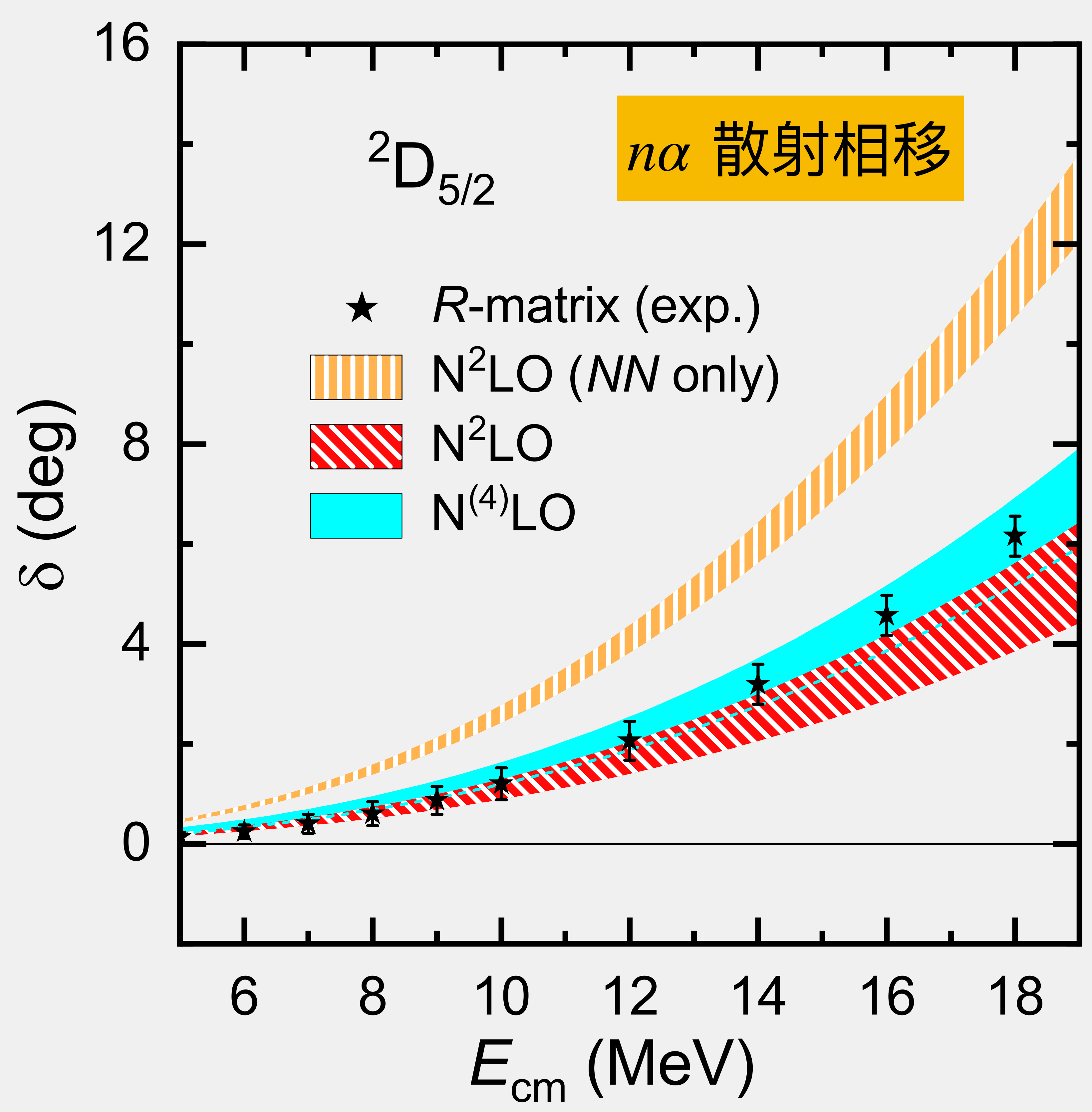
中子-阿尔法散射是一个探测**长程三体力**的灵敏探针！

多体核力



多体关联

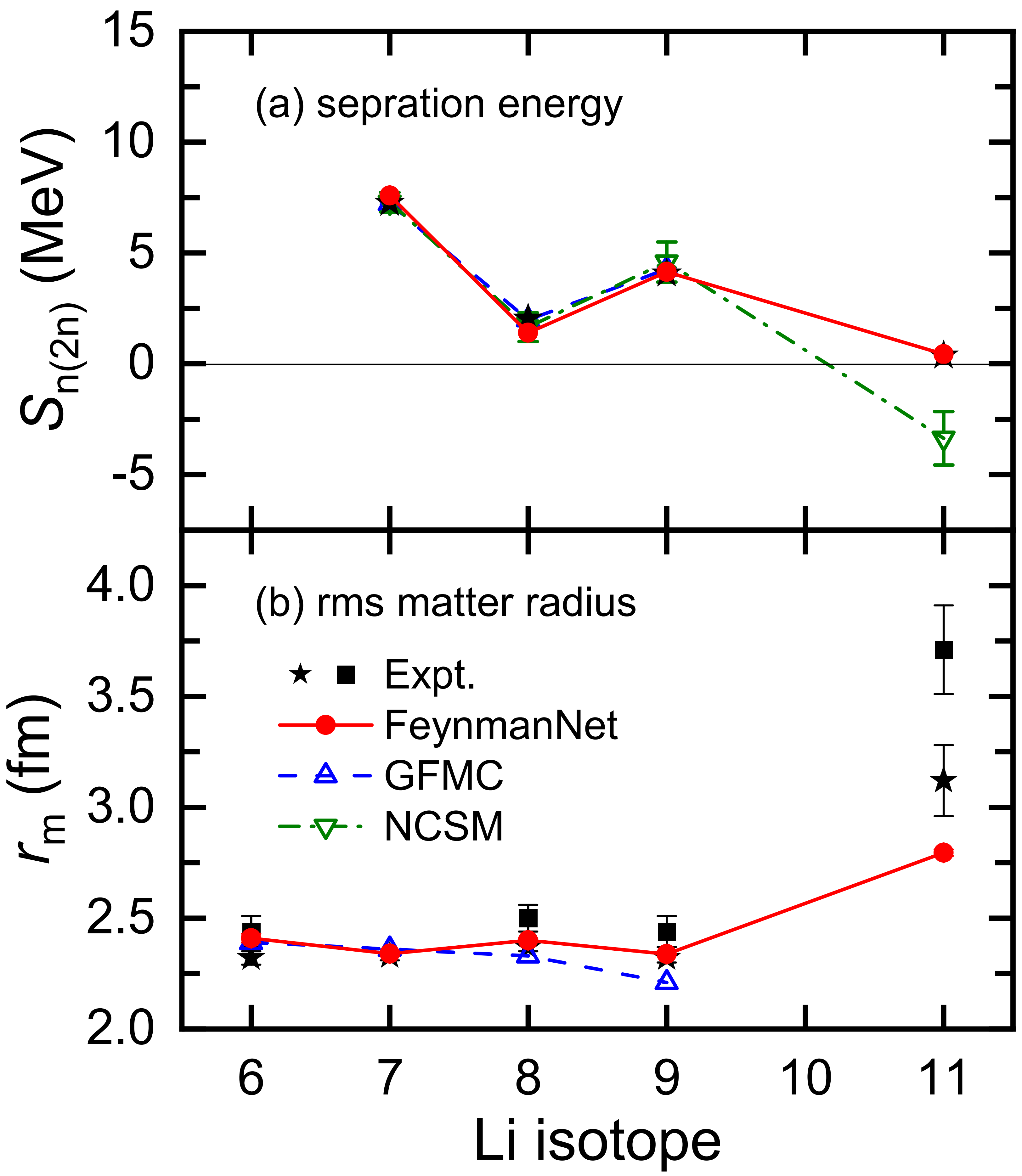


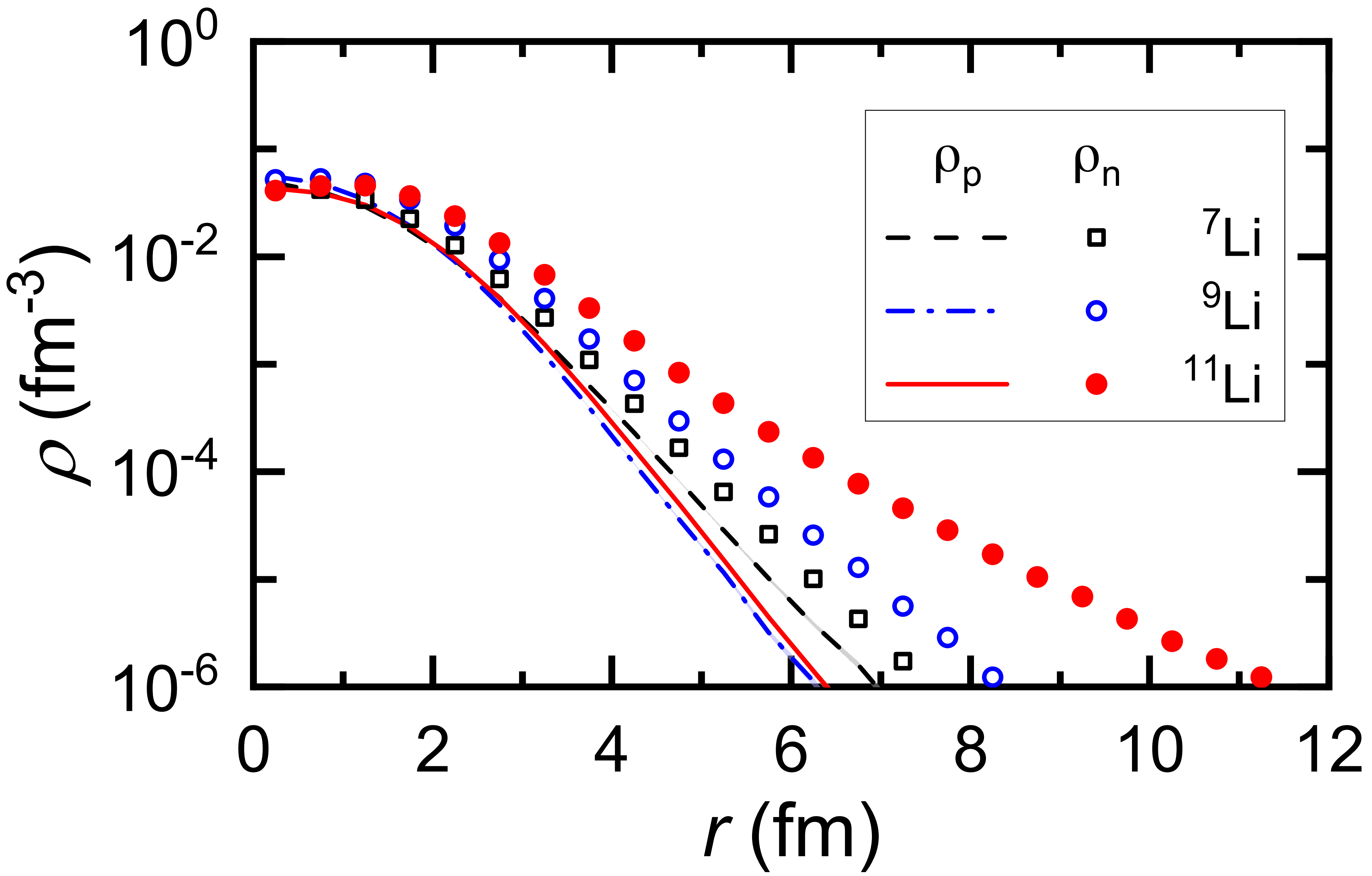


Yang, Epelbaum*, Meng*, Meng, **PWZ***, PRL 135, 172502 (2025)

