北京大学

Seminar at Institute of Theoretical Physics,
Chinese Academy of Sciences

December 4, 2025,

Neural-network quantum Monte Carlo approaches for *ab initio* nuclear theory

Yilong Yang

Peking University

Supervisor: Jie Meng, Pengwei Zhao

Email: yl_yang@pku.edu.cn

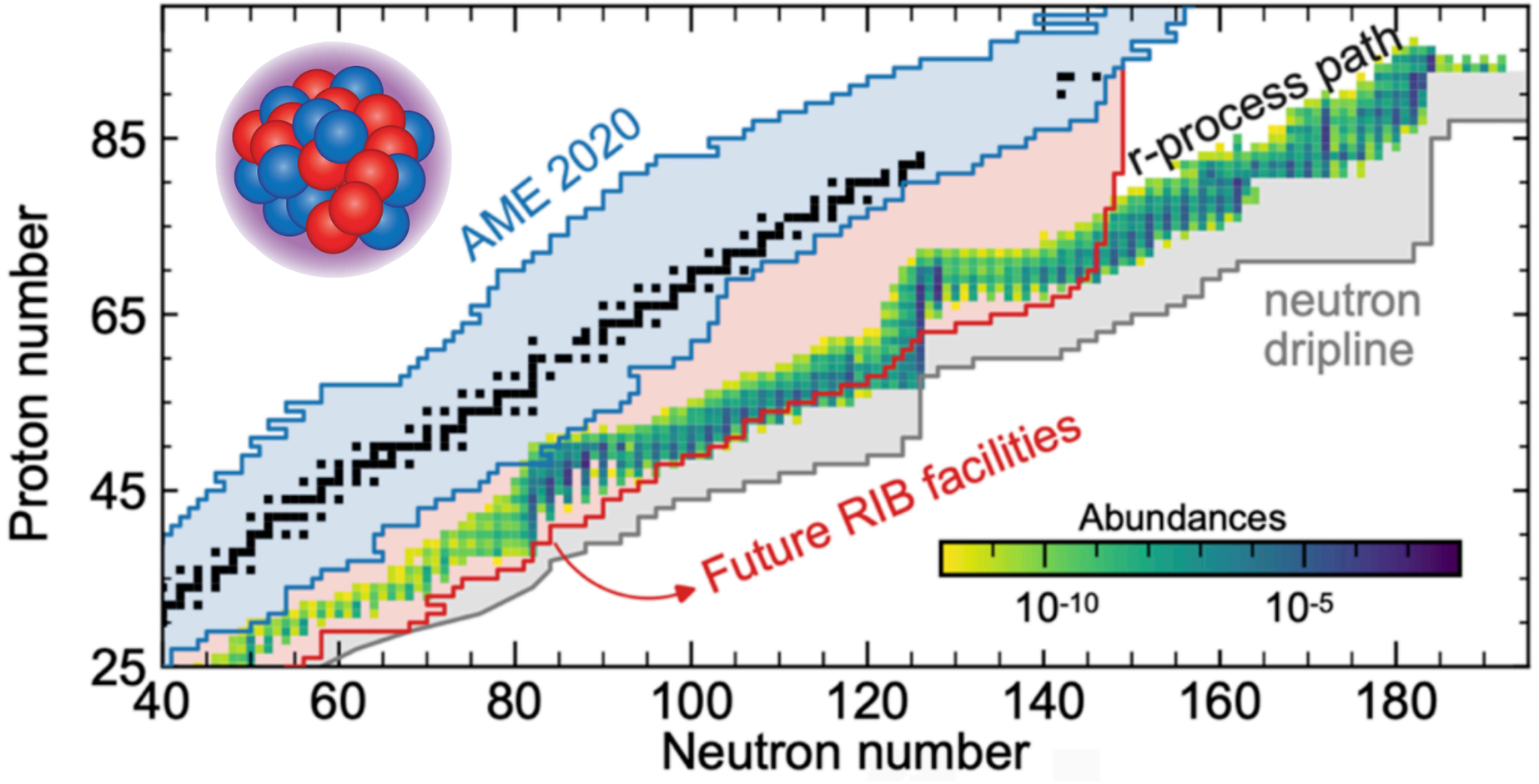
Outline

- ***Ab initio* nuclear theory**
- Neural-network quantum Monte Carlo
- Probing long-range 3N forces in peripheral neutron-α scattering
- Summary and outlook

Nuclear Physics Frontiers

- How do nuclei and nuclear matter emerge from the underlying fundamental interactions?
- What is the limit of nuclear existence and which phenomena arise from open quantum systems?
- How can nuclear structure and reaction dynamics contribute to astrophysics, hadron physics and fundamental symmetries?
- …

The NuPECC Long Range Plan 2024 for European Nuclear Physics



Ab initio nuclear theory

- **Goal:** Develop a predictive understanding of nuclei in terms of the nuclear forces between constituent nucleons
- **Definition:** solving the nuclear many-body Schrödinger equation for all consitituent nucleons explicitly and the nuclear forces between them

