利用神经网络求解第一性原理核多体问题

杨一龙

北京大学物理学院

导师：孟杰、赵鹏巍

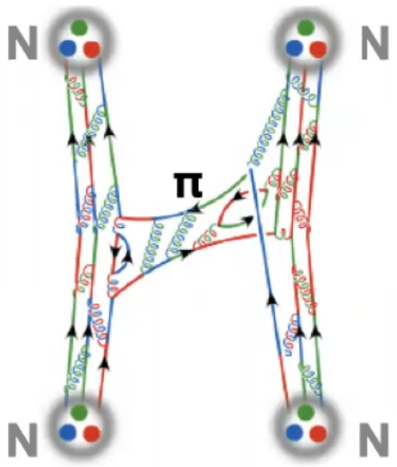
Email: yl_yang@pku.edu.cn

目录

核多体问题

- 原子核：核子组成的强相互作用量子多体系统

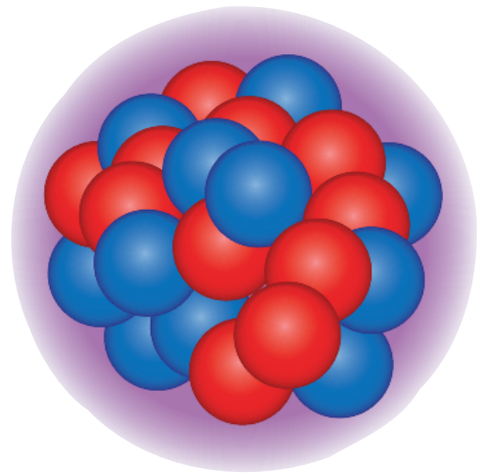
核力



$$H = -\frac{1}{2M_N}\sum_i^A \nabla_i^2 + \sum_{ij}^A v_{ij} + \dots$$

$$H\Psi(\boldsymbol{r}_1, \dots, \boldsymbol{r}_A) = E\Psi(\boldsymbol{r}_1, \dots, \boldsymbol{r}_A)$$

原子核结构

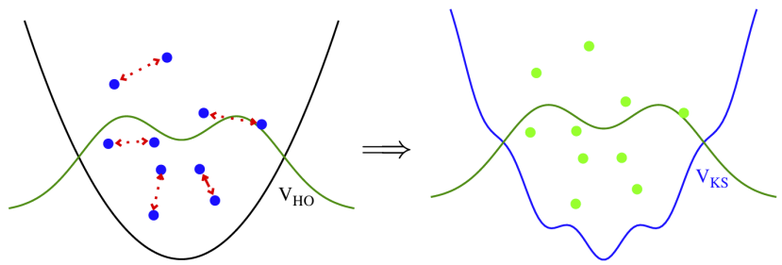


- 精确求解核多体问题是核结构研究的关键挑战
  - 从波函数提取可观测量: 结合能、半径、密度分布…
  - 求解面临的挑战：核力的强排斥芯、Hilbert 空间维度的指数增长…

原子核的第一性原理计算

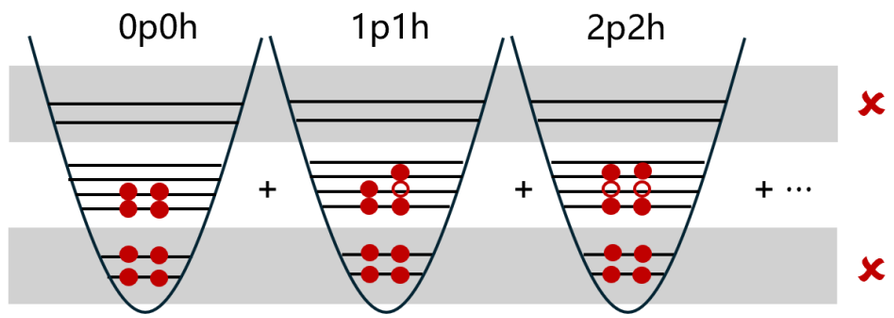
- Hartree-Fock 平均场模型，密度泛函理论

$\Psi(\boldsymbol{r}_1, \ldots, \boldsymbol{r}_A) \Rightarrow$ Slater 行列式　　$H \Rightarrow E[\rho(\boldsymbol{r})]$



- 组态相互作用壳模型

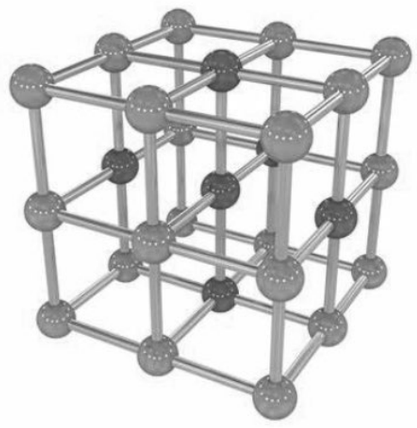
$\Psi(\boldsymbol{r}_1, \ldots, \boldsymbol{r}_A) \Rightarrow \Psi(\boldsymbol{r}_{\text{val}})$　　$H \Rightarrow H_{\text{eff}}$



- **第一性原理计算：从自由空间的核力出发，求解多体波函数 $\Psi(\boldsymbol{r}_1, \ldots, \boldsymbol{r}_A)$**

$$\left(\sum_{i=1}^{A} -\frac{\nabla_i^2}{2m} + \sum_{i<j} \hat{v}_{ij} + \sum_{i<j<k} \hat{V}_{ijk} \right) \Psi(\boldsymbol{r}_1, \ldots, \boldsymbol{r}_A) = E\Psi(\boldsymbol{r}_1, \ldots, \boldsymbol{r}_A)$$

Hilbert 空间的维度指数增长：　$A = 6$　　$N_{\text{grid}} \sim 10^{18}$



变分蒙特卡洛（VMC）

- **蒙特卡洛**：利用随机数计算高维度的积分
- **变分蒙特卡洛**：结合蒙特卡洛与变分原理求解薛定谔方程

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

变分原理

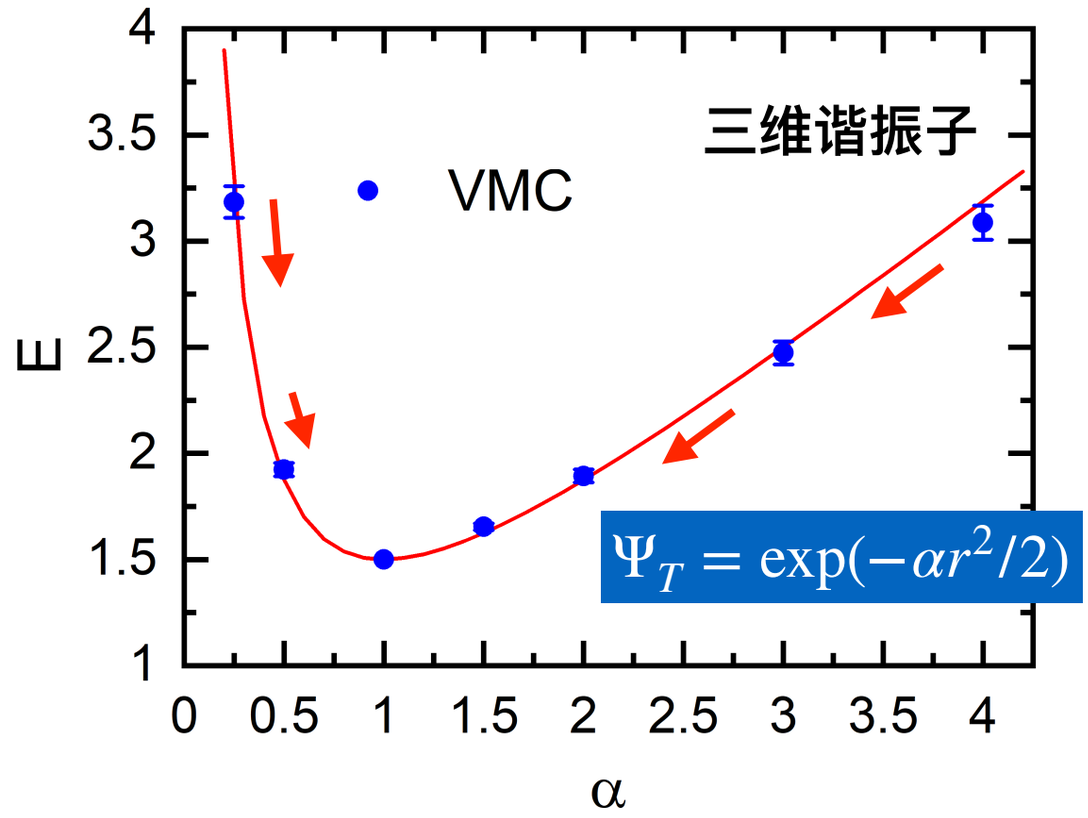
$$E_0 = \min_{\Psi} \langle \hat{H} \rangle_{\Psi} = \min_{\Psi} \frac{\langle \Psi | \hat{H} | \Psi \rangle}{\langle \Psi | \Psi \rangle}$$

蒙特卡洛积分

$$\langle \hat{H} \rangle_{\Psi} = \frac{\int \mathrm{d}\boldsymbol{R} \Psi^{\dagger}(\boldsymbol{R}) \hat{H} \Psi(\boldsymbol{R})}{\int \mathrm{d}\boldsymbol{R} |\Psi(\boldsymbol{R})|^2}$$

$$= \frac{1}{N} \sum_{n=1}^{N} \frac{\hat{H}\Psi(\boldsymbol{R}^{(n)})}{\Psi(\boldsymbol{R}^{(n)})} \pm \sigma$$

$\boldsymbol{R} = (\boldsymbol{r}_1, \ldots, \boldsymbol{r}_A)$



Metropolis et al., J. Chem. Phys. 21, 1087 (1953)

变分蒙特卡洛（VMC）

- **蒙特卡洛**：利用随机数计算高维度的积分
- **变分蒙特卡洛**：结合蒙特卡洛与变分原理求解薛定谔方程

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

变分原理

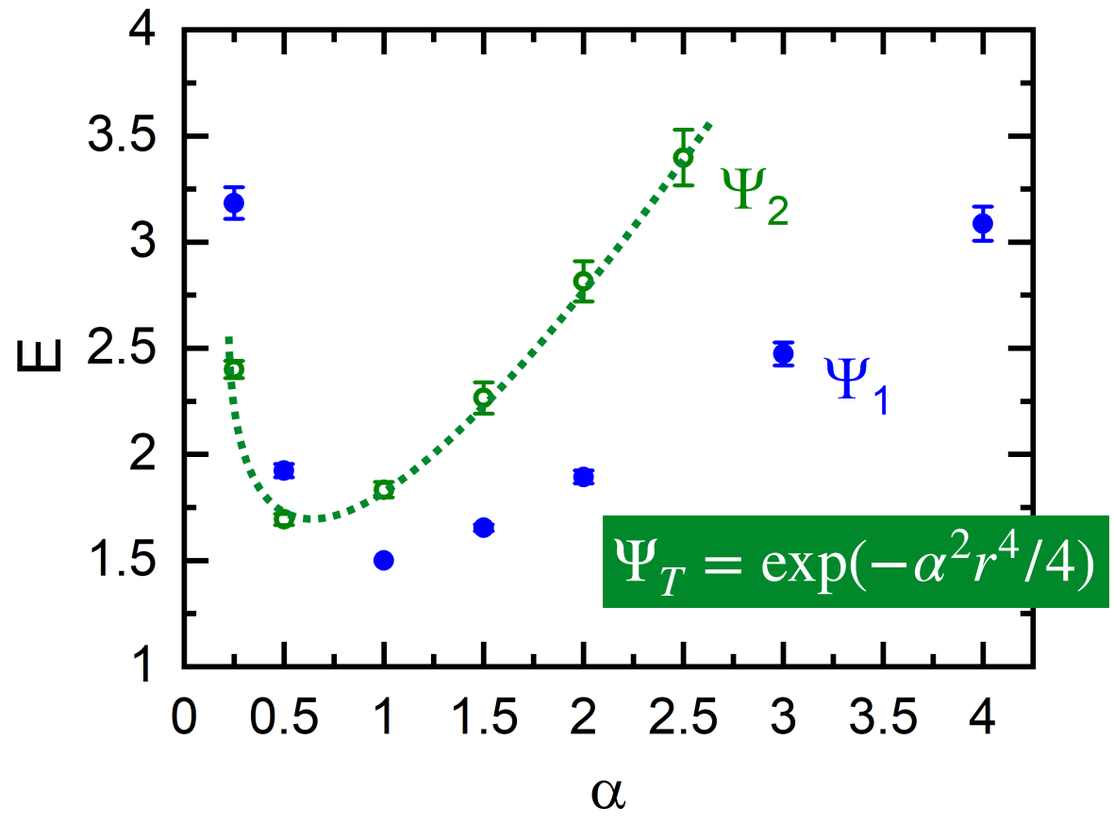
$$E_0 = \min_{\Psi} \langle \hat{H} \rangle_{\Psi} = \min_{\Psi} \frac{\langle \Psi | \hat{H} | \Psi \rangle}{\langle \Psi | \Psi \rangle}$$