FeynmanNet的应用：晕核 ^{11}Li

再现了 Li 同位素半径和分离能的实验值，给出了晕核的特征

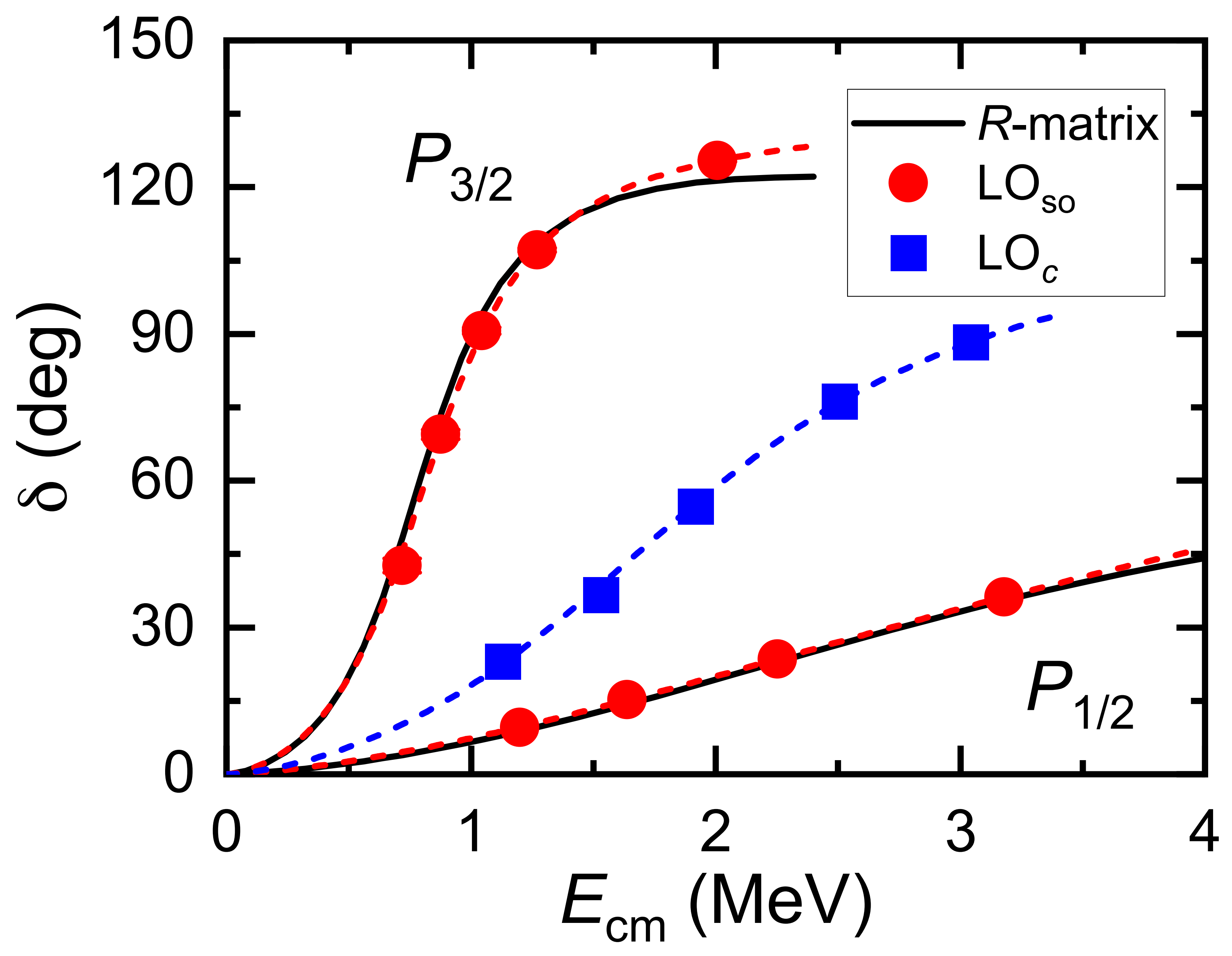


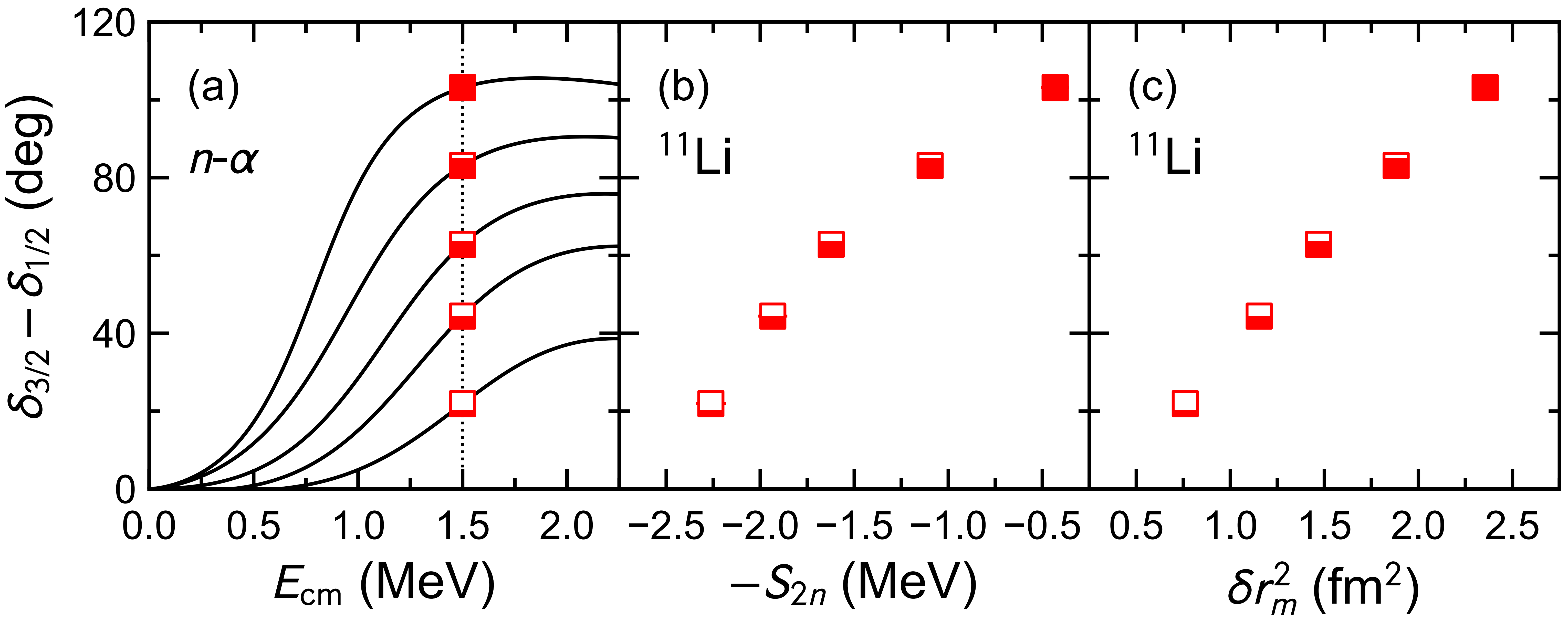


Yang, **PWZ***, submitted

FeynmanNet的应用：晕的形成机制

^{11}Li 的晕结构与中子-阿尔法 ***P* 波散射相移劈裂**紧密相关！

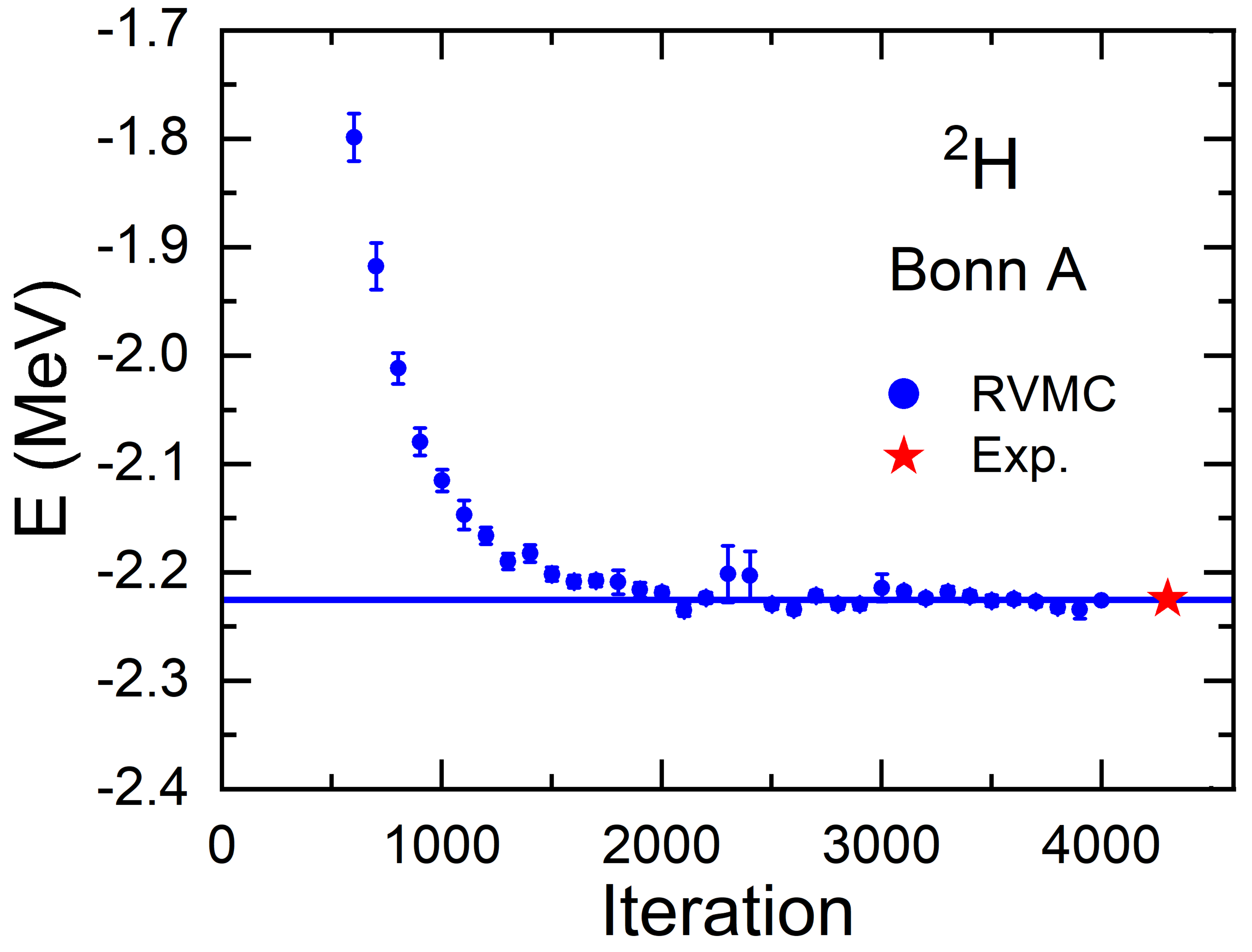


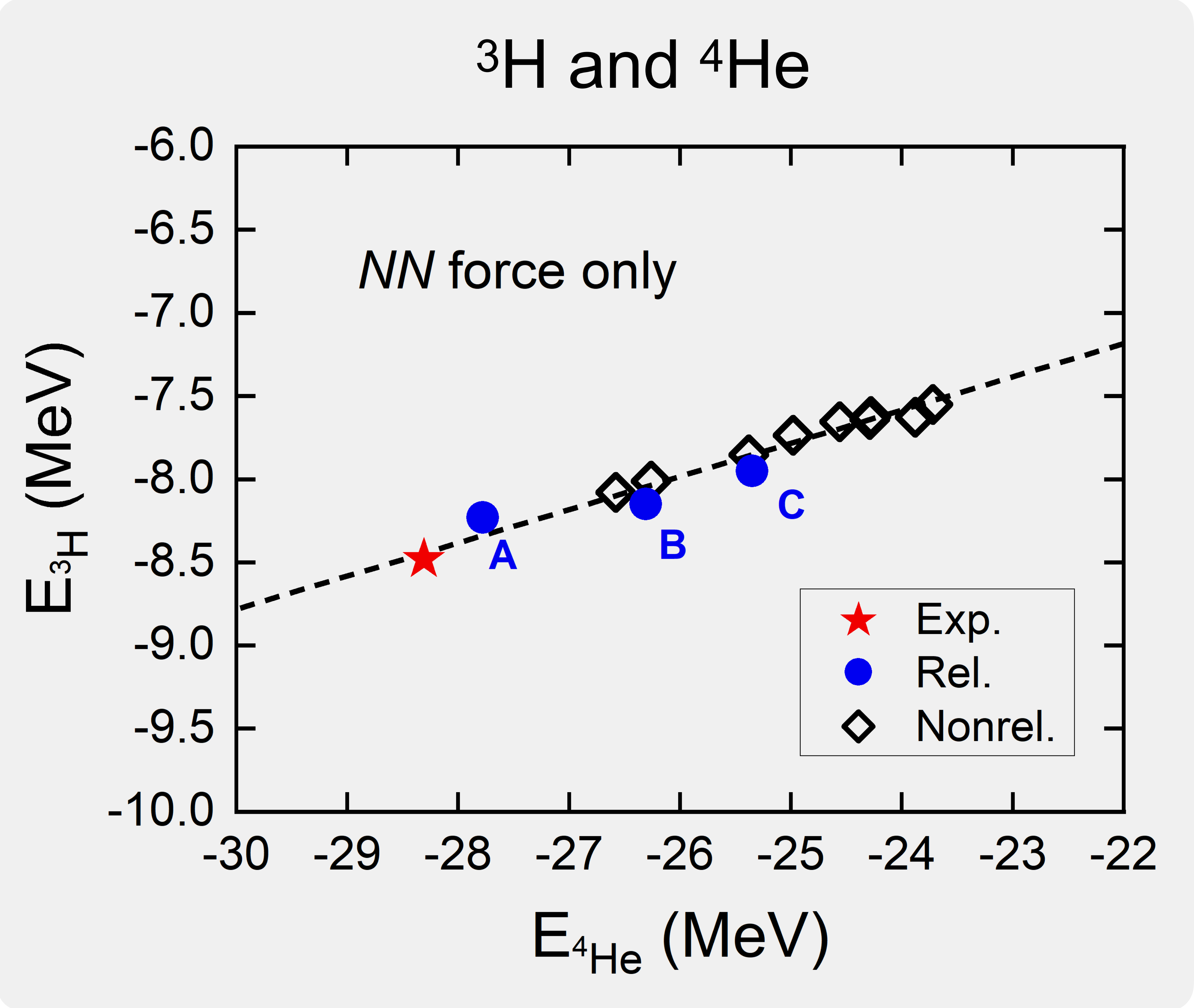


Yang, **PWZ***, submitted