Nucleon-nucleon (NN), few-N scattering data, …

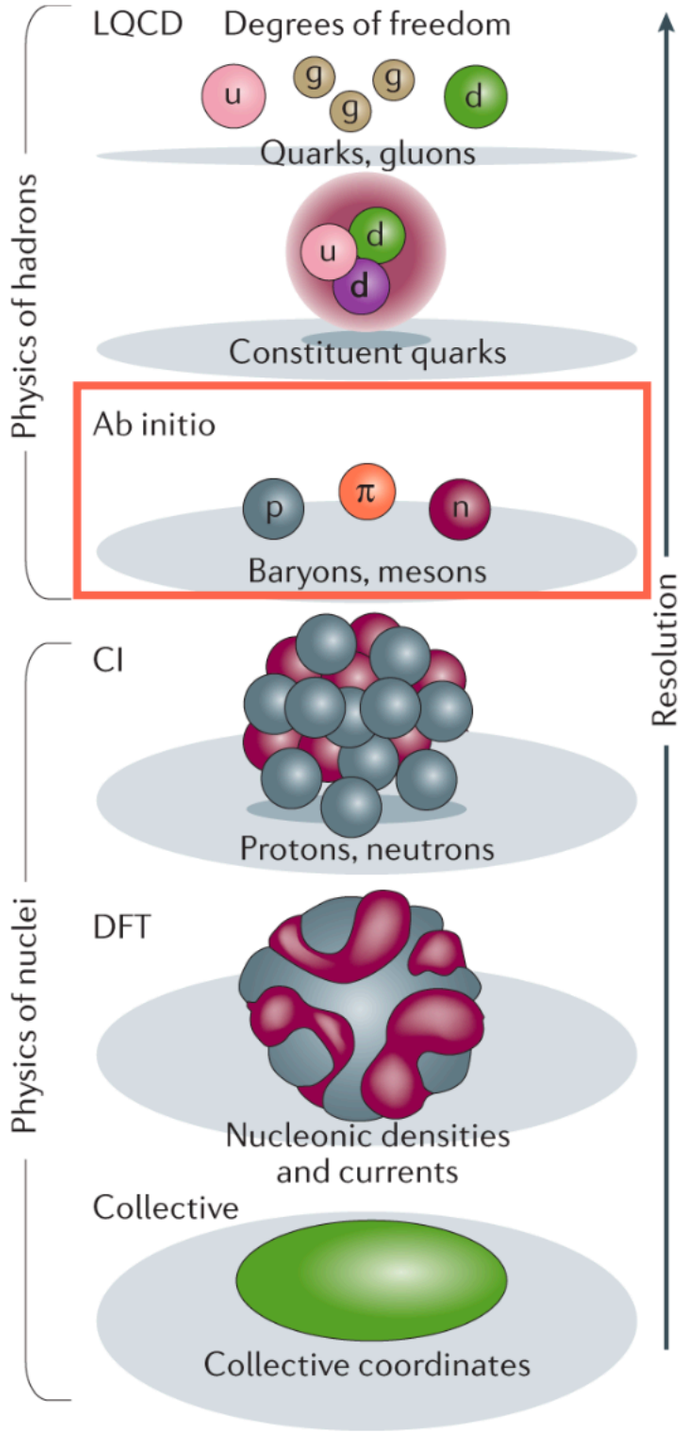
↓ Determine (nuclear force)

$$H = \sum_{i=1}^{A} \frac{-\nabla_i^2}{2M} + \sum_{i<j} v_{ij} + \sum_{i<j<k} V_{ijk}$$

↓ Predict (*ab initio* methods)

Nuclear spectra, transitions, Nuclear matter EoS,

Disentangling new physics ($0\nu\beta\beta$, EDM, …)



Nuclear forces

- Strong spin-isospin dependence, manifest by complicated operator structures

Wiringa, Stoks, and Schiavilla, PRC 51, 38 (1995)

AV18 *NN* interaction: $v_{ij} = v_{ij}^{\gamma} + v_{ij}^{\pi} + v_{ij}^{I} + v_{ij}^{S} = \sum_p v_p(r_{ij}) O_{ij}^p$