蒙特卡洛积分

$$\langle \hat{H} \rangle_{\Psi} = \frac{\int \mathrm{d}\boldsymbol{R} \Psi^{\dagger}(\boldsymbol{R}) \hat{H} \Psi(\boldsymbol{R})}{\int \mathrm{d}\boldsymbol{R} |\Psi(\boldsymbol{R})|^2}$$

$$= \frac{1}{N} \sum_{n=1}^{N} \frac{\hat{H}\Psi(\boldsymbol{R}^{(n)})}{\Psi(\boldsymbol{R}^{(n)})} \pm \sigma$$

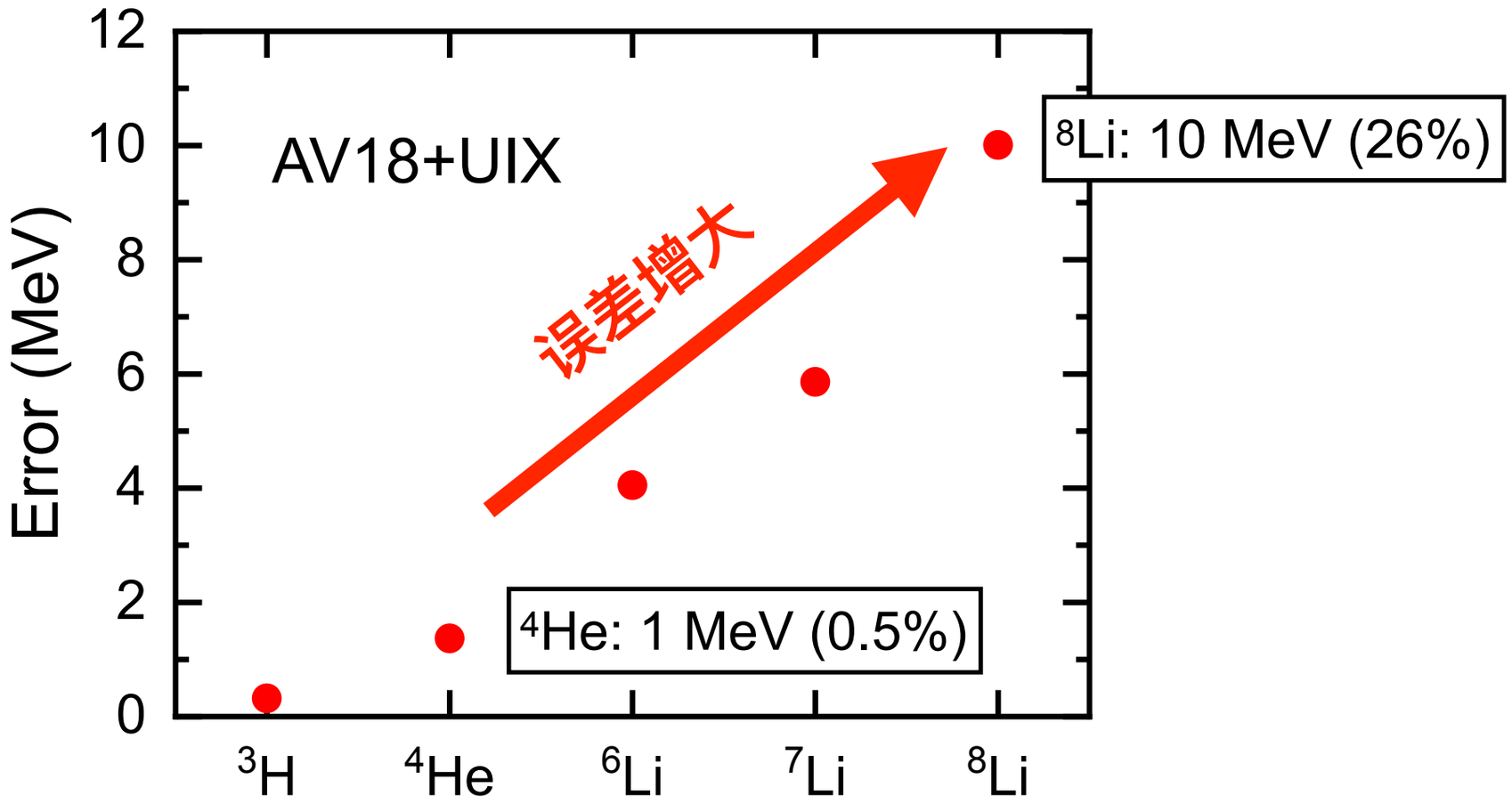
$\boldsymbol{R} = (\boldsymbol{x}_1, \ldots, \boldsymbol{x}_A)$



依赖于精确的试探波函数形式

构建核多体波函数的困难

- 传统的试探波函数精度较低



$$\Psi(\boldsymbol{r}_1, \ldots, \boldsymbol{r}_A) = \mathcal{S}\left(\prod_{i<j} \hat{U}_{ij}\right) \det[\phi_\mu(\boldsymbol{r}_i)]$$

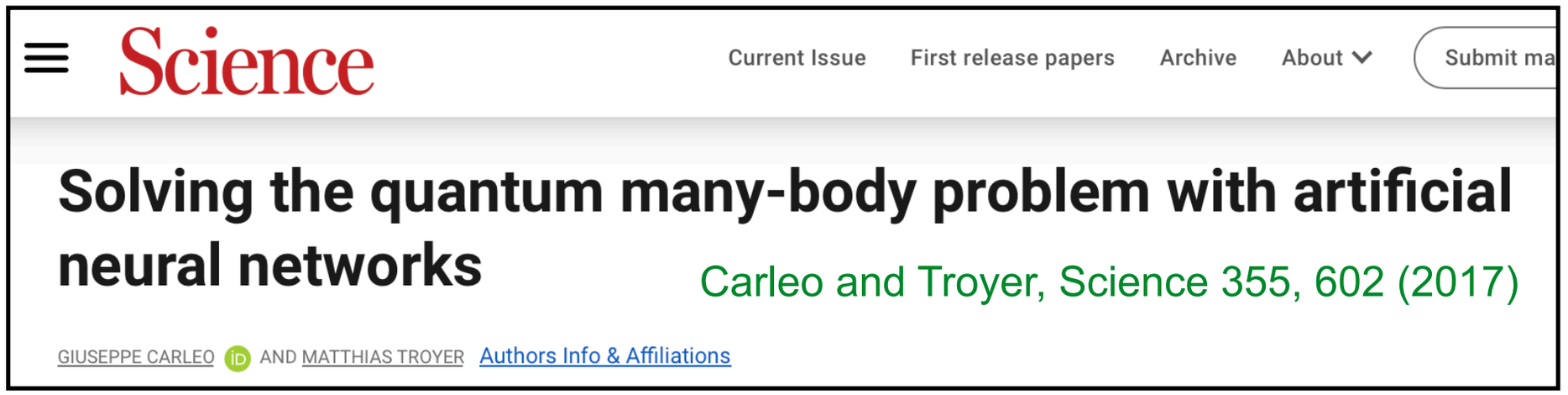
Results taken from Wiringa, Pieper, Carlson and Pandharipande, PRC 62, 014001 (2000)

如何为核多体系统构建更精确的试探波函数?

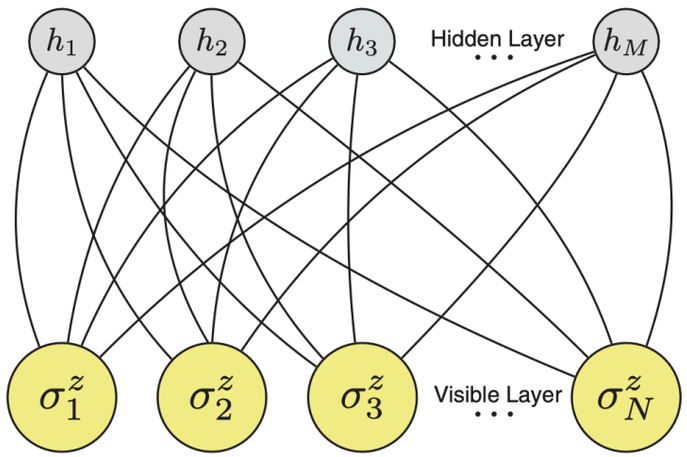
利用神经网络构建试探波函数

利用神经网络构建试探波函数

神经网络具有表示复杂高维函数的强大能力，可作为量子多体系统的试探波函数



$$\Psi\left(\quad\right) =$$



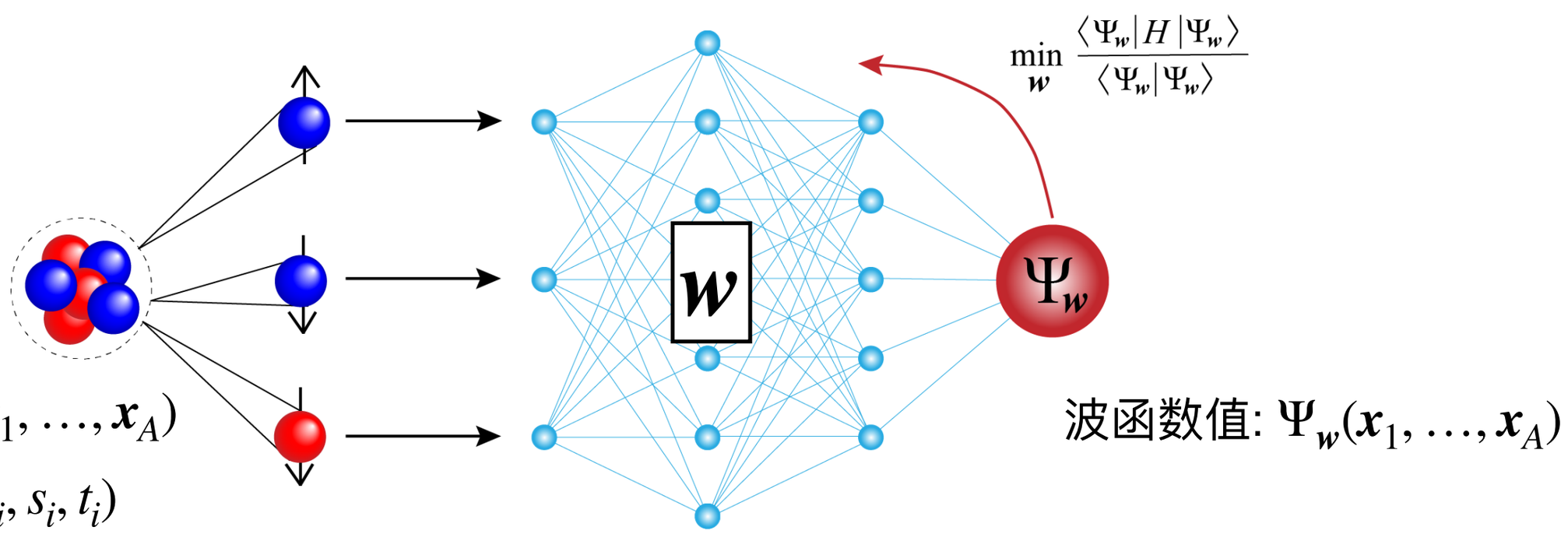
第一性原理量子化学

FermiNet PauliNet

Pfau et al., Phys. Rev. Res. 2, 033429 (2020)
Hermann et al., Nat. Chem. 12, 891 (2020)