Relativistic calculations with realistic forces

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



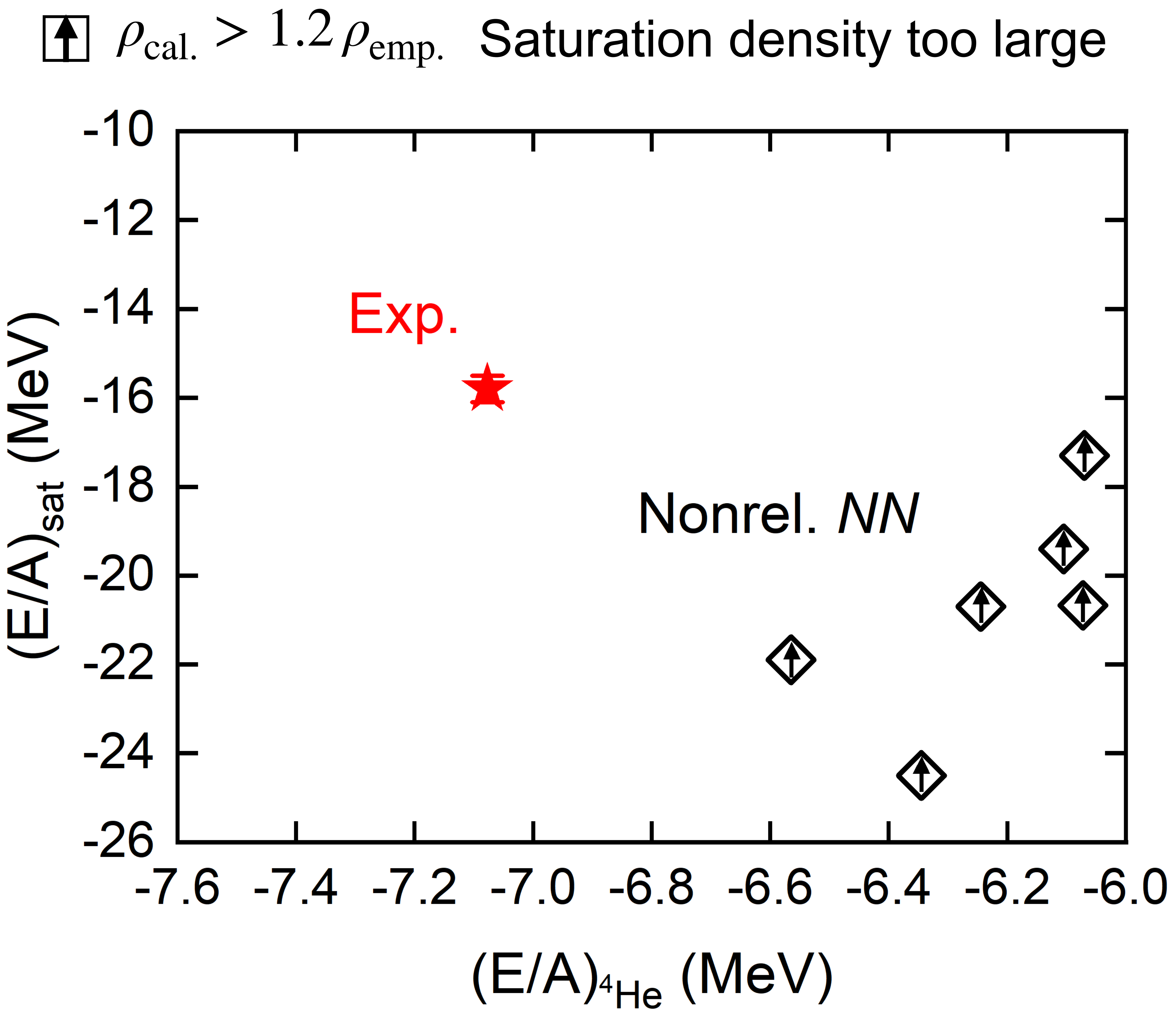


Yang and **PWZ***, CPL, 42 051201 (2025) “Express Letter”

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"



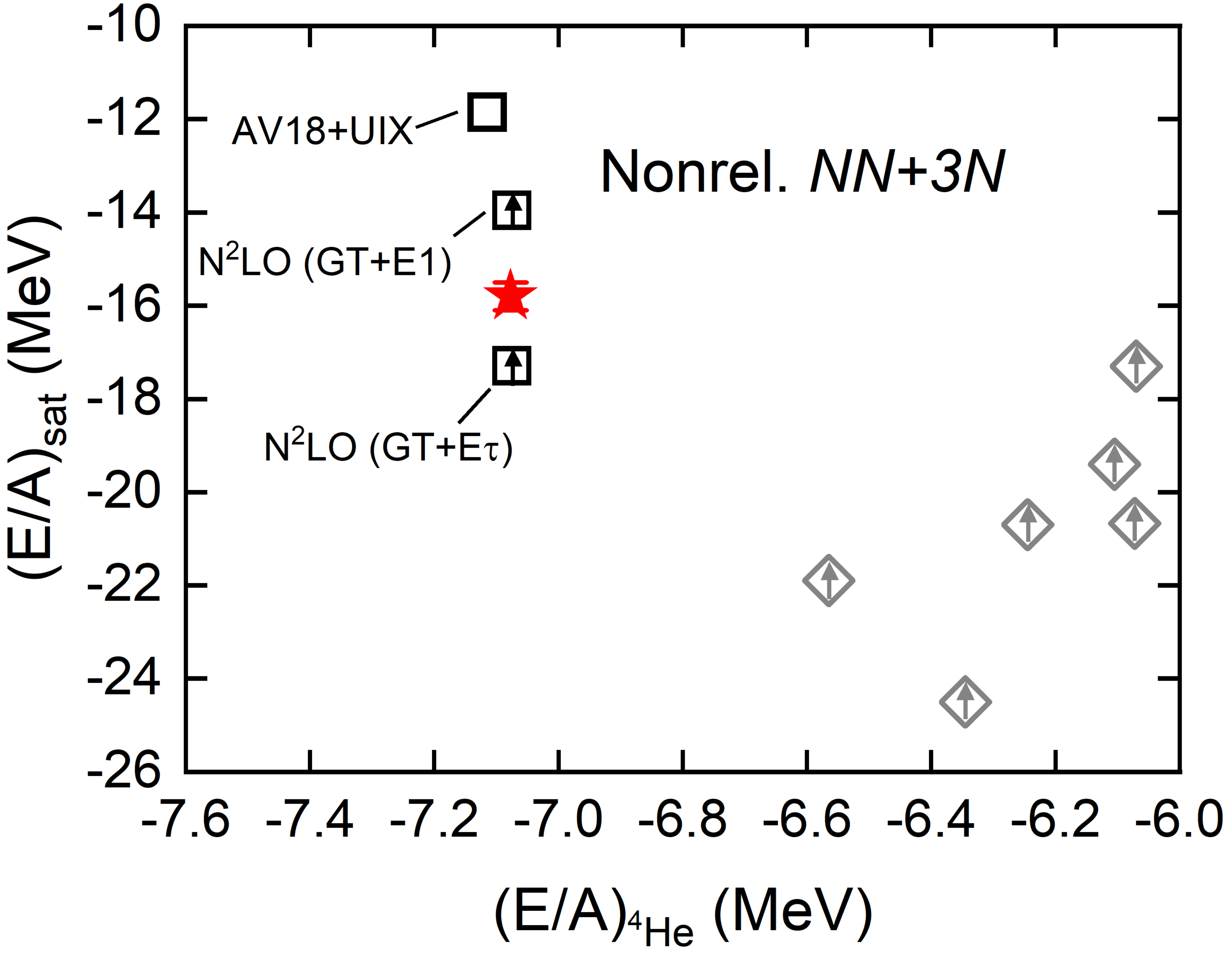
	^{4}He	Nucl. Matt.
NN	Underbind	Overbind