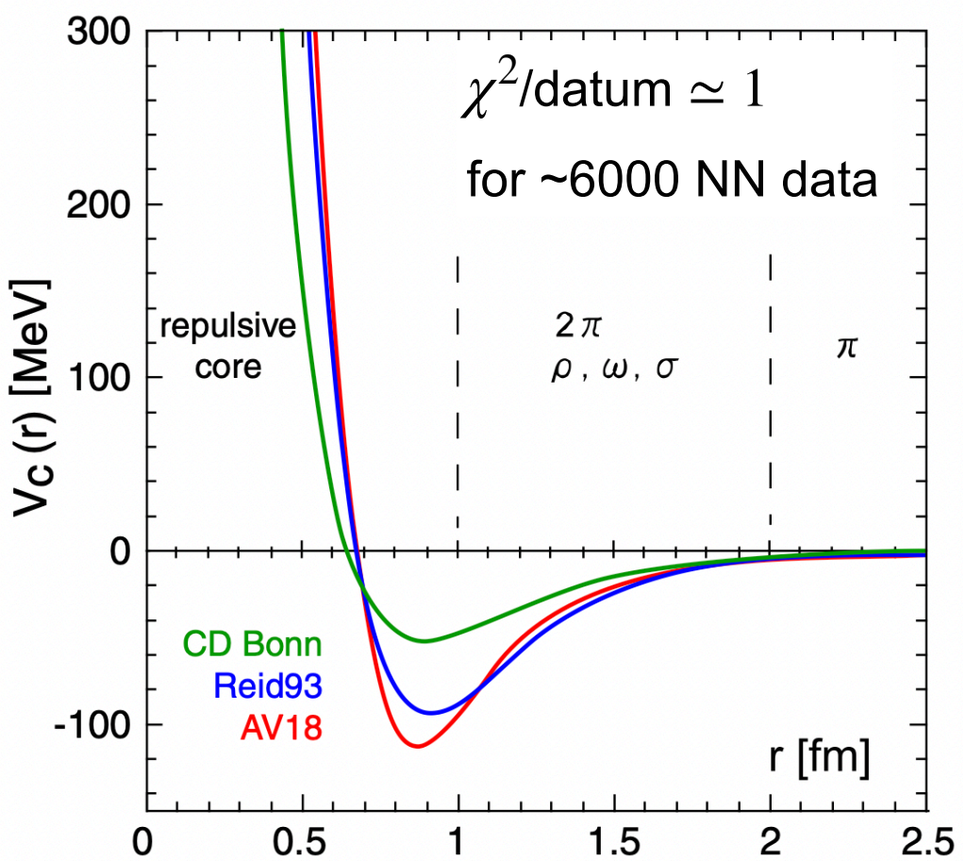
$$O_{ij}^{p=1,14} = 1, \boldsymbol{\tau}_i\cdot\boldsymbol{\tau}_j, \boldsymbol{\sigma}_i\cdot\boldsymbol{\sigma}_j, (\boldsymbol{\sigma}_i\cdot\boldsymbol{\sigma}_j)(\boldsymbol{\tau}_i\cdot\boldsymbol{\tau}_j), S_{ij}, S_{ij}(\boldsymbol{\tau}_i\cdot\boldsymbol{\tau}_j), \mathbf{L}\cdot\mathbf{S}, \mathbf{L}\cdot\mathbf{S}(\boldsymbol{\tau}_i\cdot\boldsymbol{\tau}_j),$$
$$L^2, L^2(\boldsymbol{\tau}_i\cdot\boldsymbol{\tau}_j), L^2(\boldsymbol{\sigma}_i\cdot\boldsymbol{\sigma}_j), L^2(\boldsymbol{\sigma}_i\cdot\boldsymbol{\sigma}_j)(\boldsymbol{\tau}_i\cdot\boldsymbol{\tau}_j), (\mathbf{L}\cdot\mathbf{S})^2, (\mathbf{L}\cdot\mathbf{S})^2(\boldsymbol{\tau}_i\cdot\boldsymbol{\tau}_j) .$$

$$O_{ij}^{p=15,18} = T_{ij}, (\boldsymbol{\sigma}_i\cdot\boldsymbol{\sigma}_j)T_{ij}, S_{ij}T_{ij}, (\tau_{zi} + \tau_{zj})$$

- Short- and intermediate range constrained by *NN* scattering data

$$v_{ij}^I = \sum_{p=1}^{18} I^p T^2(\mu r_{ij}) O_{ij}^p, \; v_{ij}^S = \sum_{p=1}^{18} [P^p + Q^p r + R^p r^2] W(r) O_{ij}^p,$$

An organization scheme? Connection to QCD?



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

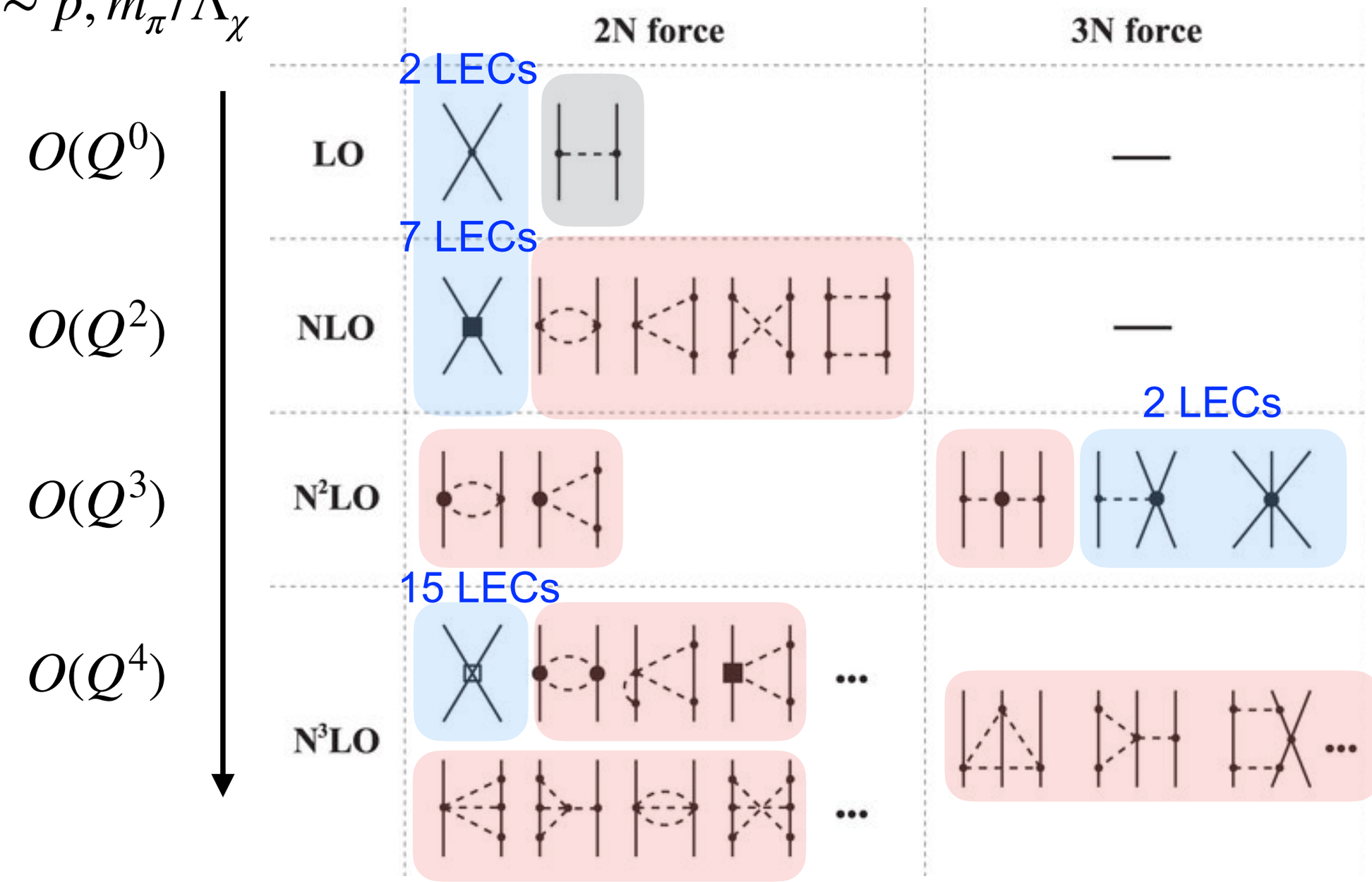
Nuclear forces from chiral effective field theory (EFT)