神经网络量子蒙特卡洛方法

- 基于神经网络 (ANN) 构建试探波函数

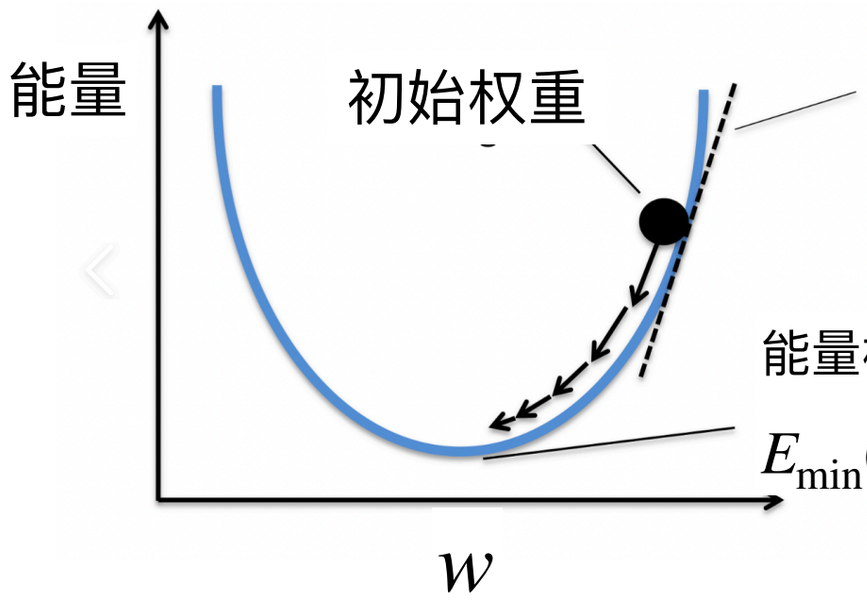


核子变量: $X = (x_1, \ldots, x_A)$

$x_i = (r_i, s_i, t_i)$

波函数值: $\Psi_w(x_1, \ldots, x_A)$

- 变分蒙特卡洛: 基于变分原理优化神经网络

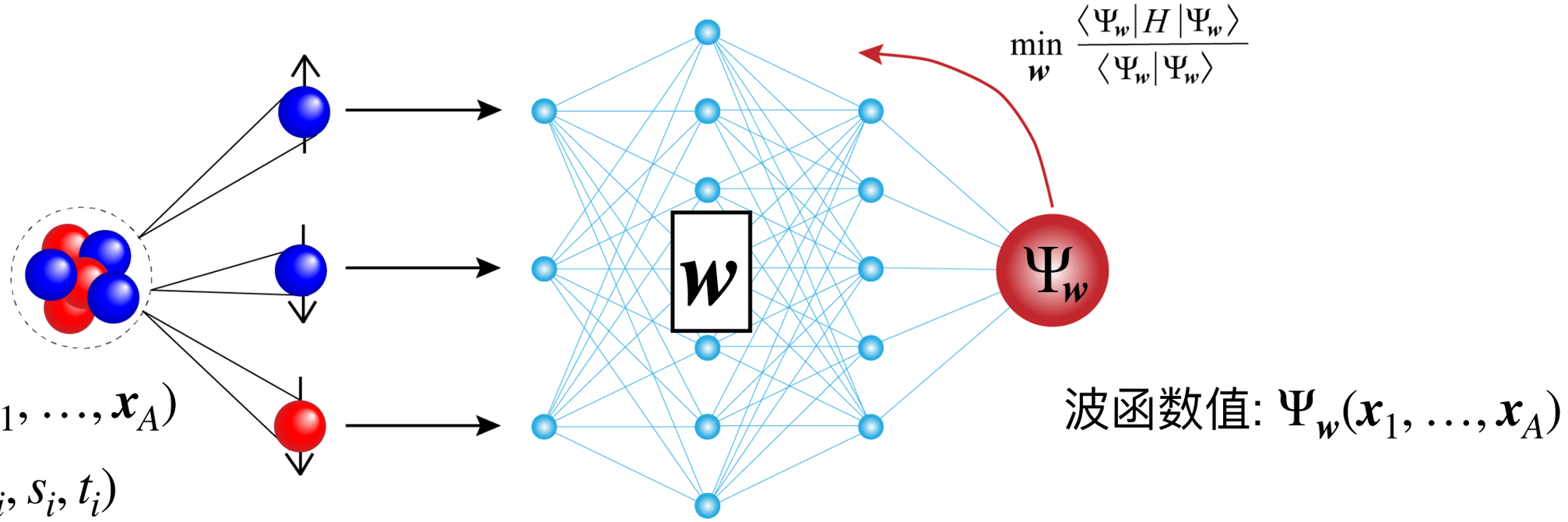


自然梯度下降法
(Stochastic reconfiguration)

Sorella, Phys. Rev. B 71, 241103(R) (2005

神经网络量子蒙特卡洛方法

- 基于神经网络 (ANN) 构建试探波函数

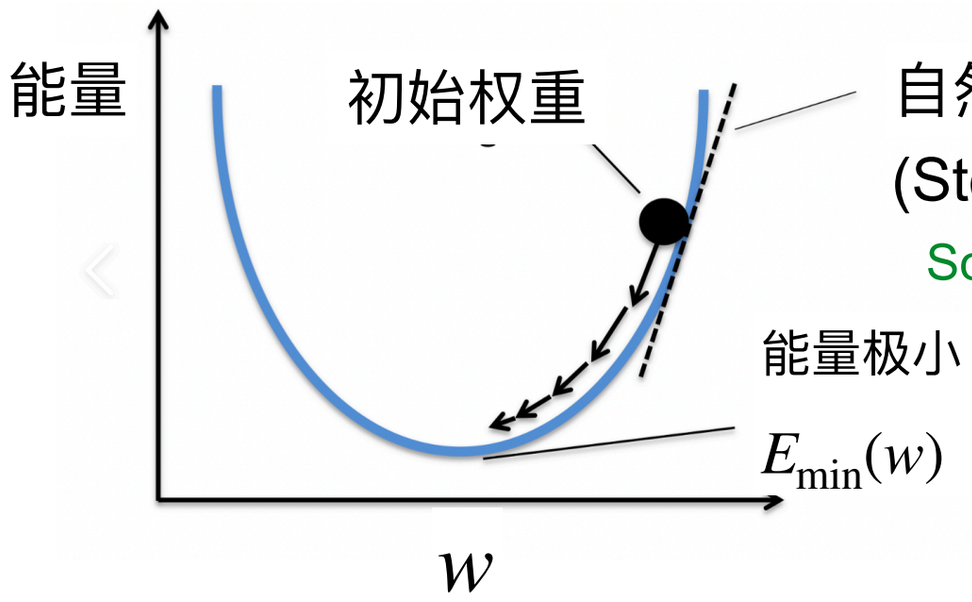


核子变量: $X = (x_1, \ldots, x_A)$

$x_i = (r_i, s_i, t_i)$

波函数值: $\Psi_w(x_1, \ldots, x_A)$

- 变分蒙特卡洛: 基于变分原理优化神经网络



自然梯度下降法
(Stochastic reconfiguration)