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”

$\boxed{\uparrow}$ $\rho_{\mathrm{cal.}} > 1.2\,\rho_{\mathrm{emp.}}$ Saturation density too large



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

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

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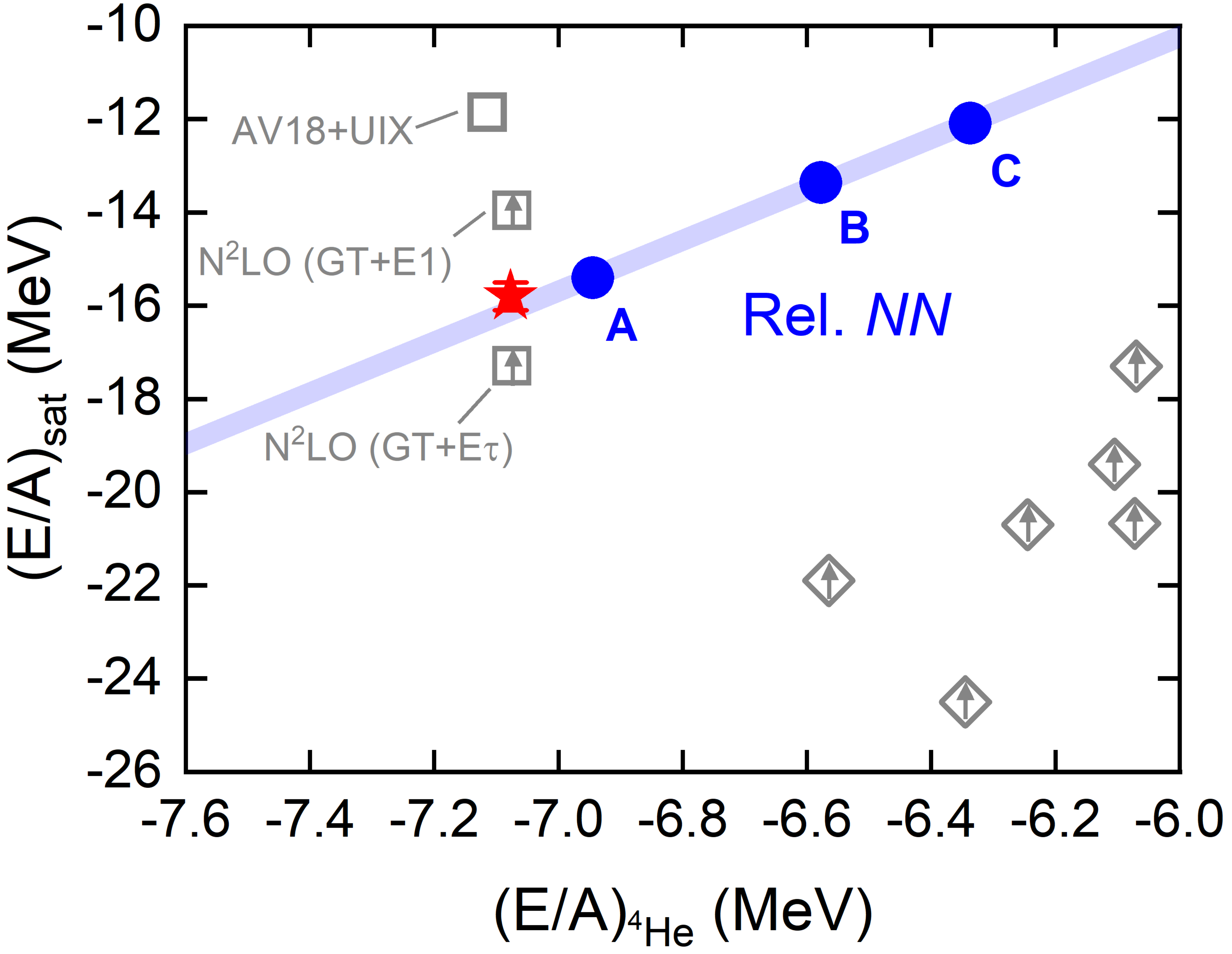

	^{4}He	Nucl. Matt.
NN	Underbind	Overbind
NN/3N	Fit	Diverse
Rel.	**Consistent !**	

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

Summary

- ✓ 第一性原理计算对直接预言原子核性质、构建具有微观基础的唯象模型等具有重要意义
- ✓ 我们发展了一种深度学习驱动的原子核第一性原理计算方法：**FeynmanNet**

  其核心在于通过**深度神经网络表示核多体波函数**，将问题从线性基展开转化为非线性函数逼近，从而**避免了费米子符号问题**，可**突破传统方法在精度和效率方面的限制**
- ✓ 中子–阿尔法散射为探测**长程三体核力**提供了灵敏探针
- ✓ ^{11}Li 的**晕结构**与**中子–阿尔法 *P* 波散射相移劈裂**之间有关联
- ✓ 相对论第一性原理计算可以**统一描述轻核与核物质**

超核体系，多夸克体系，…

张子啸, 杨一龙, 何万兵, 赵鹏巍, 吕炳楠, 马余刚, PLB 874, 140285 (2026)

吴伟霖, 孟璐, 朱世琳, PRL 136, 071901 (2026)

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谢谢！

FeynmanNet 的构造

★ **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**

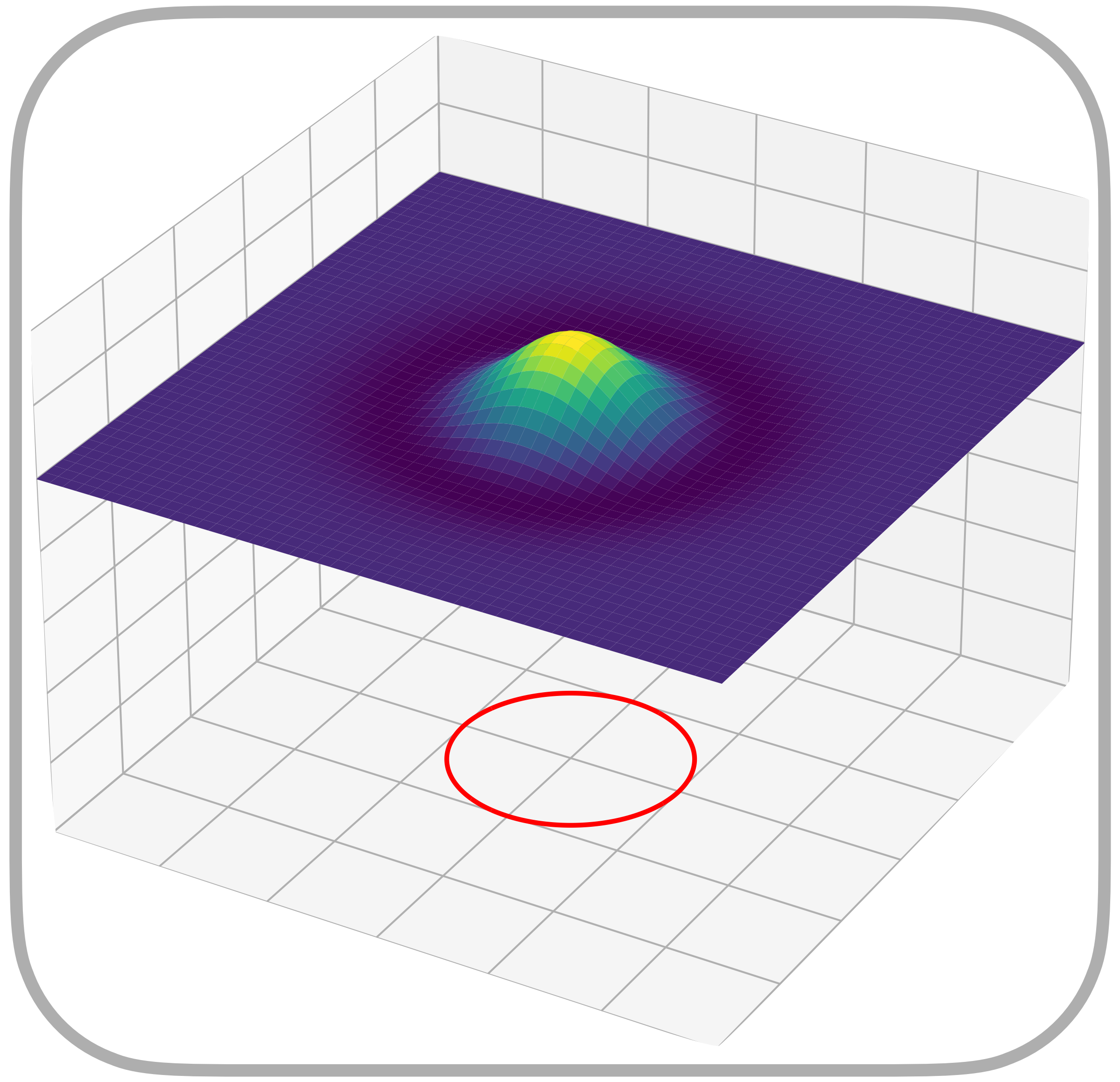
★ **多行列式叠加**：节点面之间的干涉叠加，节点重组，改变节点面拓扑结构　　**拓扑修正**