Chiral nuclear force = Short-range terms + 1π exchange + 2π exchange + …

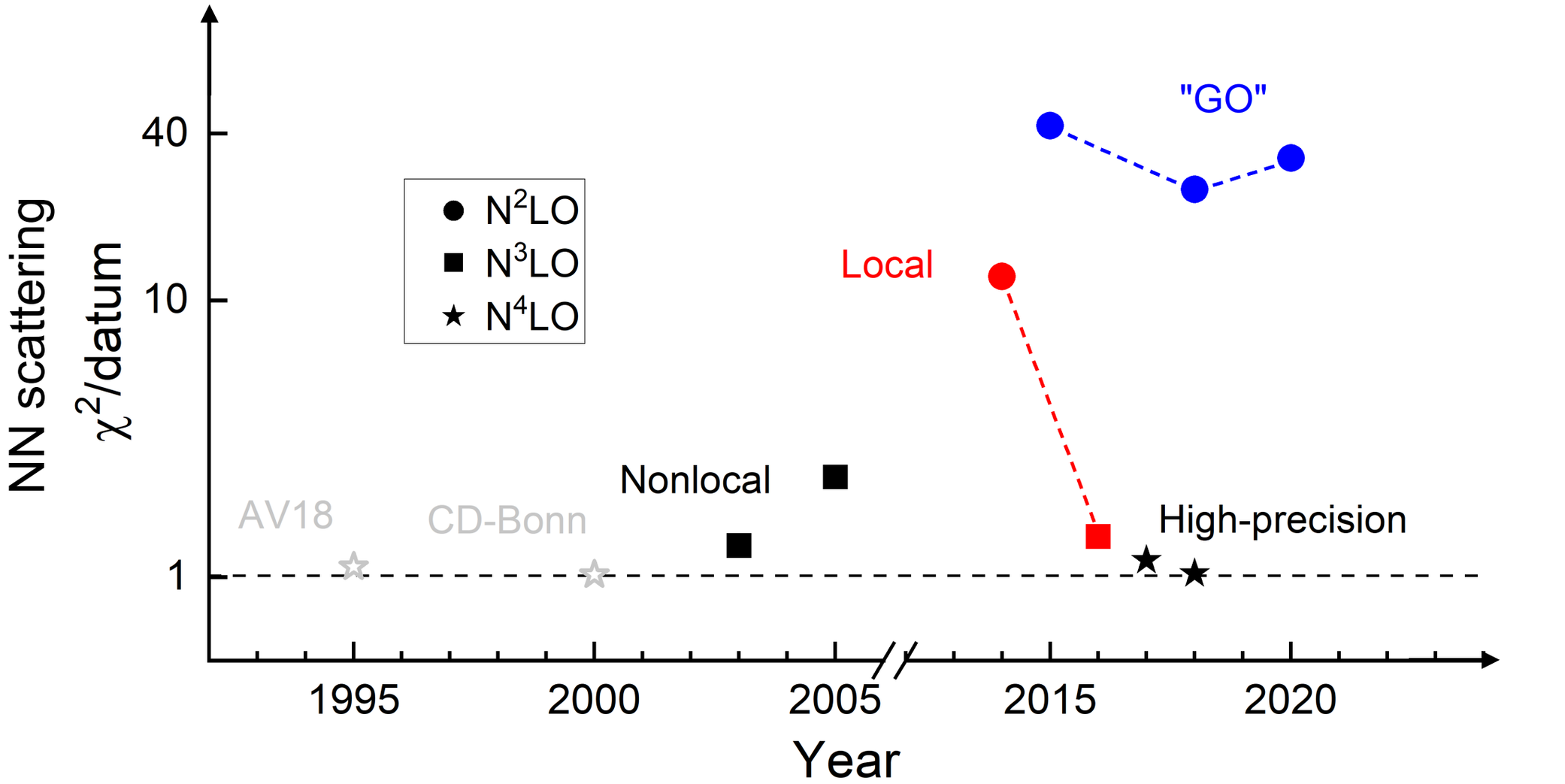
(Phenomenology) (Chiral symmetry)