Sorella, Phys. Rev. B 71, 241103(R) (2005

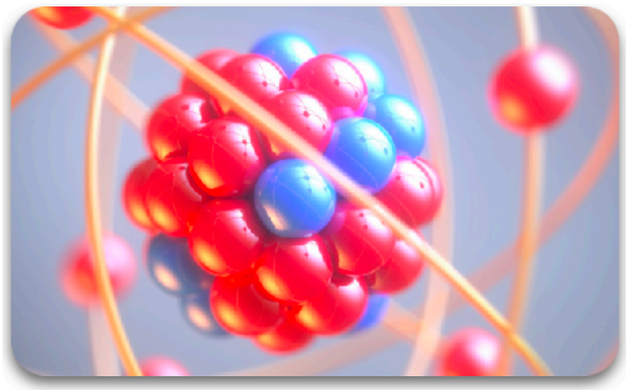
强化学习

强化学习框架

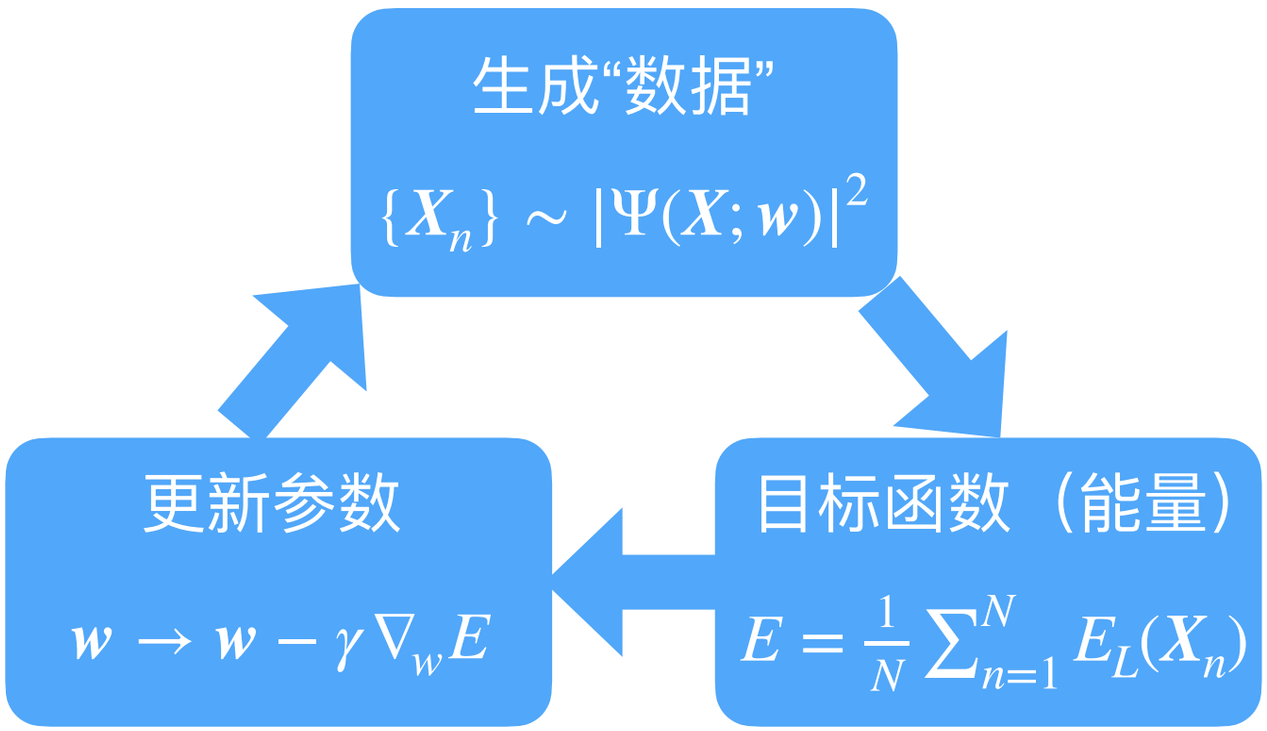
游戏规则 ⟷ 变分原理

自博弈 ⟷ 迭代变分

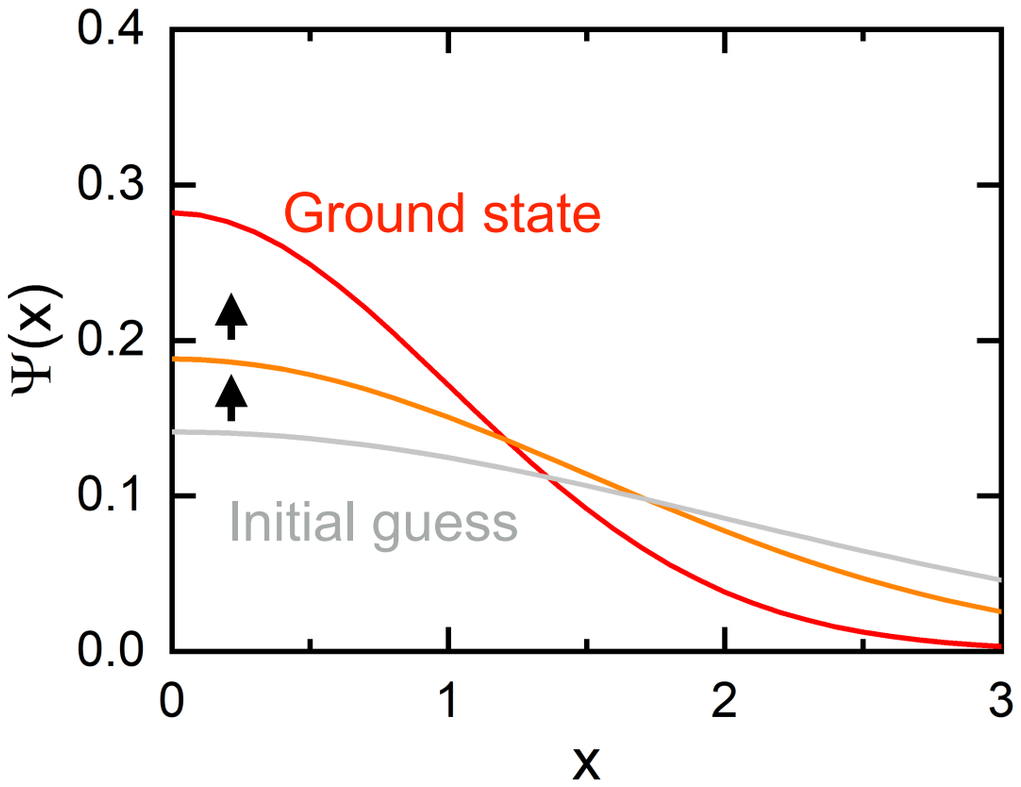
无需先验数据



迭代过程



神经网络波函数



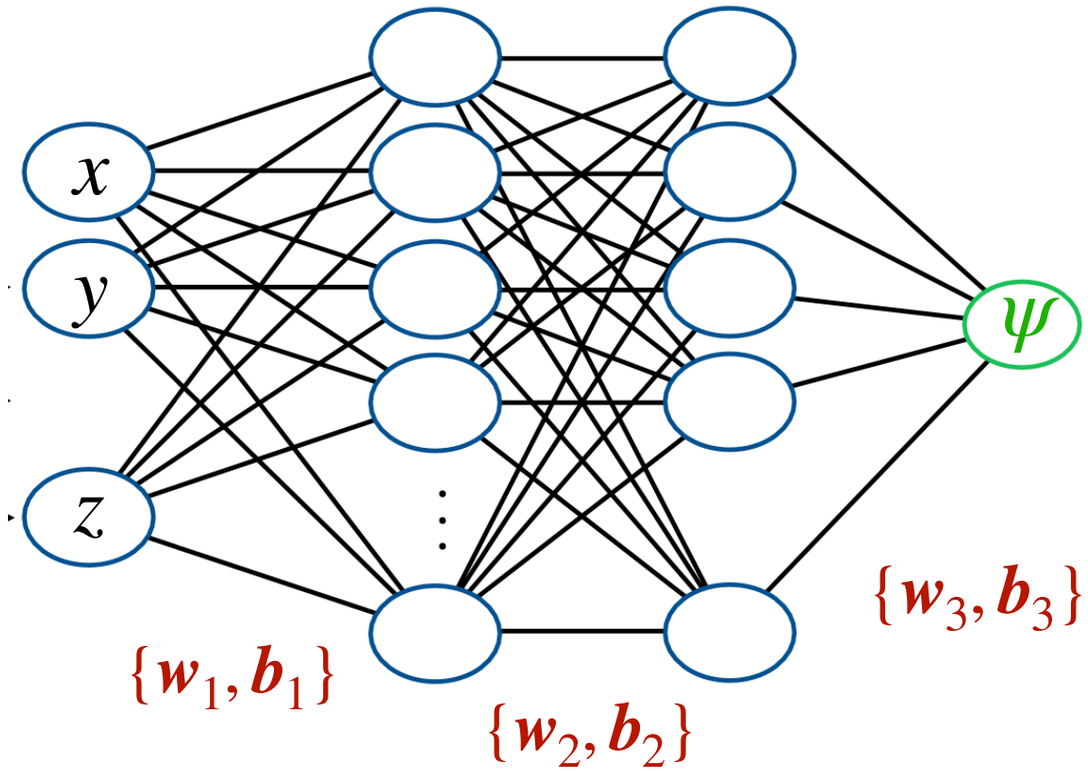
示例：求解单粒子薛定谔方程

- 考虑一个核子位于 Wood-Saxon 势阱中

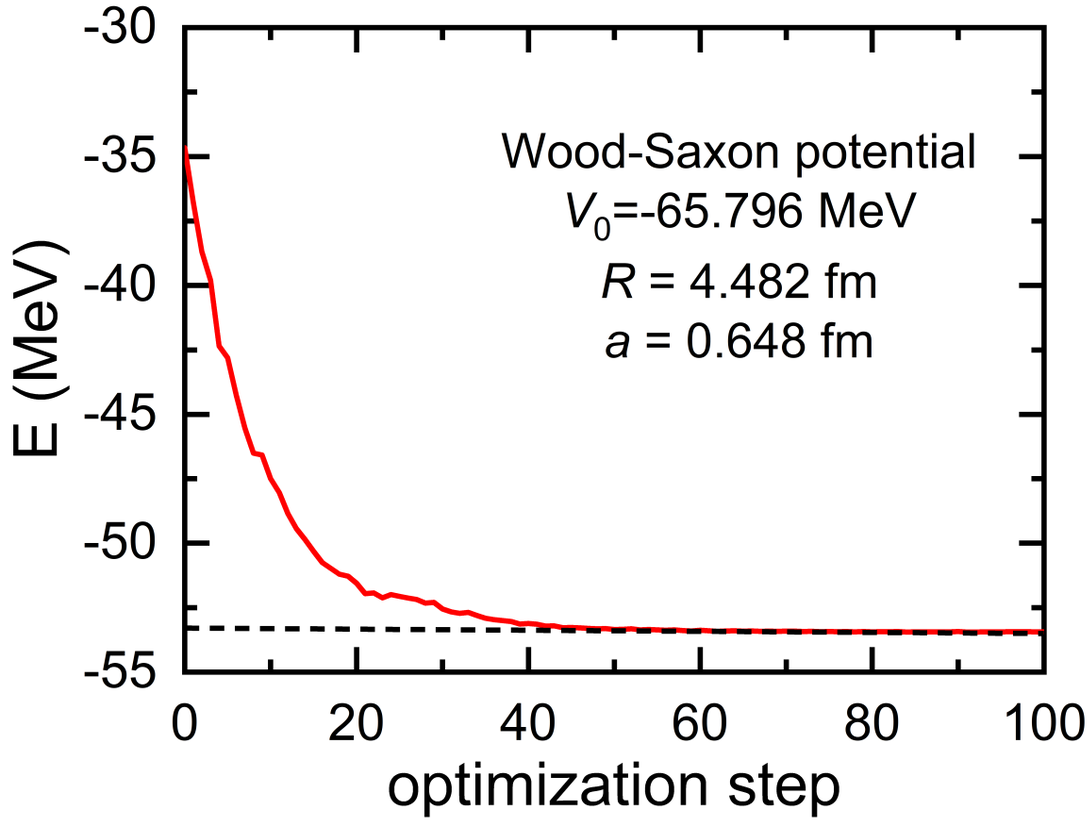
$$-\frac{\nabla^2}{2M_N}\psi(\boldsymbol{r}) + \frac{V_0}{1+\exp[(r-R_0)/a]}\psi(\boldsymbol{r}) = E\psi(\boldsymbol{r})$$

- 强化学习过程

前馈神经网络



自然梯度下降



核多体波函数

- 核多体波函数包含空间、自旋、同位旋自由度 $x_i = (\boldsymbol{r}_i, s_i, t_i)$，且需要满足核子之间的交换反对称性

$$\Psi(\ldots, x_i, \ldots, x_j, \ldots) = -\Psi(\ldots, x_j, \ldots, x_i, \ldots)$$

- 最简单的核多体波函数是一个 Slater 行列式，不包含多体关联

$$\det[\Phi] = \begin{vmatrix} \phi_1(x_1), & \phi_1(x_2), & \cdots, & \phi_1(x_A) \\ \phi_2(x_1), & \phi_2(x_2), & \cdots, & \phi_2(x_A) \\ \vdots, & \cdots, & \ddots, & \vdots \\ \phi_A(x_1), & \phi_A(x_2), & \cdots, & \phi_A(x_A) \end{vmatrix}$$

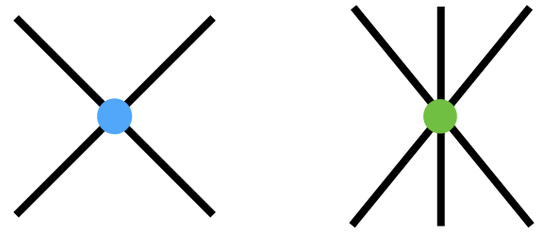
- **保证交换反对称性，针对核力的特点，设计神经网络结构来引入多体关联**

基于领头阶核力的基态计算

YLY and Pengwei Zhao, PRC 107, 034320 (2023)

- 领头阶的无 π 介子有效场论核力

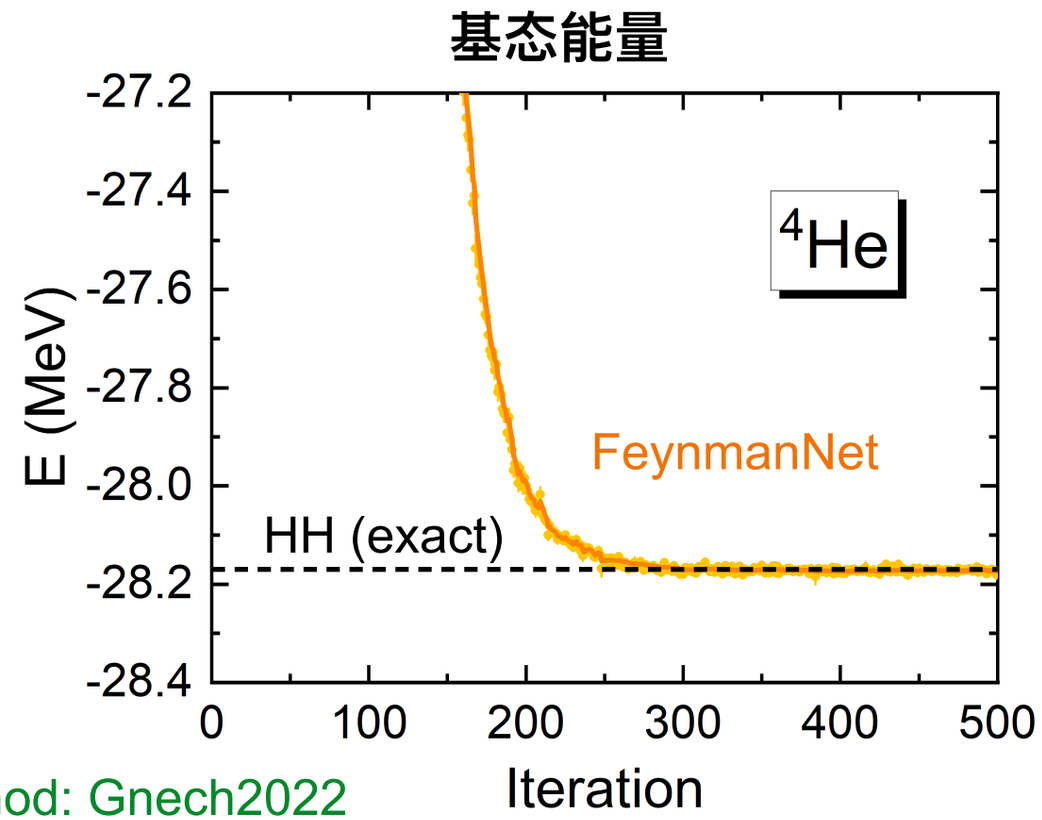
  Schiavilla et al., Phys. Rev. C 103, 054003 (2021)

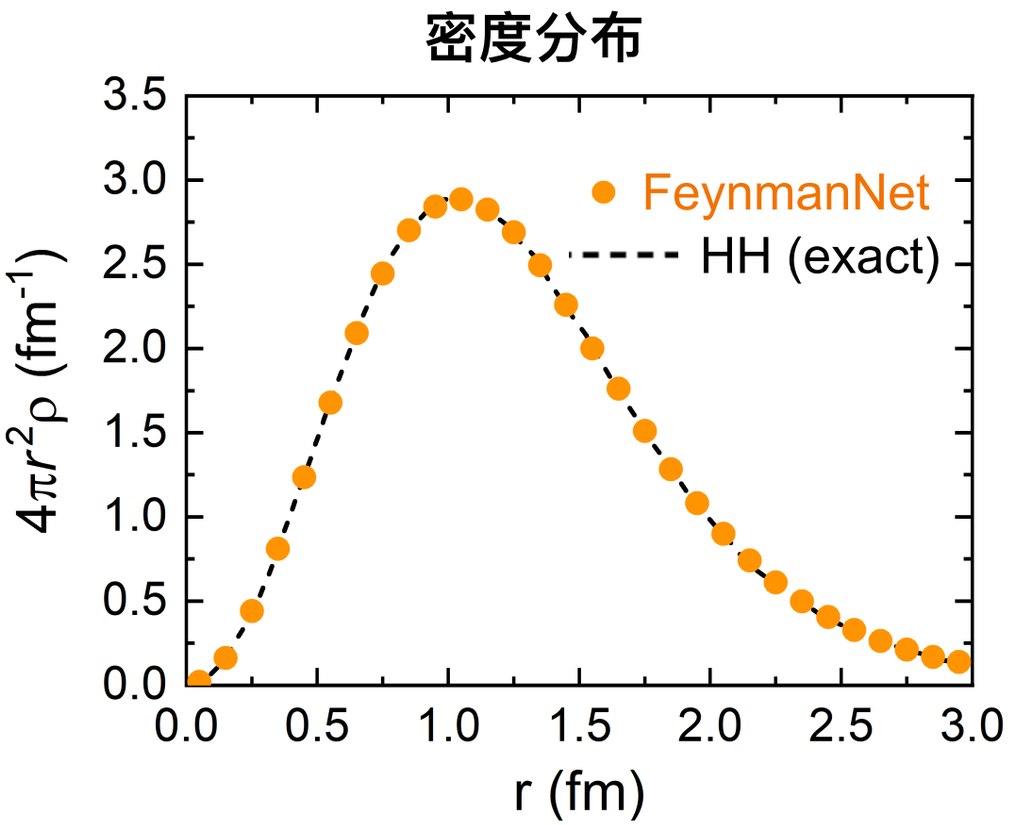


- FeynmanNet 架构: 基于 ANN 的 backflow 变换

Backflow in ^{3}He liquid: Feynman and Cohen, Phys. Rev. 102, 1189 (1956)

$$|\Psi\rangle = \mathrm{e}^{-\mathcal{U}(\boldsymbol{x}_1,\ldots,\boldsymbol{x}_A)} \sum_n \det[\mathbf{f}^{(n)}(\boldsymbol{x}_1,\ldots,\boldsymbol{x}_A)]$$





HH method: Gnech2022

激发态计算

- 谷歌 DeepMind、哈佛大学、麻省理工学院团队的最新工作将神经网络波函数应用于量子化学问题中激发态的精确计算
- 文章中引用了我们针对核多体问题建立的 FeynmanNet 方法

RESEARCH ARTICLE

QUANTUM CHEMISTRY

Accurate computation of quantum excited states with neural networks

David Pfau[1,2]*, Simon Axelrod[1,3,4], Halvard Sutterud[2], Ingrid von Glehn[1], James S. Spencer[1]

We present an algorithm to estimate the excited states of a quantum system by variational Monte Carlo, which has no free parameters and requires no orthogonalization of the states, instead transforming the problem into that of finding the ground state of an expanded system. Arbitrary observables can be calculated, including off-diagonal expectations, such as the transition dipole moment. The method works particularly well with neural network ansätze, and by combining this method with the FermiNet and Psiformer ansätze, we can accurately recover excitation energies and oscillator strengths on a range of molecules. We achieve accurate vertical excitation energies on benzene-scale molecules, including challenging double excitations. Beyond the examples presented in this work, we expect that this technique will be of interest for atomic, nuclear, and condensed matter physics.