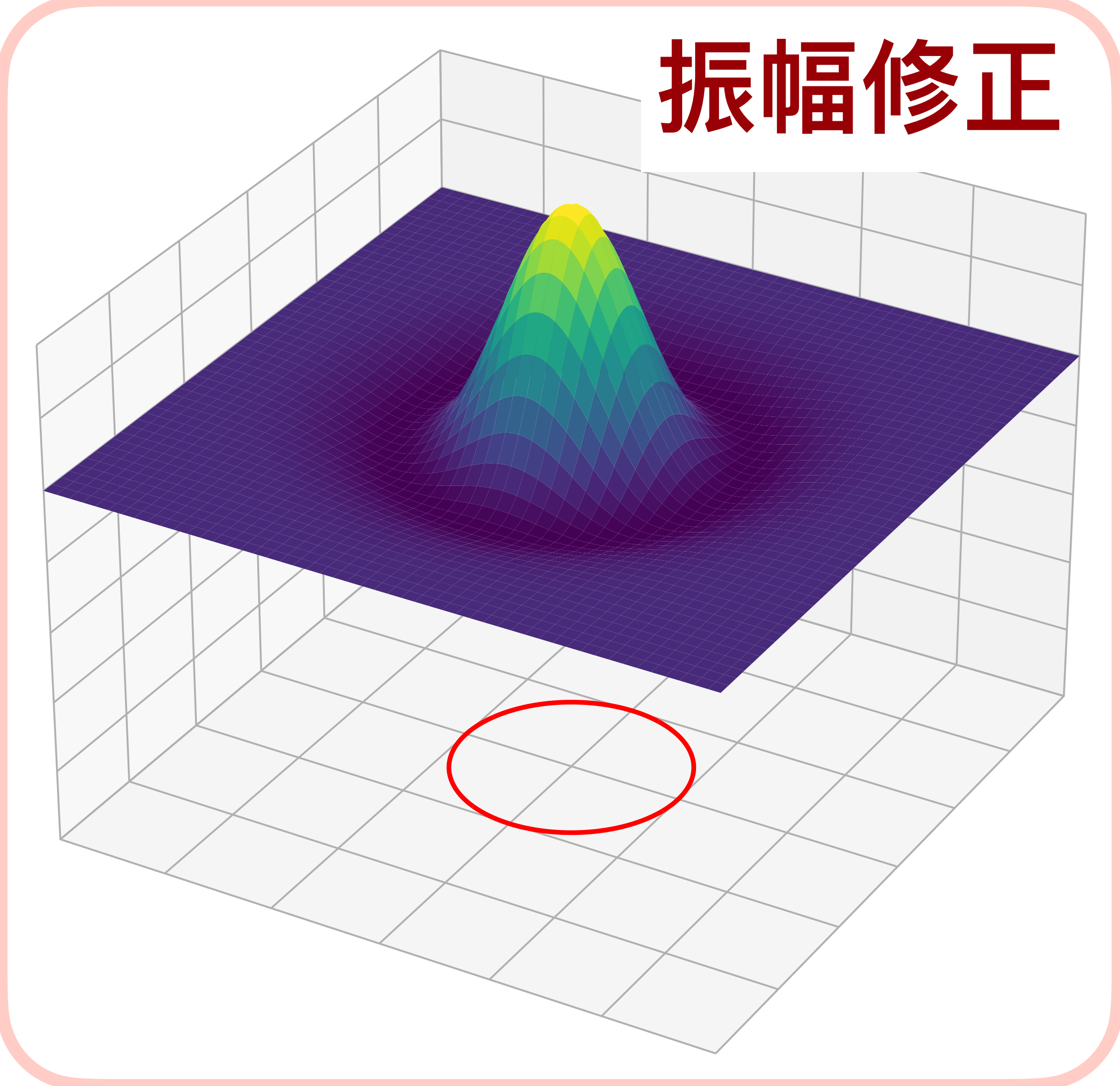
$$\Psi^{(\alpha)}(\boldsymbol{x}_1,\ldots,\boldsymbol{x}_A) = \mathrm{e}^{\mathcal{U}^{(\alpha)}(\boldsymbol{x}_1,\ldots,\boldsymbol{x}_A)} \sum_n w_n \det \boldsymbol{\Phi}^{(\alpha,n)}(\boldsymbol{x}_1,\ldots,\boldsymbol{x}_A), \quad \alpha = \mathrm{R},\mathrm{I}.$$

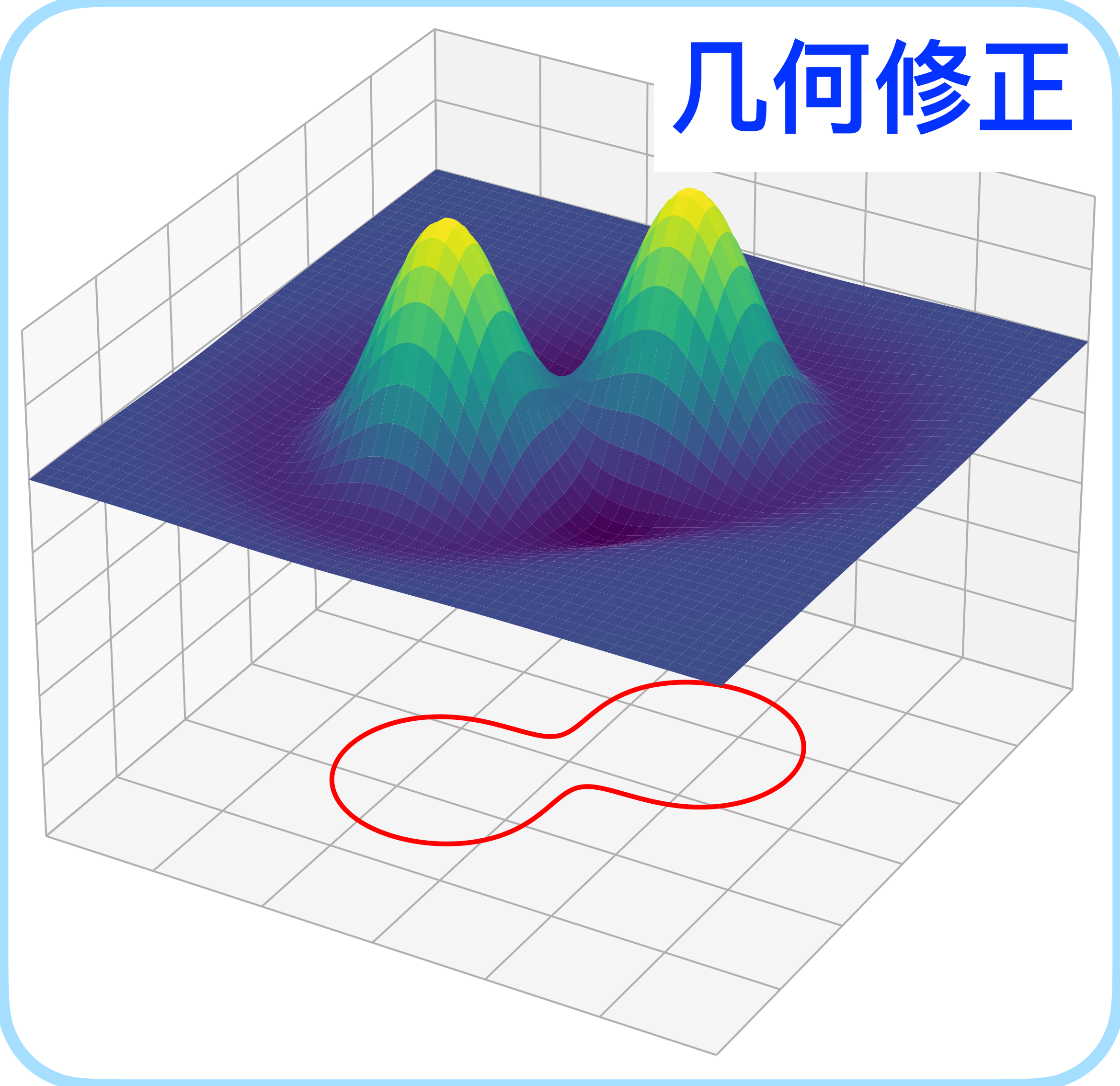
Complexed valued network!

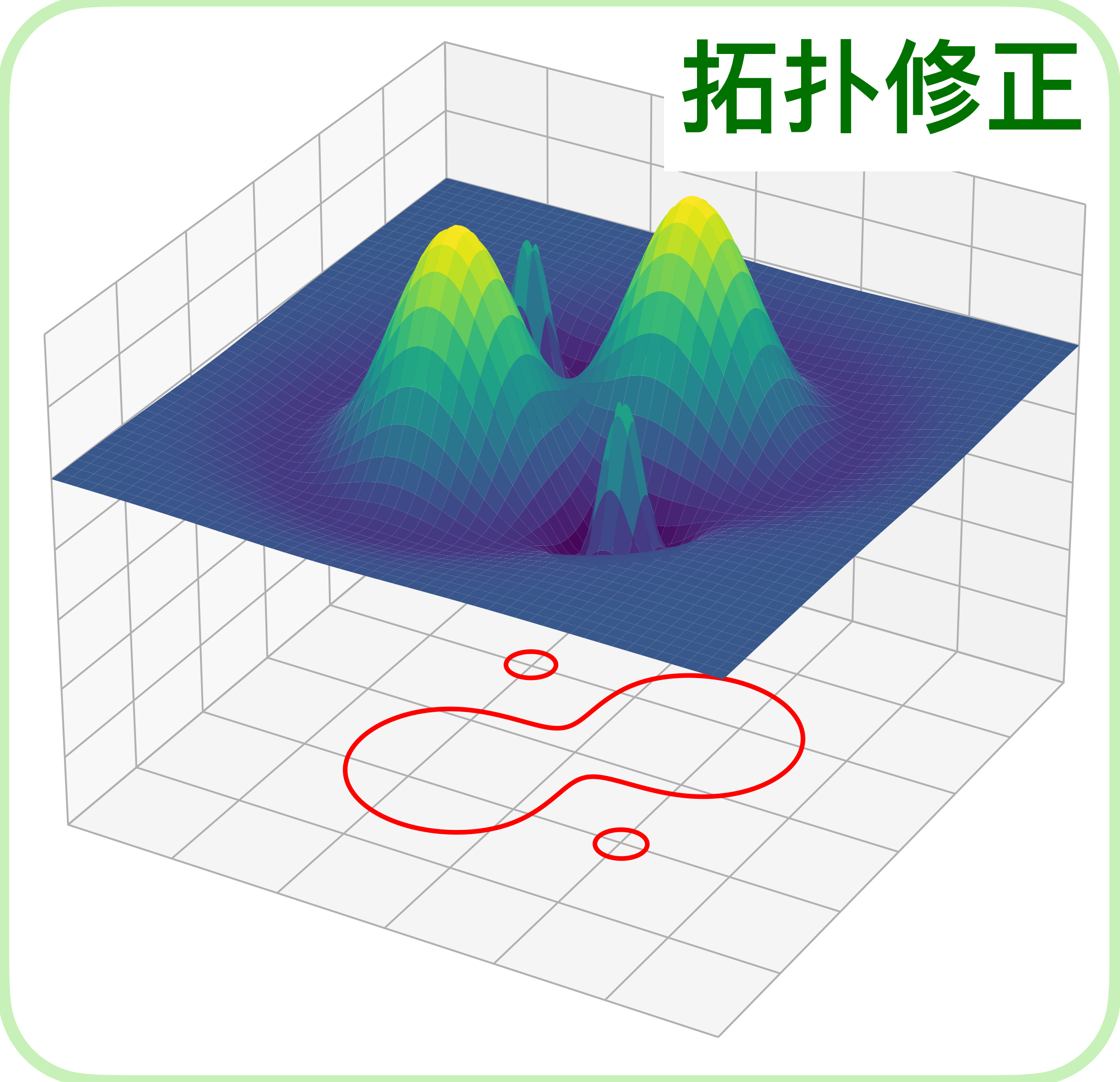
$$[\boldsymbol{\Phi}^{(\alpha,n)}]_{i\mu} = \mathbf{f}^{(\alpha,n)}_{i\mu}(\boldsymbol{x}_1,\ldots,\boldsymbol{x}_A)\varphi_\mu(\boldsymbol{x}_i)$$