Weinberg, PLB 251, 288 (1990); NPB 363, 3 (1991)
Epelbaum, Hammer, and Meißner, RMP 81, 1773 (2009)

$Q \sim p, m_\pi/\Lambda_\chi$



Progress in chiral NN forces



Review: Machleidt and Sammarruca, PPNP 137, 104117 (2024)

1. Early birds (nonlocal): The first quantitative chiral NN forces
   Entem2003, Epelbaum2005
2. *r*-space regularization (Local): Suitable for accurate quantum Monte Carlo calculations
   Gezerlis2014, Piarulli2016
3. Göteborg/Oak Ridge (GO): Less accurate description for NN scattering
   Ekström2015, 2018, 2020
4. Latest N⁴LO (high-precision): Reaching χ^2/datum $\simeq 1$ up to pion-production threshold
   Entem2017, Reinert2018

Relativistic N²LO NN forces (J. X. Lu et al. PRL 2022) not listed, as χ^2/datum not available

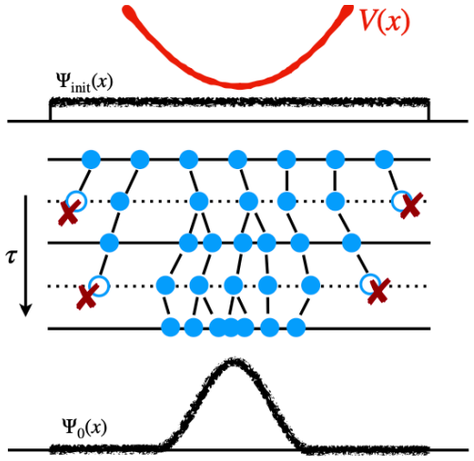
Ab initio methods

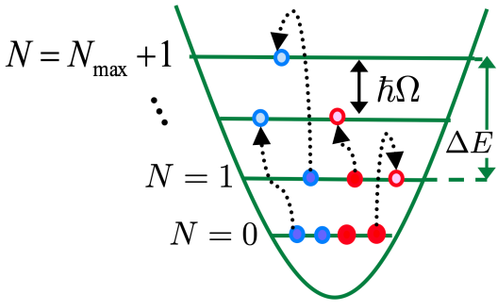
- Full many-body correlations
  - Few-body ($A \leq 4$) methods: Fadeev, …
  - Quantum Monte Carlo (QMC)

    Carlson et al., RMP 87, 1067 (2015)
  - No-core shell model

    Barrett, Navrátil, Vary, PPNP. 69, 131 (2013)
  - Nuclear lattice EFT

    Lähde & Meißner, Lect. Note. Phys. 957, 1 (2019); Lee, FP 8, 174 (2020)





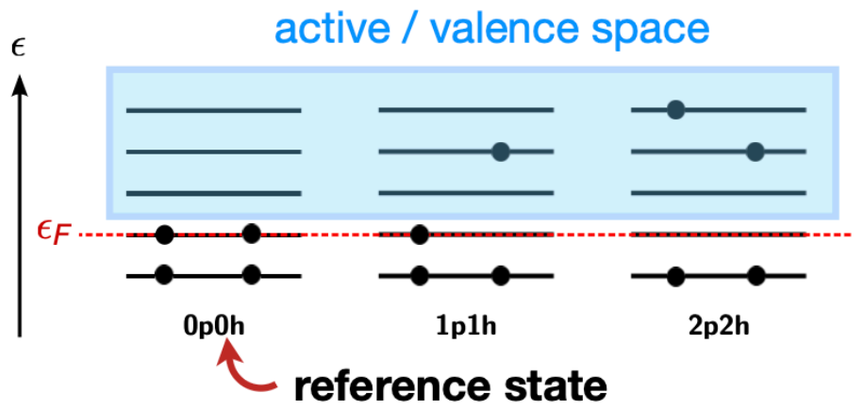
- Systematic Truncations of many-body correlations
  - Many-body perturbation theory

    Tichai, Roth, and Duguet, FP 8, 164 (2020)
  - Self-Consistent Green's Functions

    Somà, FP 8, 340 (2020)
  - Coupled Cluster (CC)