Science

Pfau et al., Science 385, 6711 (2024)

However, in recent years, advances in deep neural networks have led to their use as accurate ansätze for studying spin systems (6), electronic structure (7) and **nuclear systems (70), often reaching levels of accuracy rivaling** projector QMC methods. These advances have **led to a renewed interest** in VMC as a standalone method.

… 其**精度**通常达到与投影QMC方法**相媲美的水平**。这导致人们**重新燃起**将VMC作为一独立方法的**兴趣**。

Neural network ansätze have already been applied to **ground state calculations in some of these domains (70, 71). We are excited to see how** NES-VMC and deep neural networks can be applied to many of the most challenging open problems in many-body quantum mechanics in the future.

神经网络波函数已经应用于一些领域的**基态计算**(**70**,71)。**我们将很高兴看到**NES–VMC和深度神经网络在未来如何应用于多体量子力学中许多最具挑战性的开放问题。

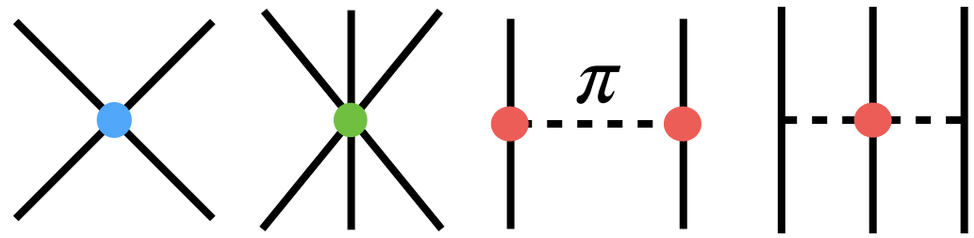
文献 (70) 即 FeynmanNet: Yang and Zhao, PRC 107, 034320 (2023)

基于高精度核力的基态计算

YLY, Evgeny Epelbaum, Chen Ji, Pengwei Zhao, arXiv:2509.01303 (2025); under review in PRL

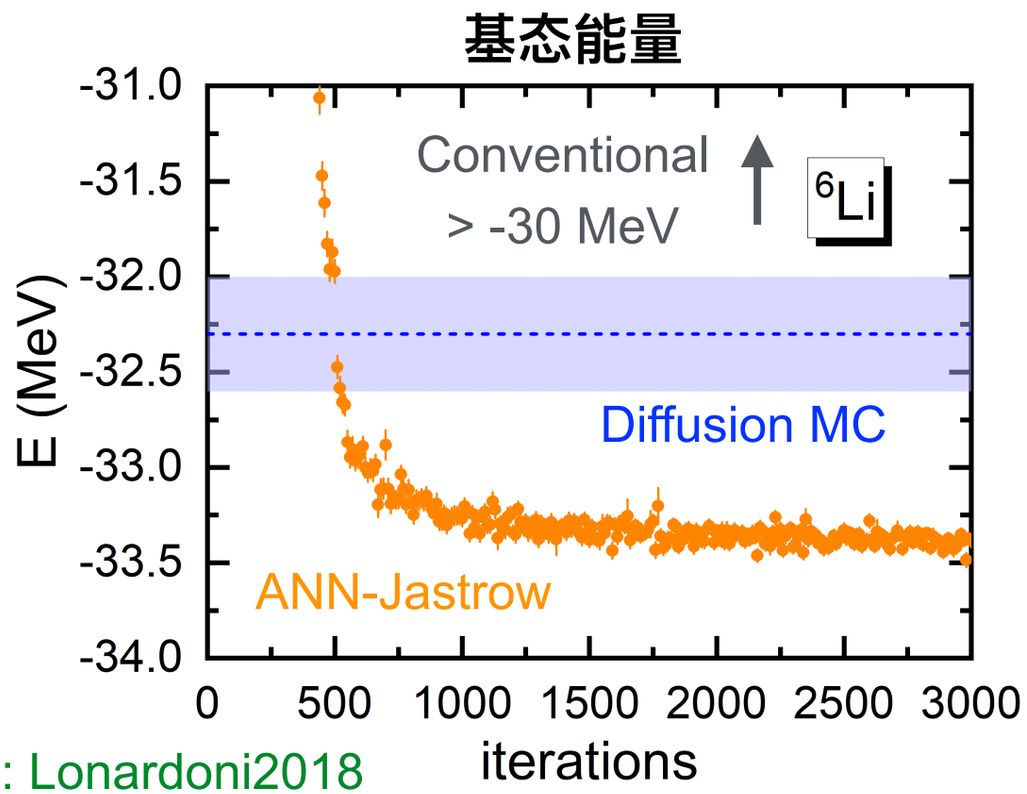
- 次次领头阶的手征有效场论核力

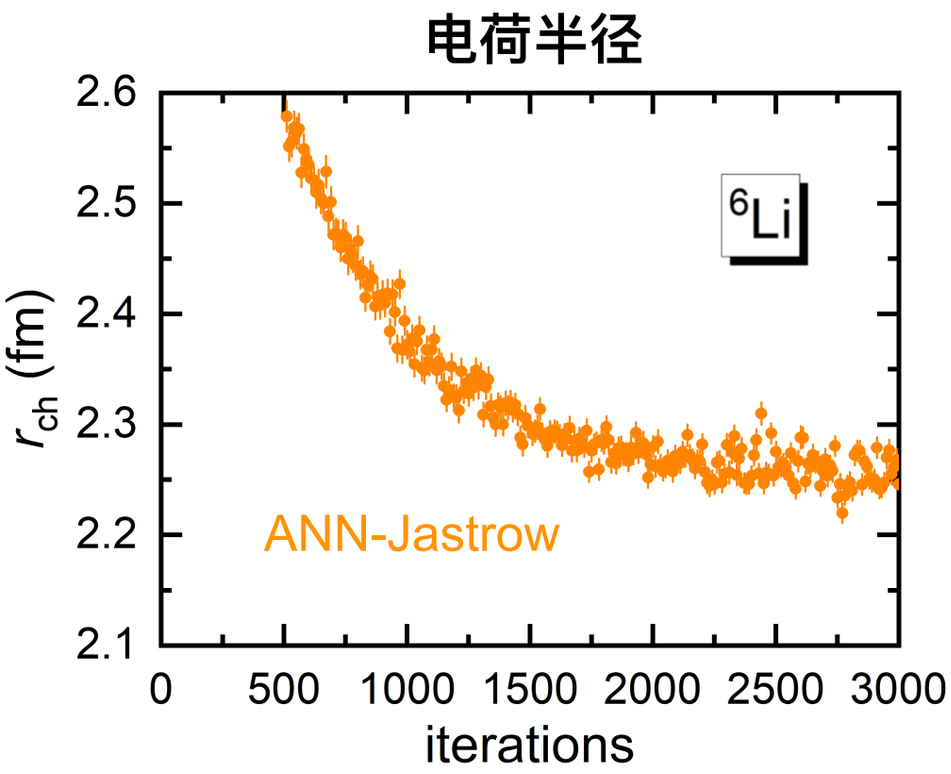
  Lynn et al. PRL 116, 062501 (2016)



- ANN-Jastrow 架构：ANN 关联函数 + 自旋依赖（张量）的算符

$$|\Psi\rangle = \prod_{n=1}^{n_J}\left[1+\sum_{i<j}\left(\sum_{p=2}^{6}u_p^{(n)}(\tilde{r}_{ij})O_{ij}^{p}+\sum_{k\neq i,j}\sum_{q=1}^{8}v_q^{(n)}(r_{ij},r_{ik},r_{jk})\tilde{O}_{ijk}^{q}\right)\right]|\Phi\rangle$$