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





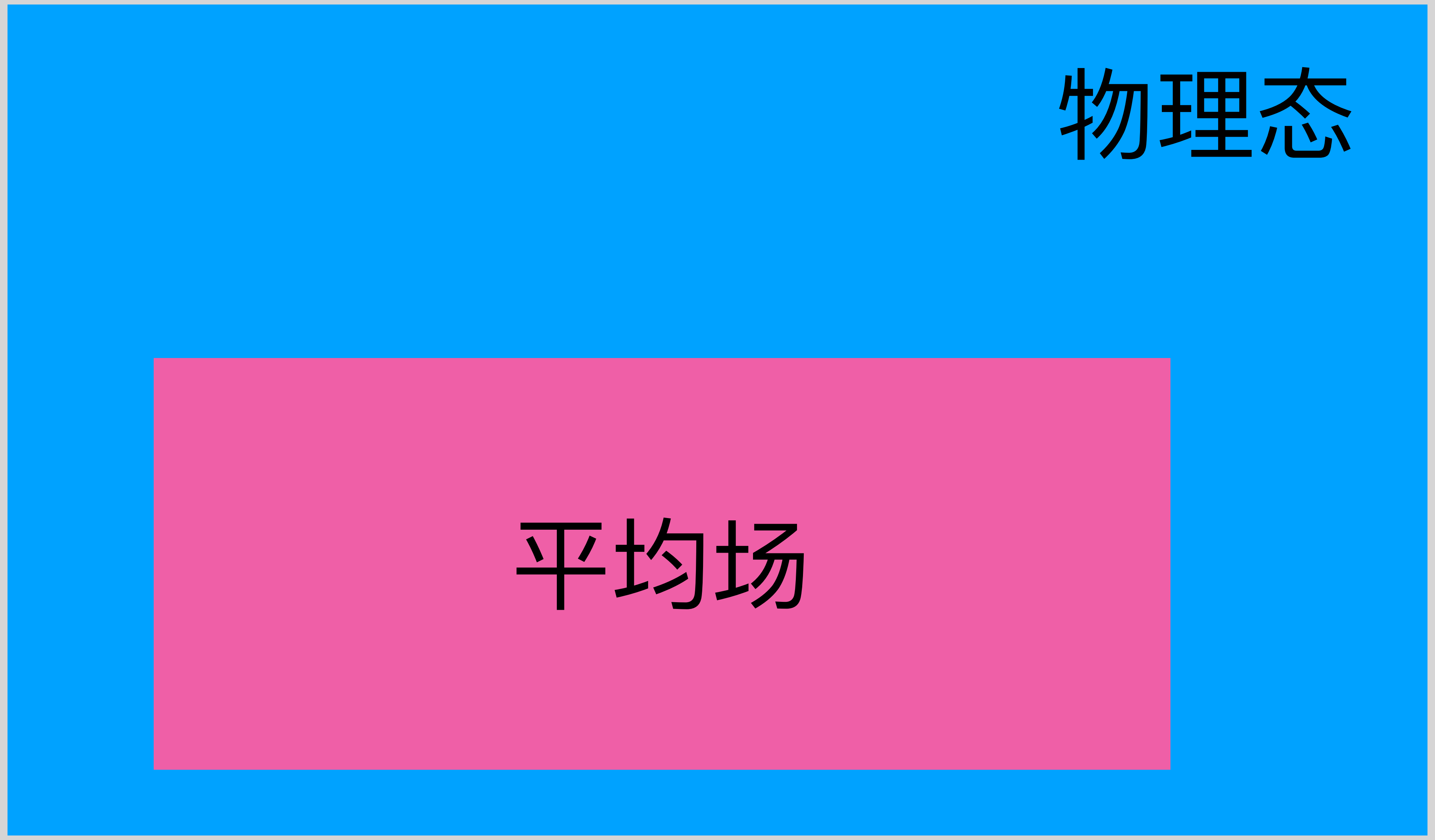


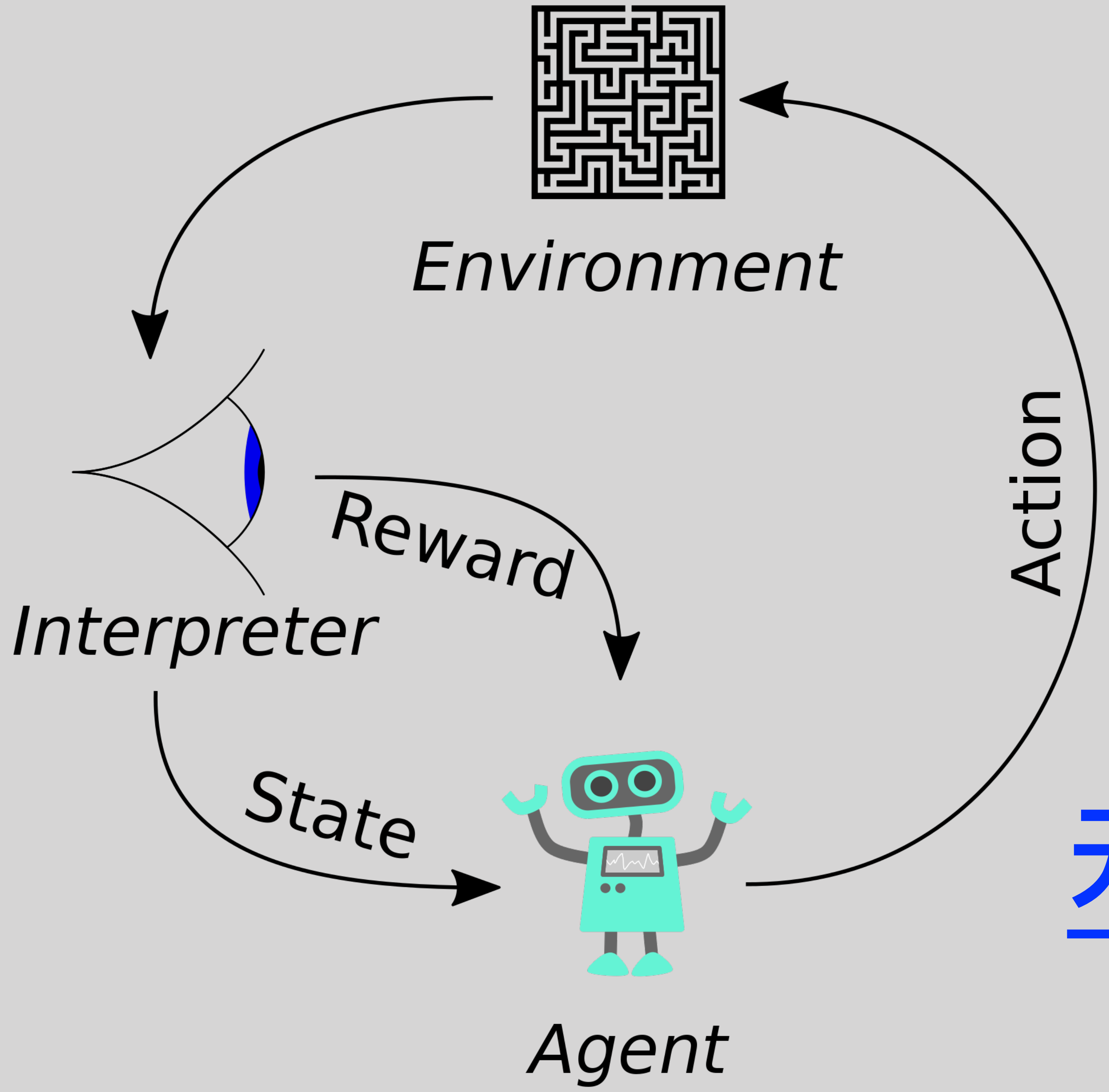


人工神经网络波函数

希尔伯特空间

$$\hat{H}\Psi = E\Psi$$

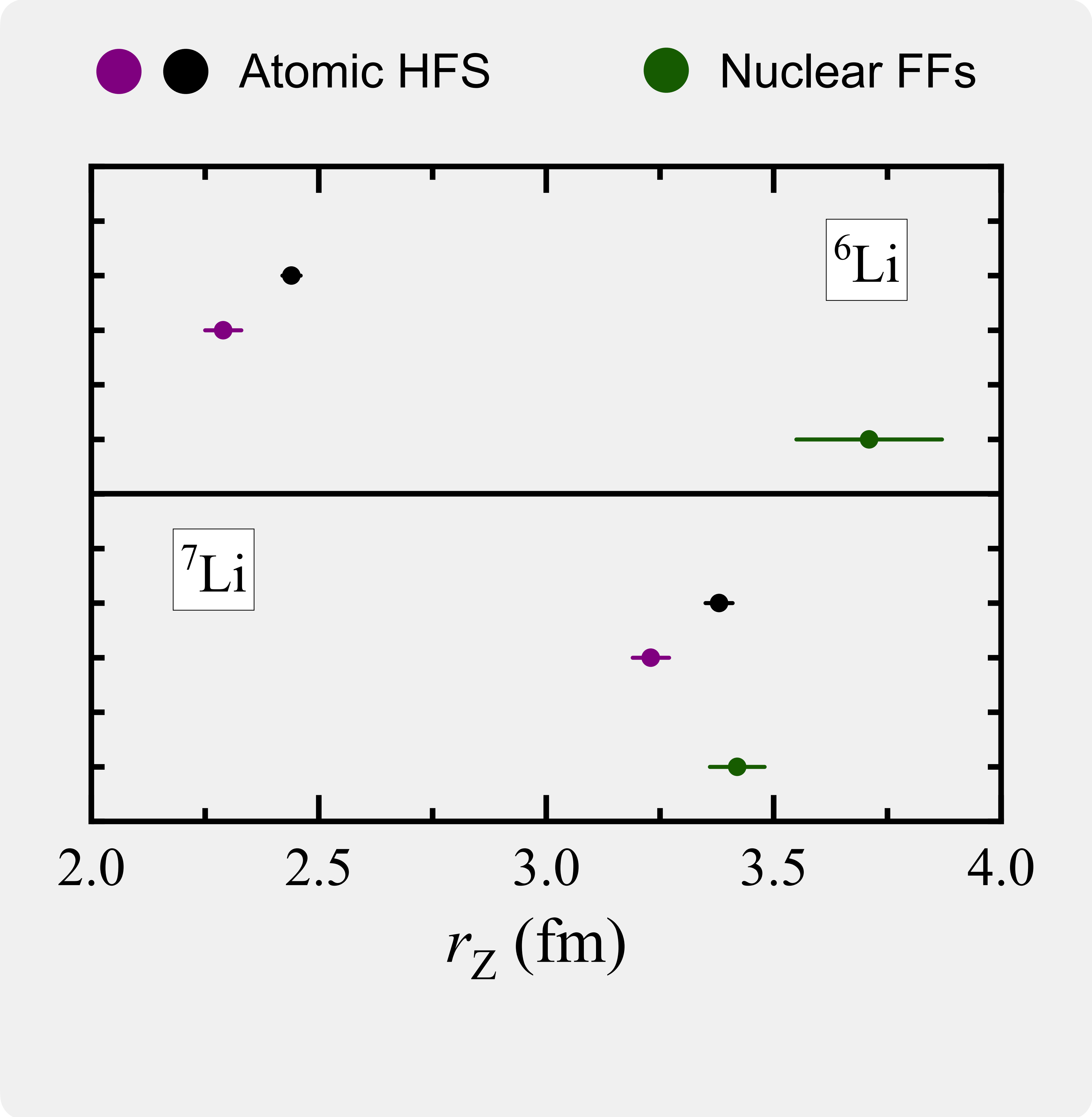




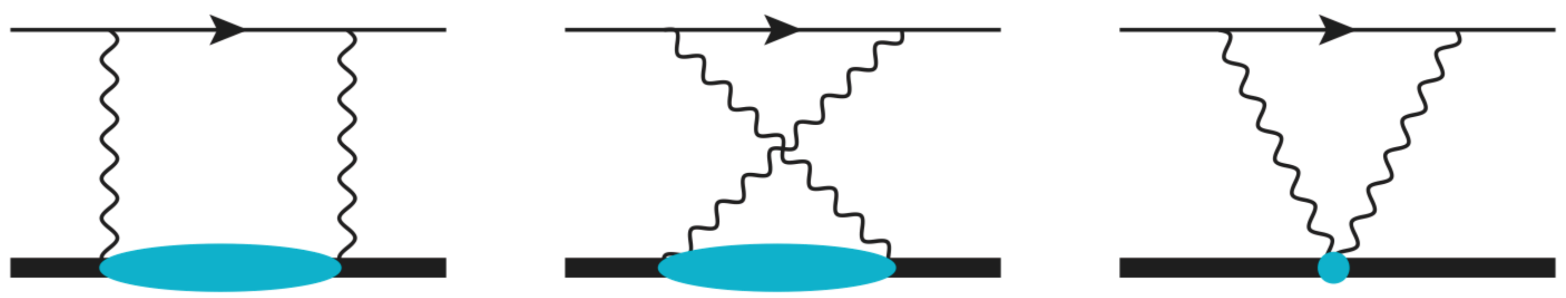
无需训练数据
强化学习

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

FeynmanNet的应用：Zemach 半径的 Li-Puzzle



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



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

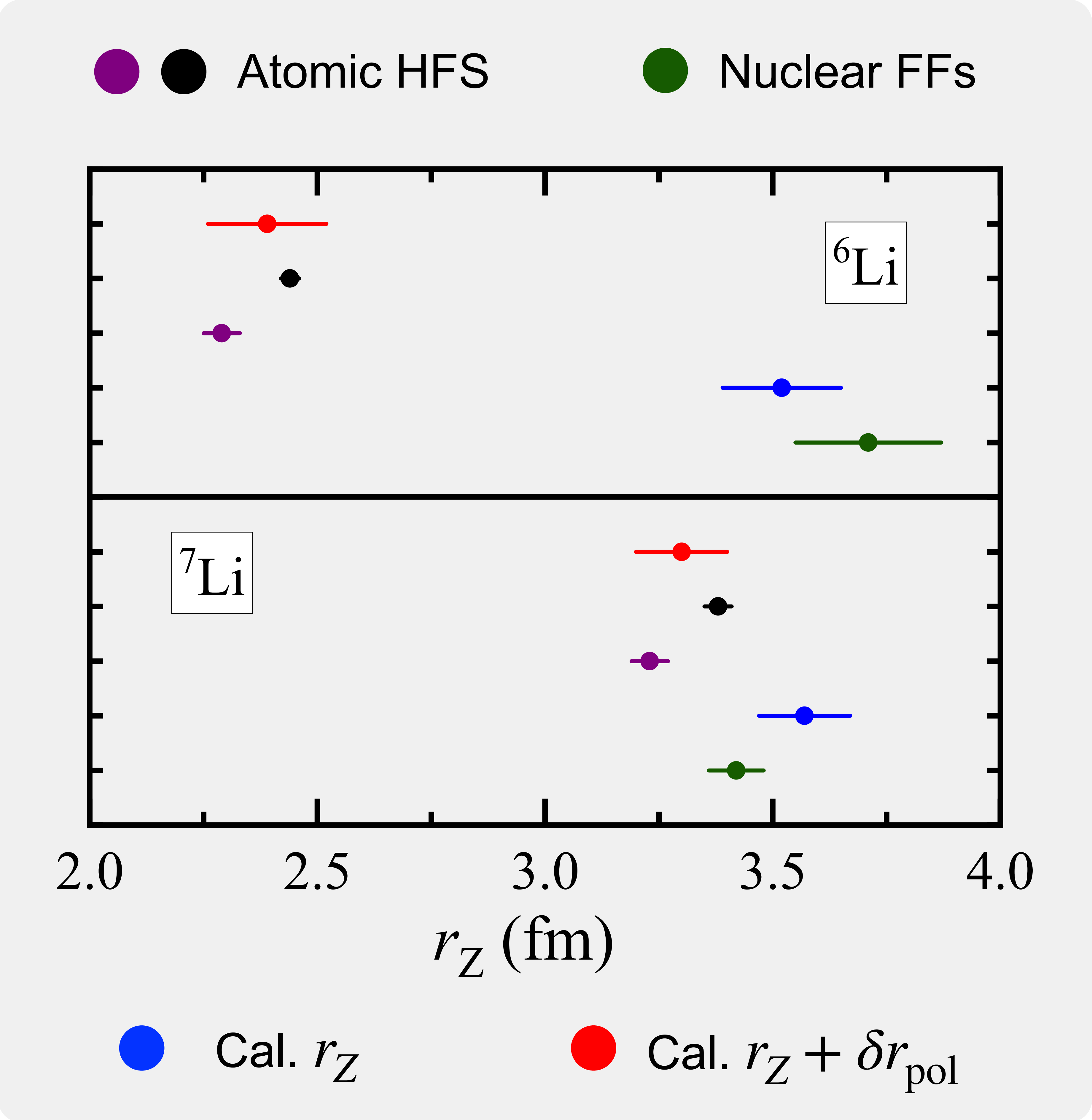