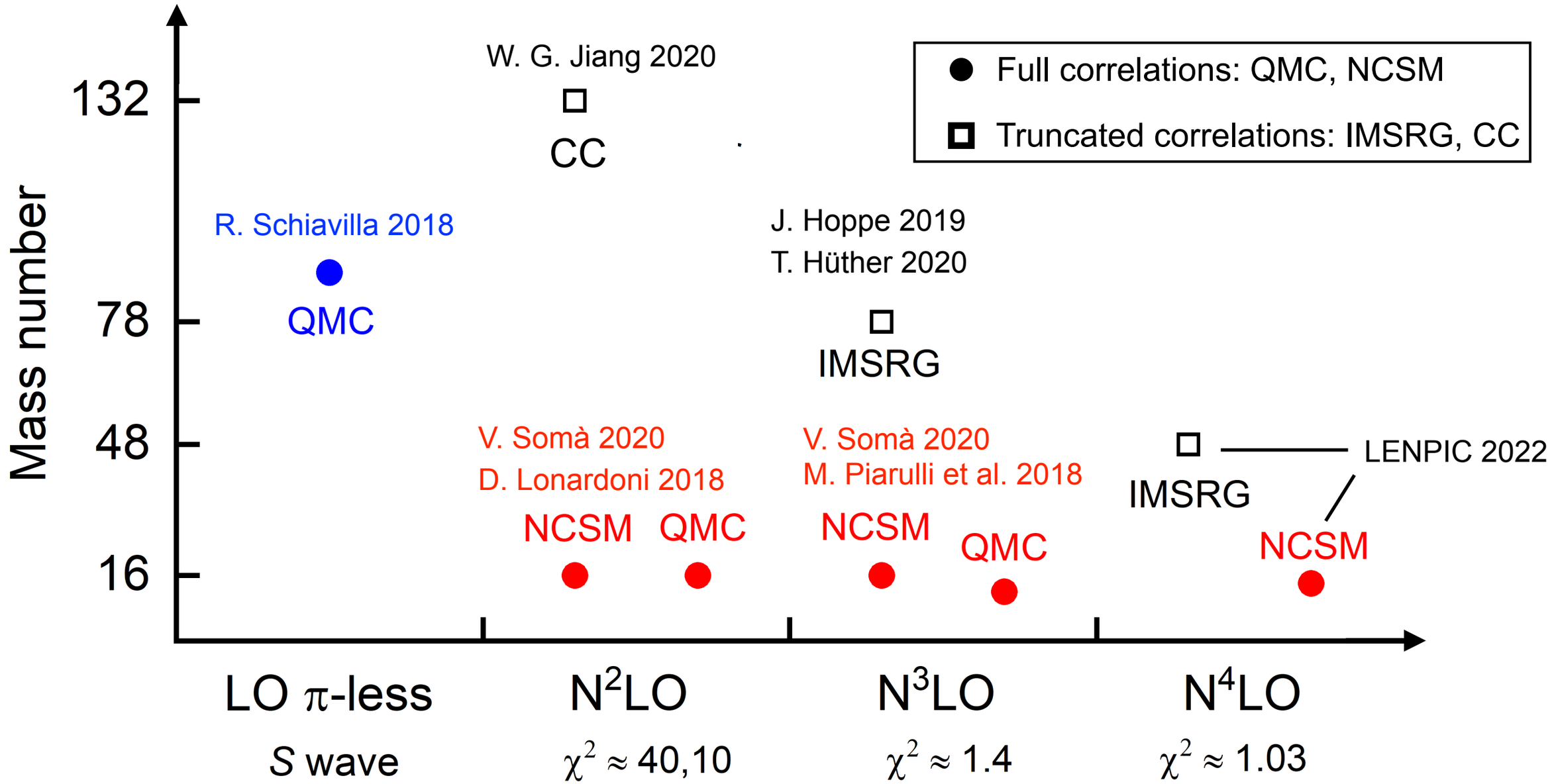
    Hagen et al., Rep. Prog. Phys. 77, 096302 (2014)
  - In-Medium Similarity Renormalization Group (IMSRG)

    Hergert et al., PR 621, 165 (2016)