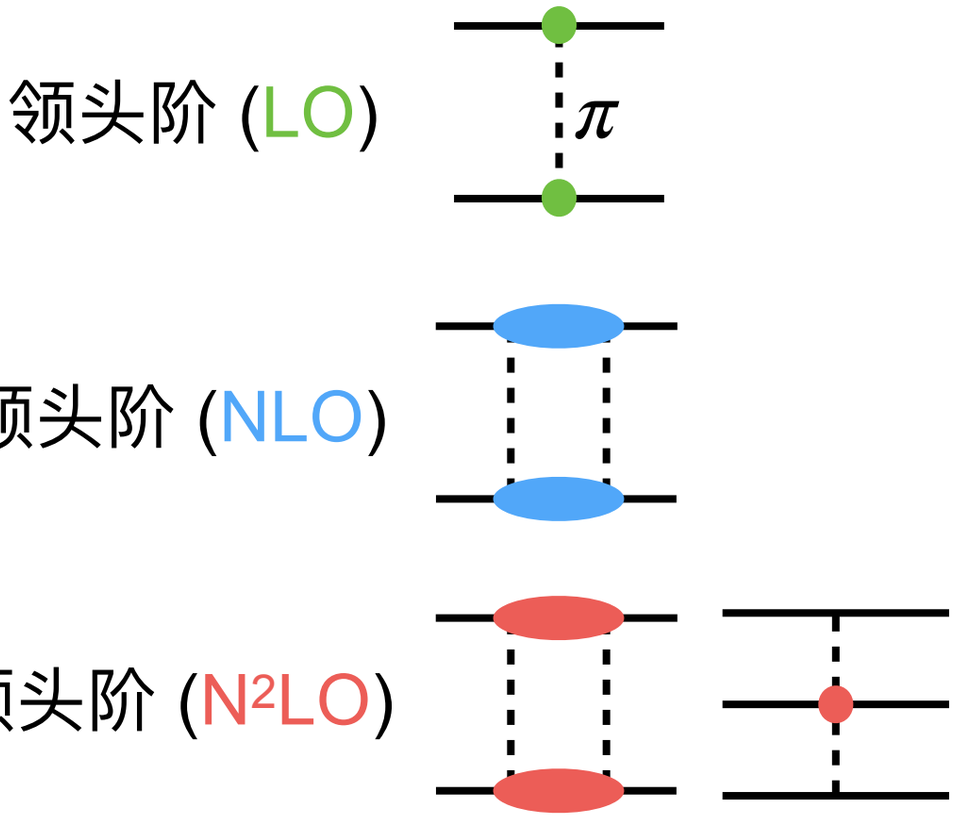
AFDMC: Lonardoni2018

基于手征核力计算低能的 n-α 擦边散射

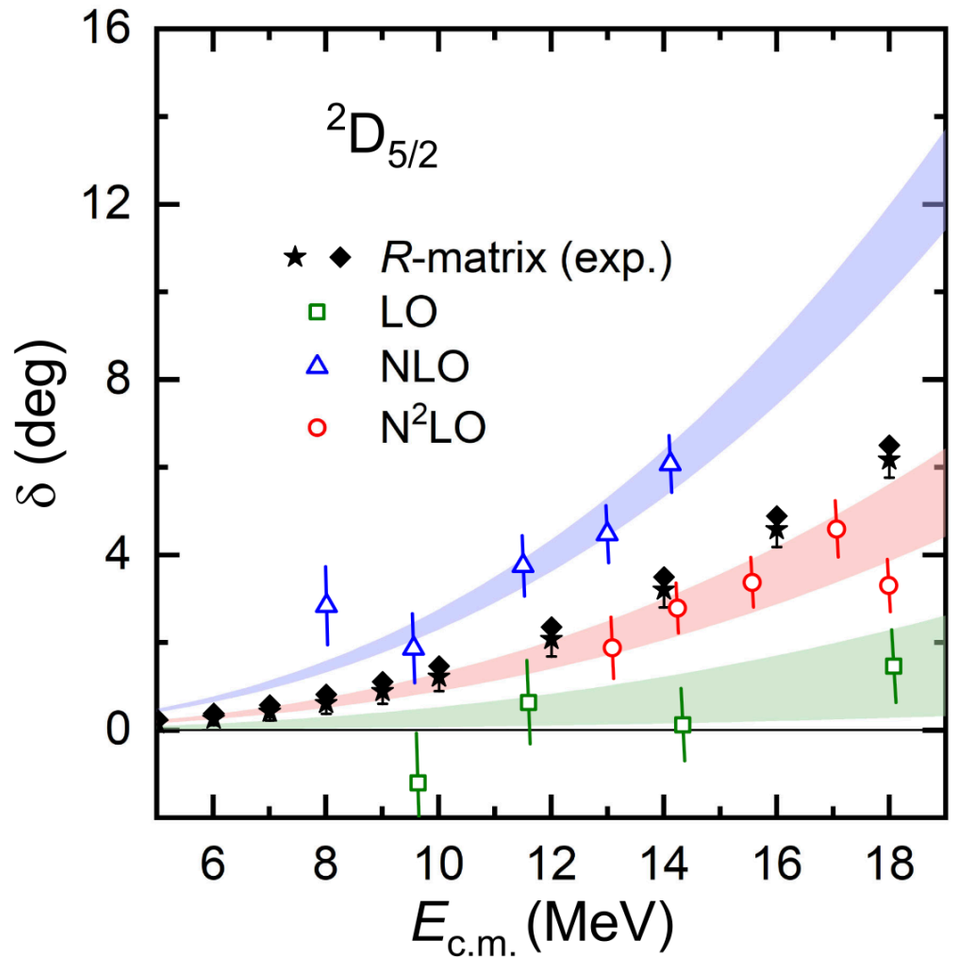
YLY, Evgeny Epelbaum, Jie Meng, Lu Meng, and Pengwei Zhao, PRL 135, 172502 (2025)

- 实现了高精度的 n-α D 波散射相移的第一性原理计算
- 提出并展示了低能的 n-α 高分波散射相移可以作为检验长程三体力的探针

手征核力中的长程 π 介子交换势



n-α D 波散射相移

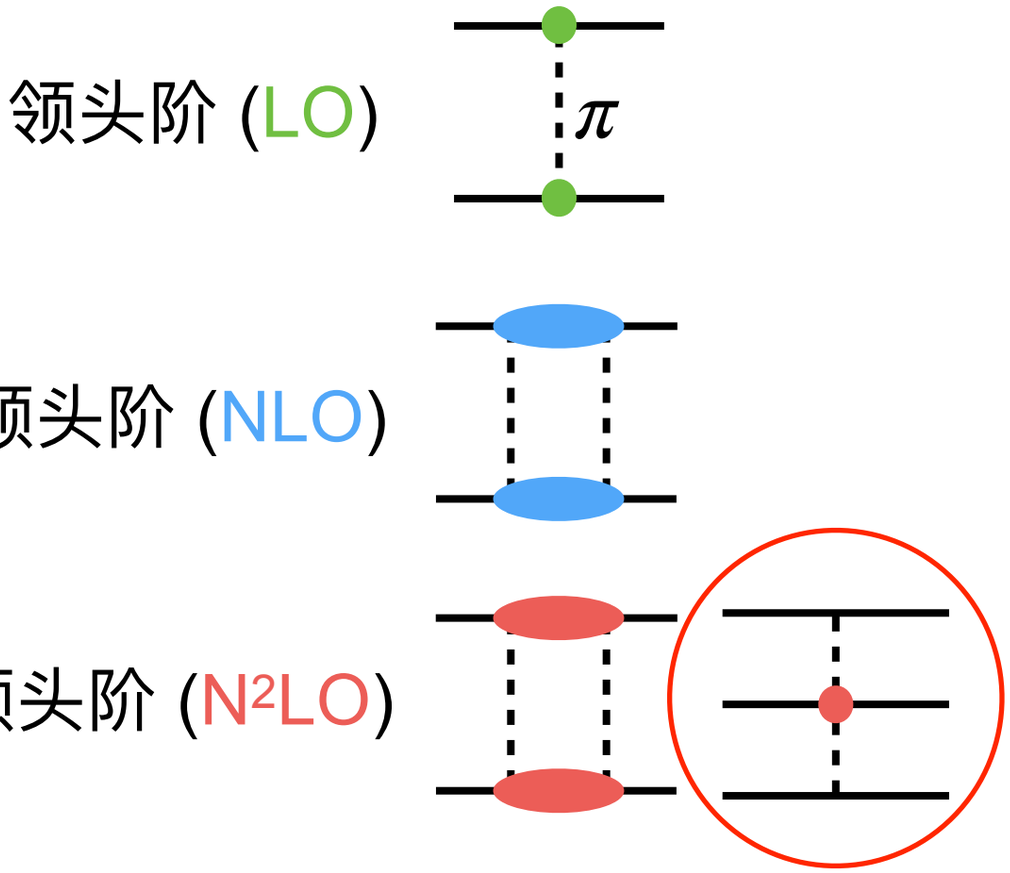


基于手征核力计算低能的 n-α 擦边散射

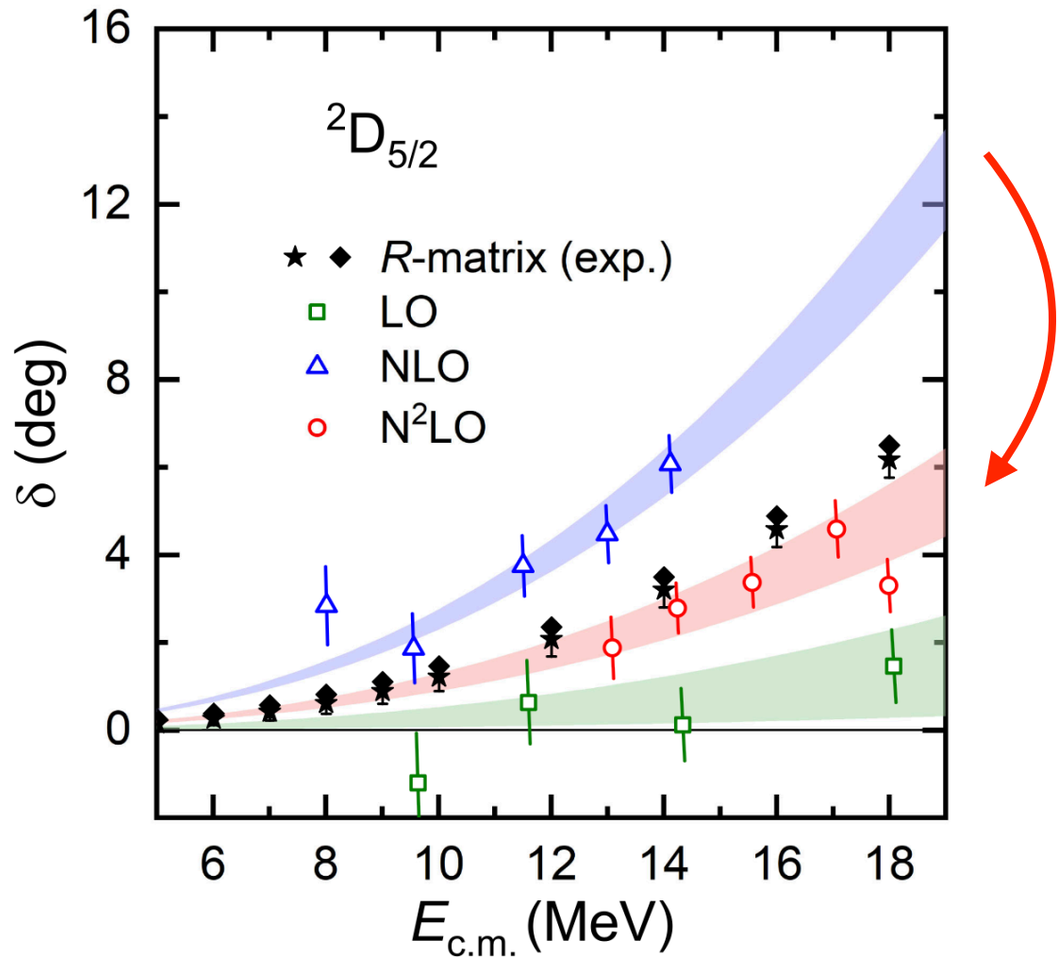
YLY, Evgeny Epelbaum, Jie Meng, Lu Meng, and Pengwei Zhao, PRL 135, 172502 (2025)

- 实现了高精度的 n-α D 波散射相移的第一性原理计算
- 提出并展示了低能的 n-α 高分波散射相移可以作为检验长程三体力的探针

手征核力中的长程 π 介子交换势



n-α D 波散射相移



总结与展望

总结：神经网络量子蒙特卡洛方法是一种新型的高精度第一性原理核多体方法

- FeynmanNet 架构：求解领头阶的无 π 介子有效场论核力

YLY and Zhao, PRC 107, 034320 (2023)

- ANN-Jastrow 架构：求解高精度的手征核力

YLY, Epelbaum, Ji, and Zhao, arXiv:2509.01303 (2025)

- 基于手征核力计算低能的 n-α 擦边散射

YLY, Epelbaum, Meng, Meng, and Zhao, PRL 135, 172502 (2025)

展望：开展原子核结构性质、电弱过程等方面的第一性原理研究

➡ 中重原子核基态与激发态、核物质状态方程

➡ 电磁跃迁、β 衰变、无中微子双 β 衰变…

基于相对论手征有效场论的两中子衰变计算：YLY and Zhao, PRL 134, 242502 (2025)

Thank you for your attention!

ALPHAGO ZERO

Article | Published: 19 October 2017

Mastering the game of Go without human knowledge

David Silver ✉, Julian Schrittwieser, Karen Simonyan, Ioannis Antonoglou, Aja Huang, Arthur Guez, Thomas Hubert, Lucas Baker, Matthew Lai, Adrian Bolton, Yutian Chen, Timothy Lillicrap, Fan Hui, Laurent Sifre, George van den Driessche, Thore Graepel & Demis Hassabis

Nature **550**, 354–359 (2017) | Cite this article

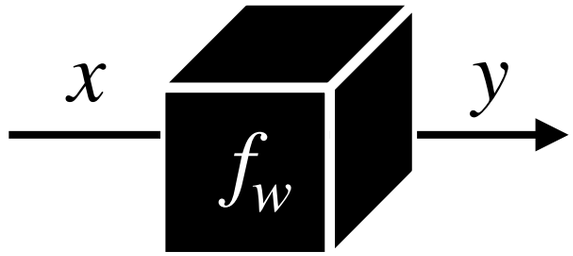
Abstract

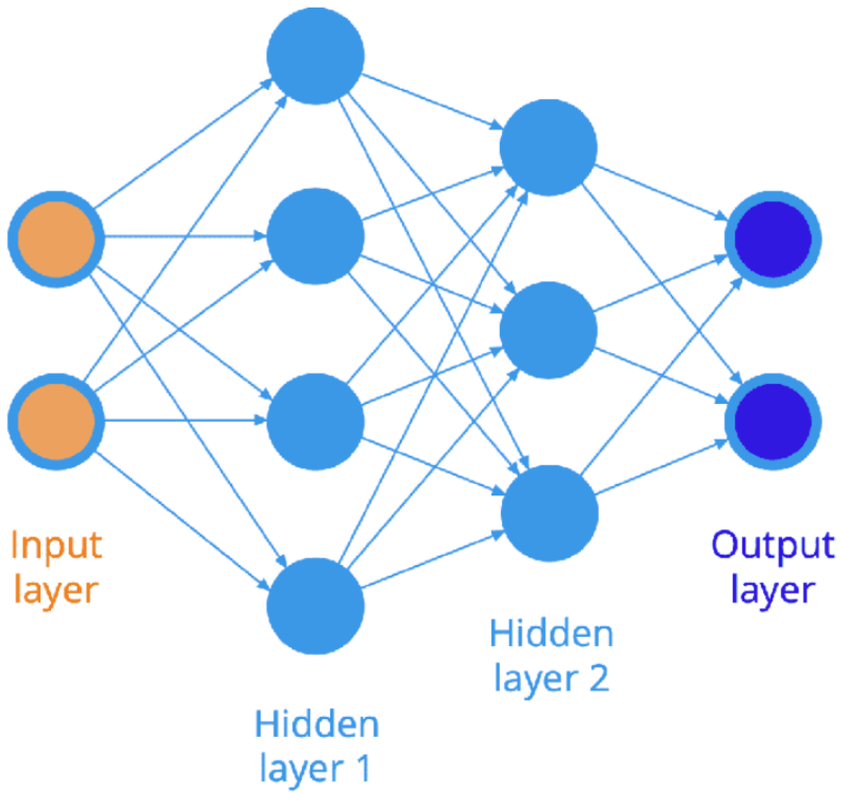
A long-standing goal of artificial intelligence is an algorithm that learns, *tabula rasa*, superhuman proficiency in challenging domains. Recently, AlphaGo became the first program to defeat a world champion in the game of Go. The tree search in AlphaGo evaluated positions and selected moves using deep neural networks. These neural networks were trained by supervised learning from human expert moves, and by reinforcement learning from self-play. Here we introduce an algorithm based solely on reinforcement learning, without human data, guidance or domain knowledge beyond game rules. AlphaGo becomes its own teacher: a neural network is trained to predict AlphaGo's own move selections and also the winner of AlphaGo's games. This neural network improves the strength of the tree search, resulting in higher quality move selection and stronger self-play in the next iteration. Starting ***tabula rasa***, our new program AlphaGo Zero achieved superhuman performance, winning 100–0 against the previously published, champion-defeating AlphaGo.