$$\simeq \begin{cases} -\dfrac{1}{Z} \dfrac{\mu_p}{\mu_p + \mu_n} \delta r_p(\bar{\omega}) & \text{odd-odd} \\ -\dfrac{1}{Z} \delta r_p(\bar{\omega}) & \text{odd-even} \\ 0 & \text{even-odd} \end{cases}$$

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

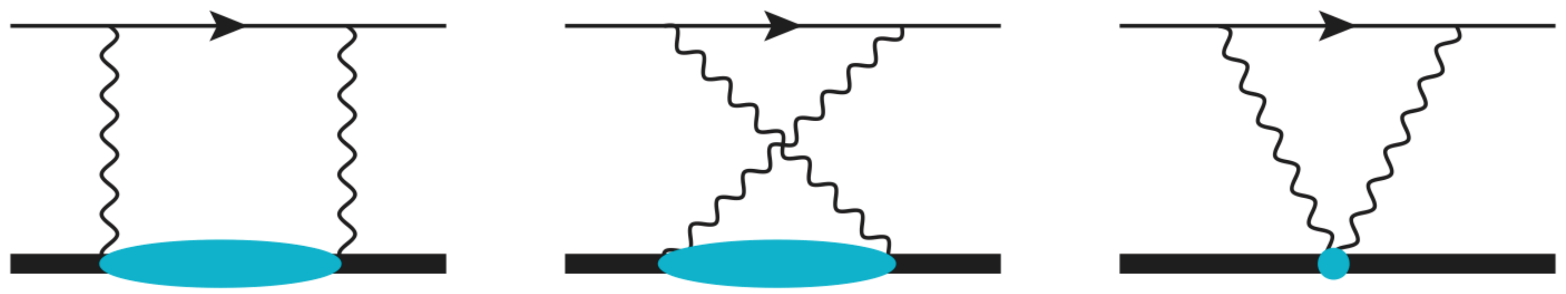
<u>Nuclear polarizability:</u> the dominant source for solving the puzzle

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

FeynmanNet的应用：Zemach 半径的 Li-Puzzle



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



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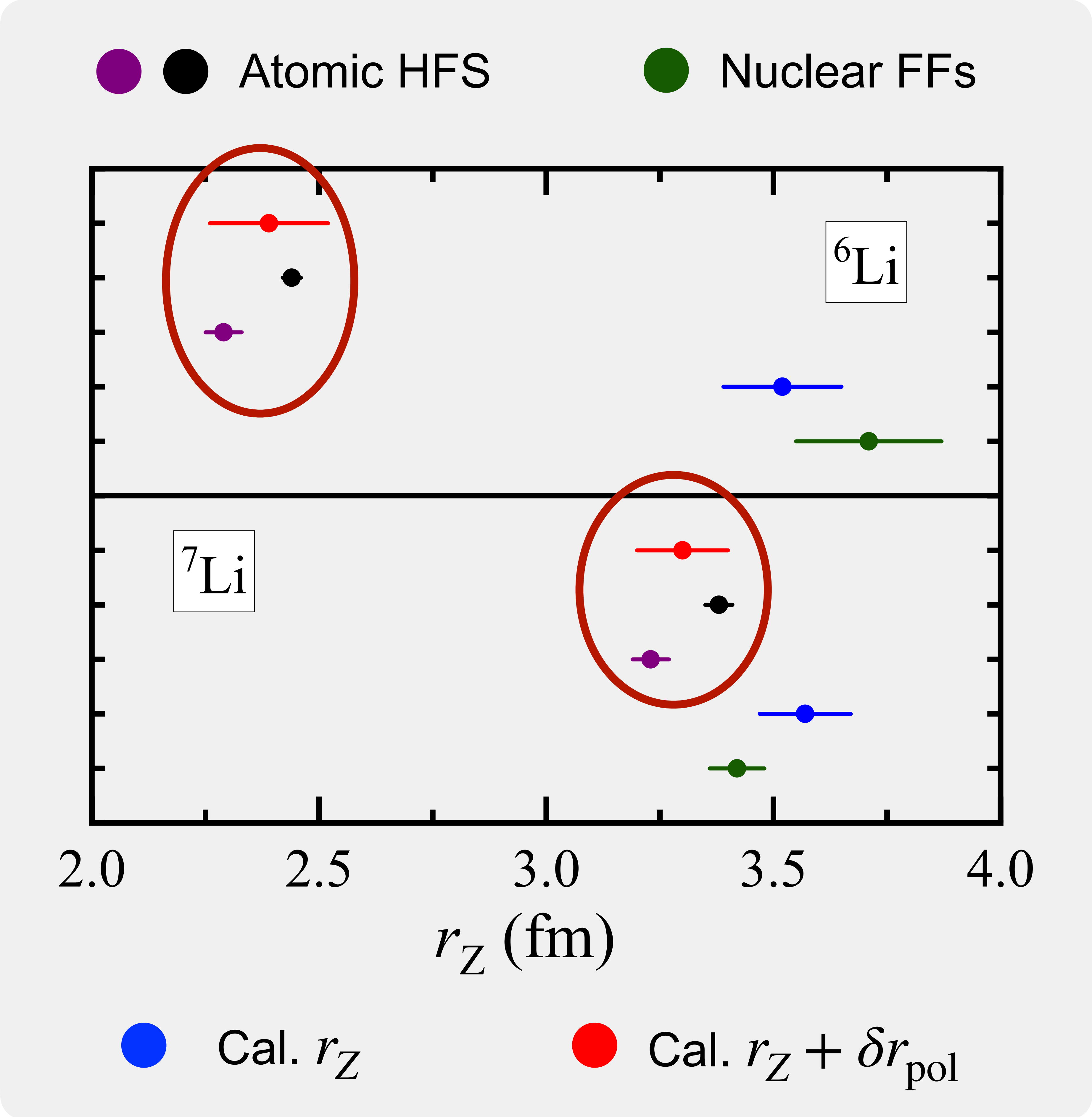