Progress in *ab initio* calculations

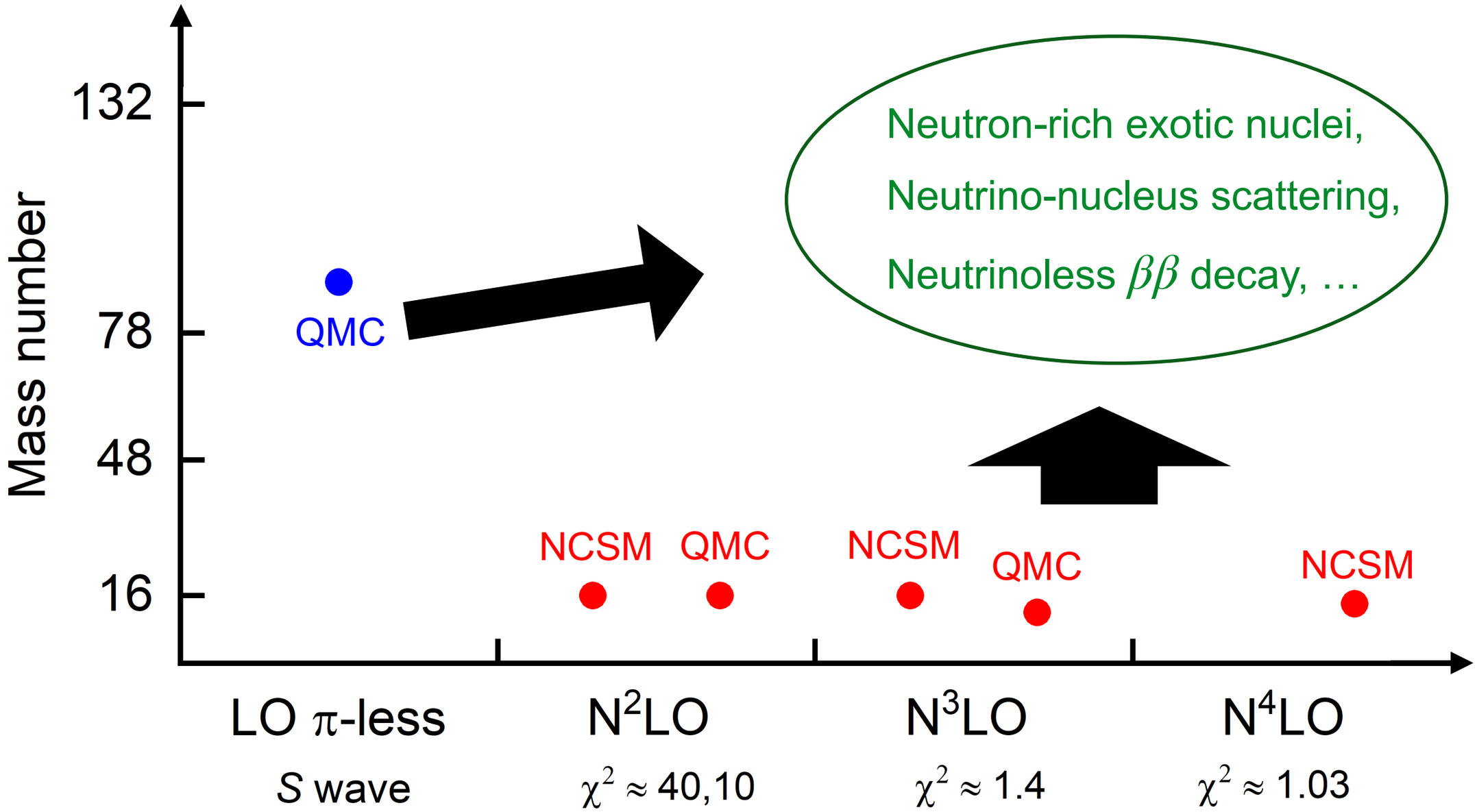
Accurate *ab initio* calculations of medium-mass nuclei are still challenging!



Lattice calculations are also actively pursued by NLEFT groups: Elhatisari et al. 2024, Z. W. Niu and B. N. Lu 2025

Concluding Remarks

Advancing *ab initio* method towards solving medium-mass nuclei with **full many-body correlations and high-precision nuclear force**