Appendix

神经网络

- 表示一个从输入到输出的函数
- 由多层线性和非线性函数嵌套构成





输出 输入

$$y_i = \sigma\left(\sum_{j=1}^{n} x_j \times w_{ij} + b_j\right)$$

w, b: 可调权重

σ: 非线性函数，例如 $\tanh(x)$, $\ln(1+\mathrm{e}^x)$, …

万能近似定理: → 理论上严格的试探波函数形式

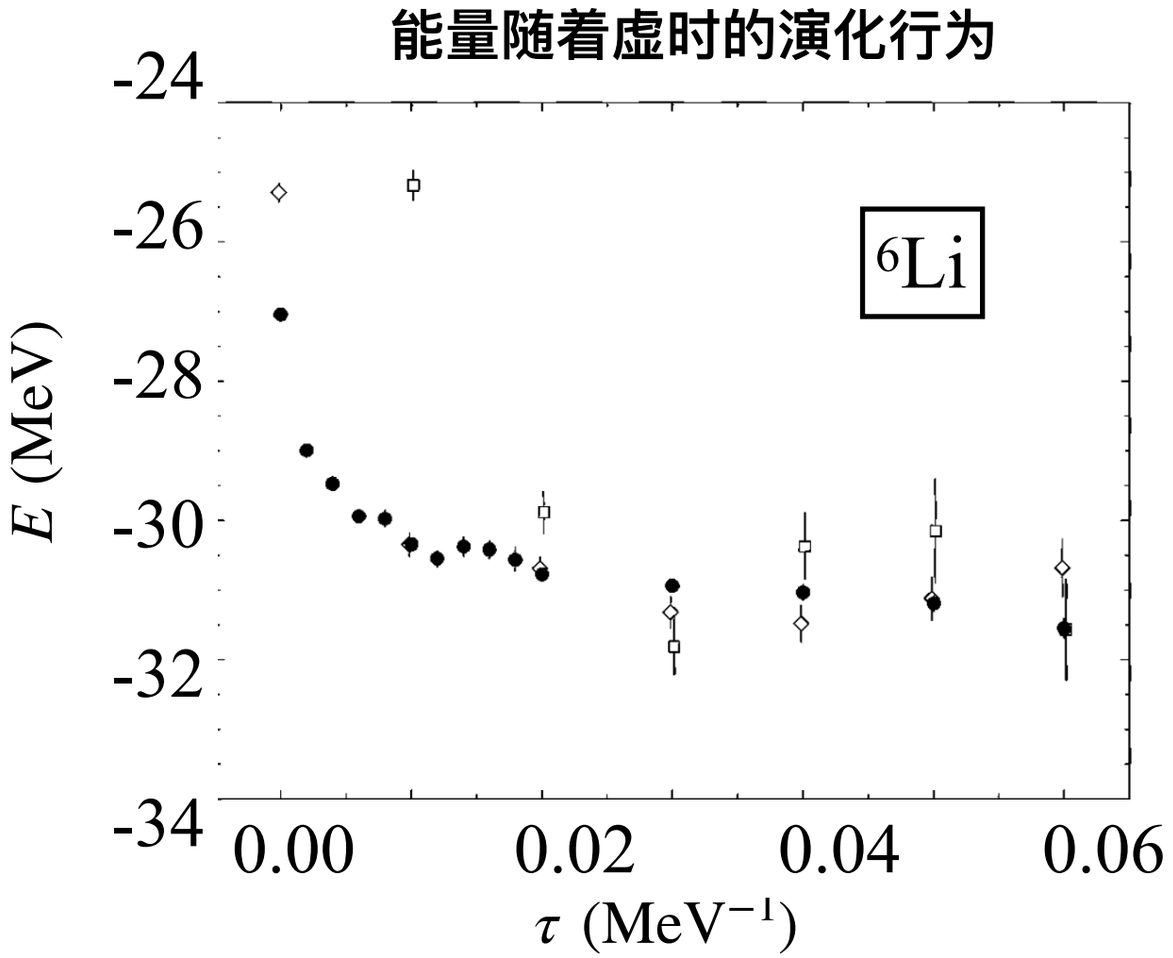
一个单隐藏层的神经网络，只需包含足够多的神经元，便能近似任何连续函数。

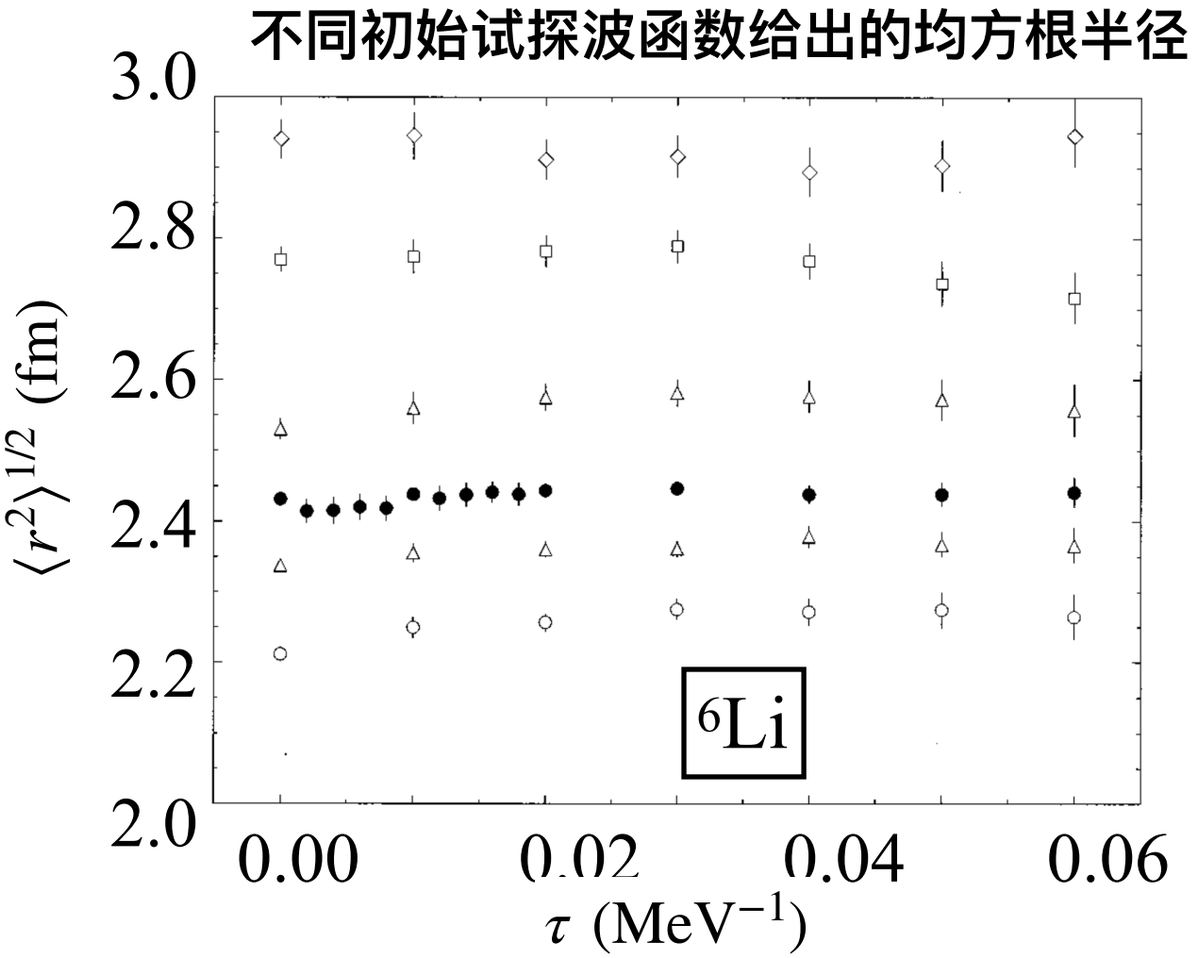
扩散蒙特卡洛方法面临的挑战

- 扩散蒙特卡洛会遭遇费米子符号问题，只能在有限的虚时 τ 内演化

$$|\Psi_0\rangle = \lim_{\tau\to\infty} \mathrm{e}^{-H\tau}|\Psi_T\rangle$$

- 许多结构性质 (半径、密度分布) 仍依赖于初始的试探波函数

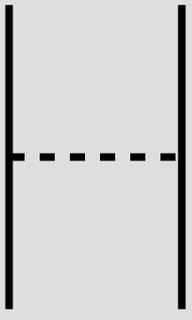




Taken from Pudiner, Pandharipande, Carlson, Pieper, and Wiringa, PRC 56, 1720 (1997)

Chiral symmetry in nuclear force

Chiral symmetry + πN data = predictions for the large-distance behavior of the nuclear forces



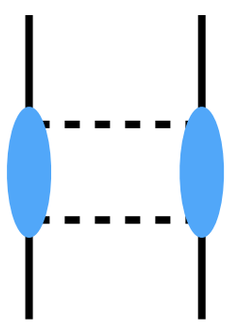
$$\mathscr{L}_{pv} = -\frac{g}{2M}\bar{N}\gamma_5\gamma^\mu\tau N\cdot\partial_\mu\pi$$

$$\mathscr{L}_{ps} = -g\bar{N}i\gamma_5\tau N\cdot\pi$$

$\Big\}\Rightarrow$

Same 1π exchange (on-shell)

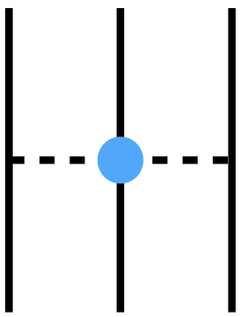
i.e., ***NOT*** contrained by χ symmetry



2π exchange strongly constrained by χ symmetry

$\mathscr{L}_{pv}$ vs $\mathscr{L}_{ps}$ matters; $\pi\pi$, $\pi\pi N$ interactions enter (fixed in πN systems)

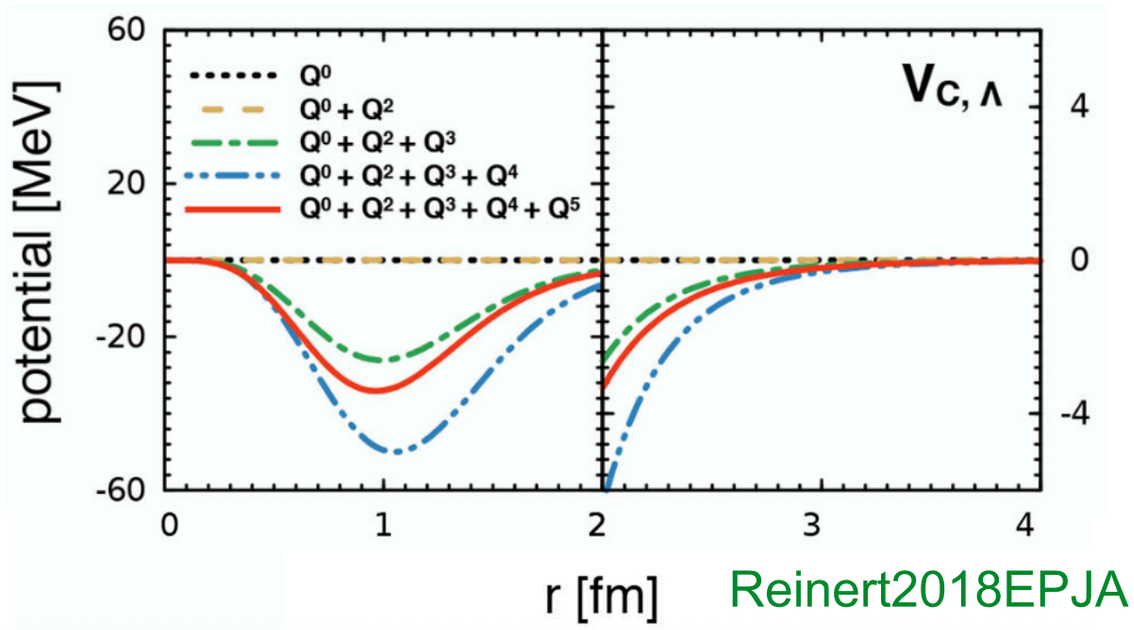
predictions for long-range NN and 3N force



e.g., a N^{2}LO contribution

$$V_C^{(3)}(r) = c_1\frac{3m_\pi^6 g_A^2}{16\pi^2 f_\pi^4}\frac{\mathrm{e}^{-2x}}{x^4}(1+x^2)$$

$$x = m_\pi r$$



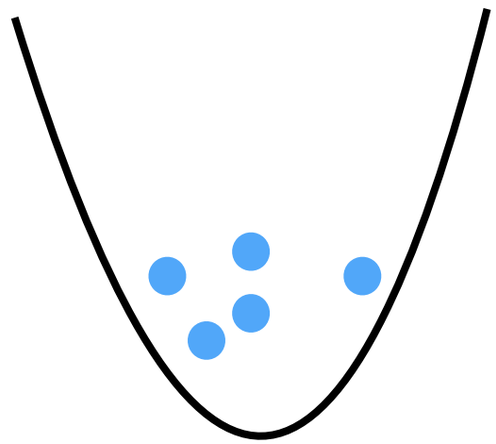
Reinert2018EPJA

QMC + BERW formula for $n\alpha$ phase shifts

YLY, Evgeny Epelbaum, Jie Meng, Lu Meng, and Pengwei Zhao, PRL 135, 172502 (2025)