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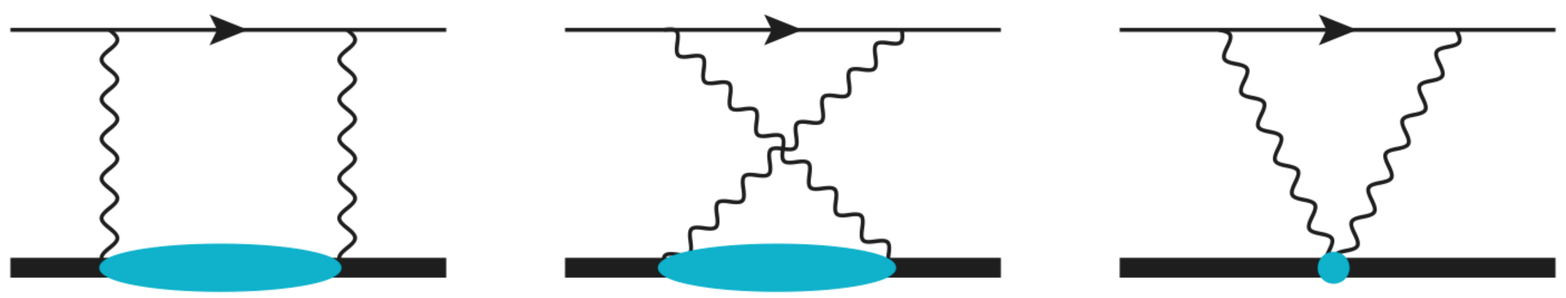

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Where do the **next ten years** take us?

到2030年，**平均场模型**与**第一性原理方法**的结合，有望对中等质量原子核乃至更重核区的核结构和核反应，提供带有定量不确定度评估的预言。 —— Long Range Plan 2023

Progress in Particle and Nuclear Physics 109 (2019) 103713

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Review

Towards an *ab initio* covariant density functional theory for nuclear structure

Shihang Shen [a,b,c], Haozhao Liang [d,e], Wen Hui Long [f,g], Jie Meng [a,h,i,*], Peter Ring [a,j]

Progress in Particle and Nuclear Physics 64 (2010) 120–168

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Review

Toward *ab initio* density functional theory for nuclei

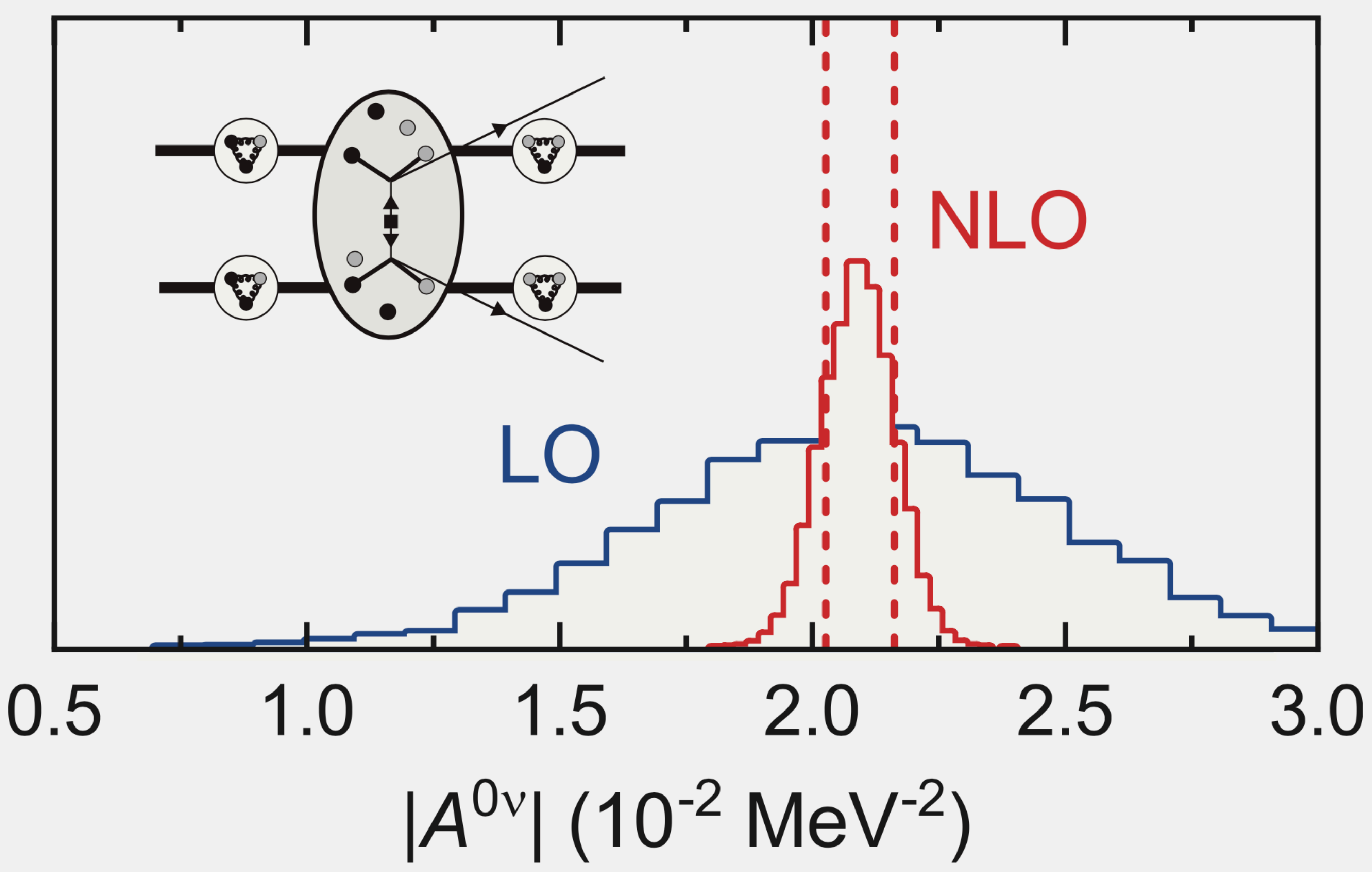
J.E. Drut, R.J. Furnstahl *, L. Platter

Department of Physics, Ohio State University, Columbus, OH 43210, United States

展望

适用于**中重核**的高精度第一性原理计算方法 **FeynmanNet+**

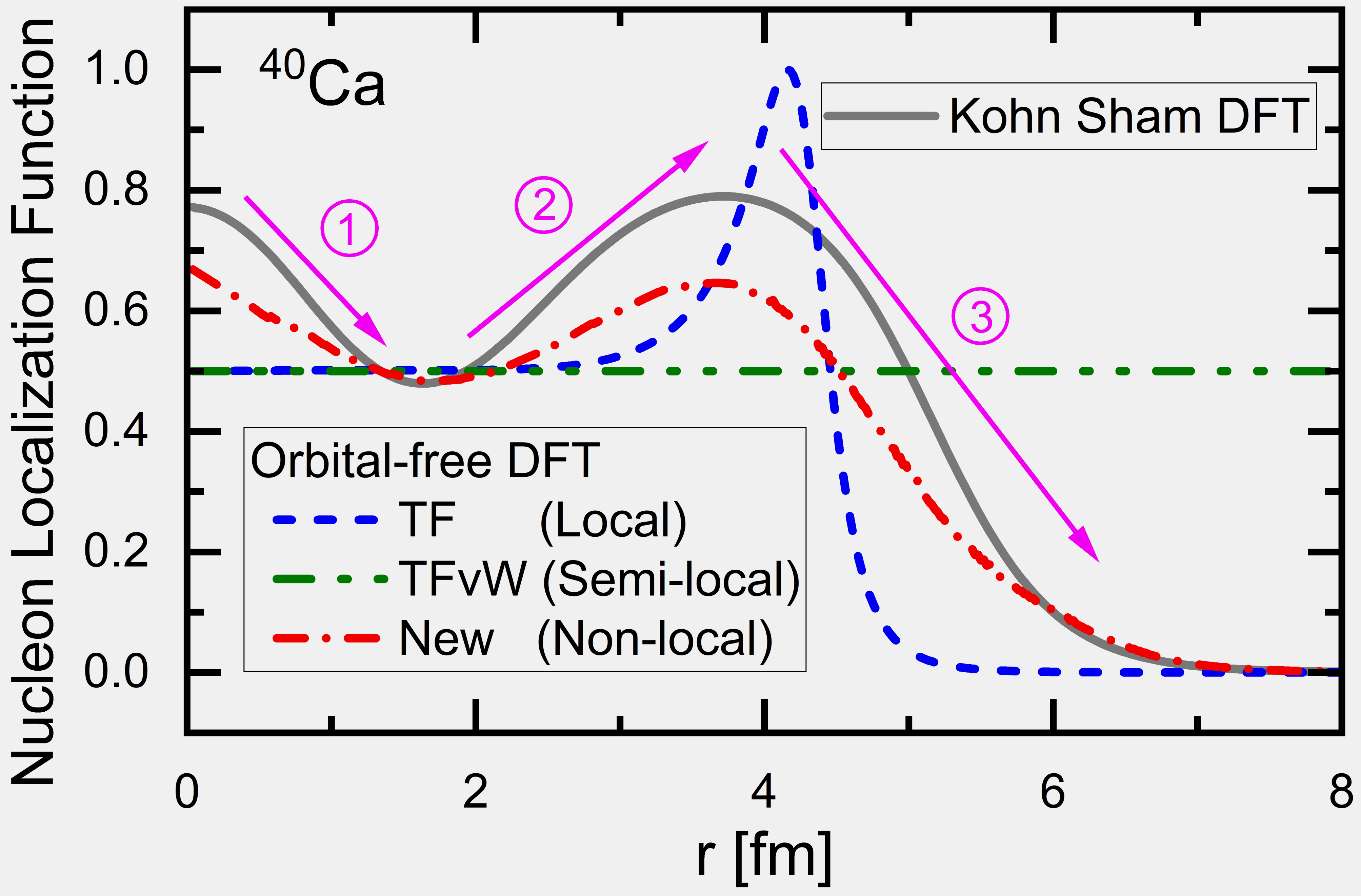
无中微子双贝塔衰变



Yang and **PWZ***, PLB 855, 138782 (2024)

Yang and **PWZ***, PRL 134, 242502 (2025)

第一性原理密度泛函



Wu, Ren, **PWZ***, PRC 105, L031303 (2022)

Wu*, Colò*, Hagino*, **PWZ***, PRL 136, 092501 (2026)