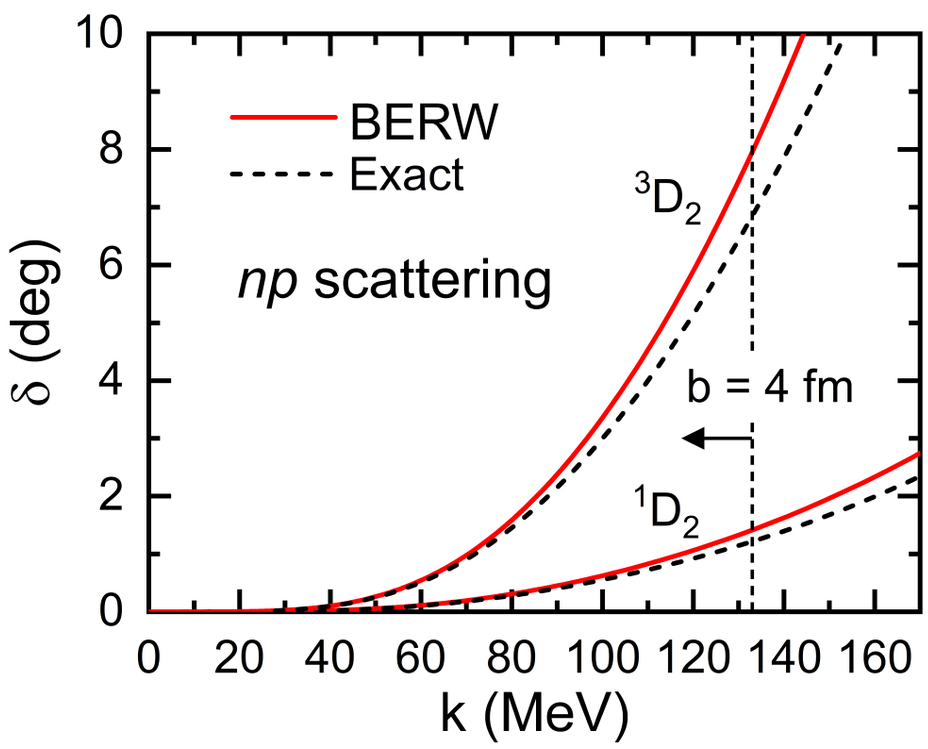
- $n\alpha$ phase shifts are extracted from the $^5\mathrm{He}_l$ energy in a harmonic oscillator trap

$$k^{2l+1}\cot\delta_l^{n\alpha}(k) = (-1)^{l+1}\left(4\mu\omega\right)^{l+1/2}\frac{\Gamma((3+2l)/4-\epsilon_l/(2\omega))}{\Gamma((1-2l)/4-\epsilon_l/(2\omega))}$$



Busch et al., Found. Phys. 28, 549 (2008); Suzuki et al., PRA 80, 033601 (2009)

with $\epsilon_l = E(^5\mathrm{He}_l) - E_\alpha$. We focus on the $D_{5/2}$ wave (spin-orbit splitting between $D_{5/2}$ and $D_{3/2}$ at low energies are small).



- The oscillator lengths $b > 4$ fm are used.

  much larger than interaction range $m_\pi b \geq 3$

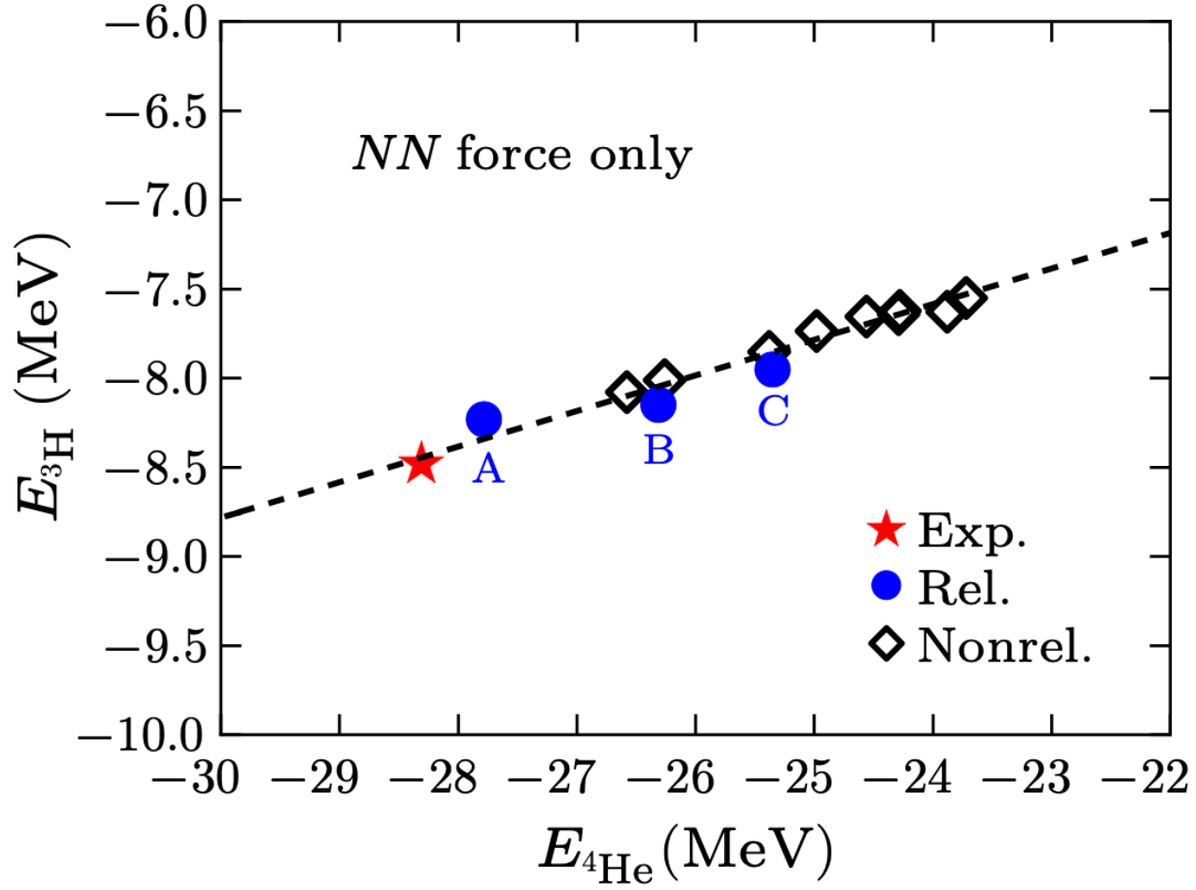
- Benchmarked in D-wave NN scattering.

  systematic error within ~10% at low energies.

基于 Bonn 势计算轻核基态

YLY and Pengwei Zhao, Chinese Phys. Lett. 42, 052101 (2025)

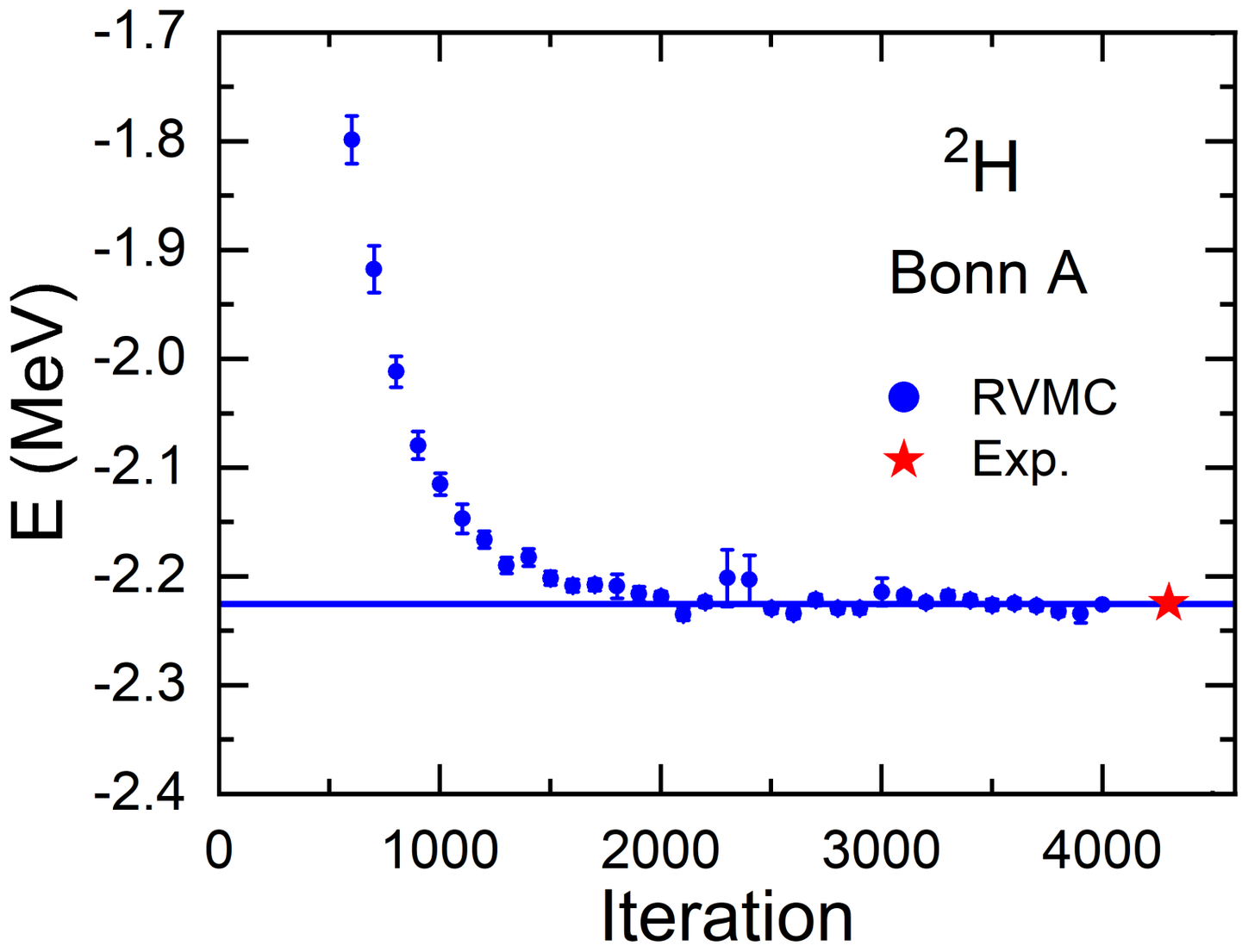
- 结合神经网络波函数，建立了相对论量子蒙特卡洛方法
- 基于 Bonn 势计算的 $A \leq 4$ 原子核的基态能量，系统地优于同样基于两体力的非相对论计算结果



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

Wiringa1995PRC, Stoks1994PRC, Wiringa1995PRC, Epelbaum2015PRL, Entem2017PRC, …

Deuteron


-1.7
-1.8
-1.9
-2.0
-2.1
-2.2
-2.3
-2.4
E (MeV)
0
1000
2000
3000
4000
Iteration
^{2}H
Bonn A
RVMC
Exp.