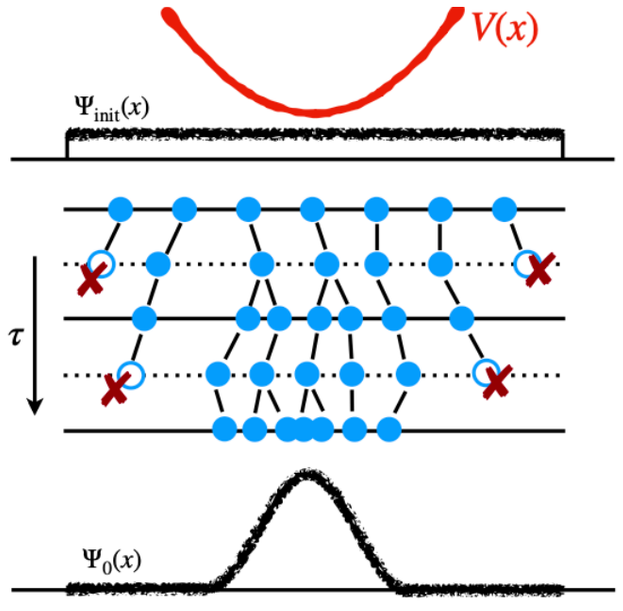


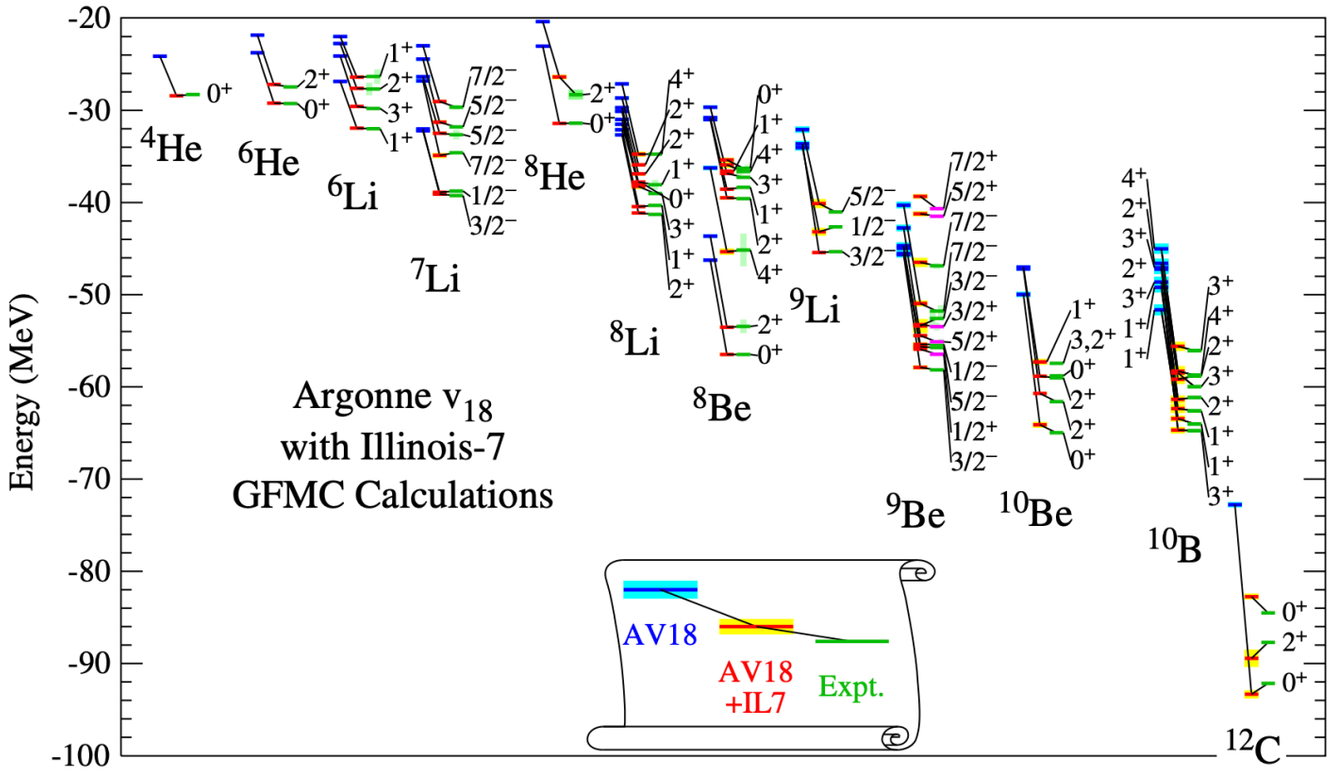
Outline

- *Ab initio* nuclear theory
- **Neural-network quantum Monte Carlo**
- Probing long-range 3N forces in peripheral neutron-α scattering
- Summary and outlook

Why Quantum Monte Carlo (QMC)?

- **Full many-body correlations**
- NO softening/SRG-evolving nuclear force
- Applicable for both ground and excited states
- Access to many properties, such as spectra, transitions, form factors, etc.





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

Lattice QCD

Nuclear Physics

Cold Atoms

Atoms/Molecules

Condensed Matter

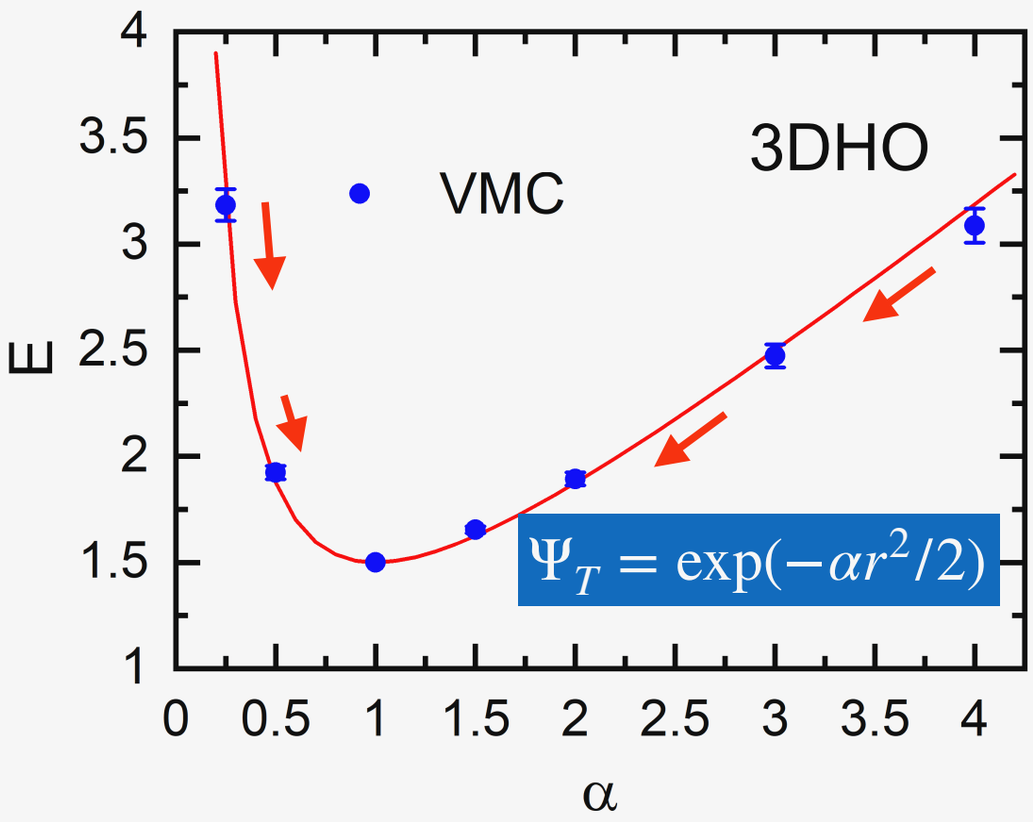
…

Quantum Monte Carlo methods

- **Monte Carlo**:
  Solve multi-dimensional intergrals by using random numbers
- **Quantum Monte Carlo**:
  Solve quantum mechanical problems using Monte Carlo

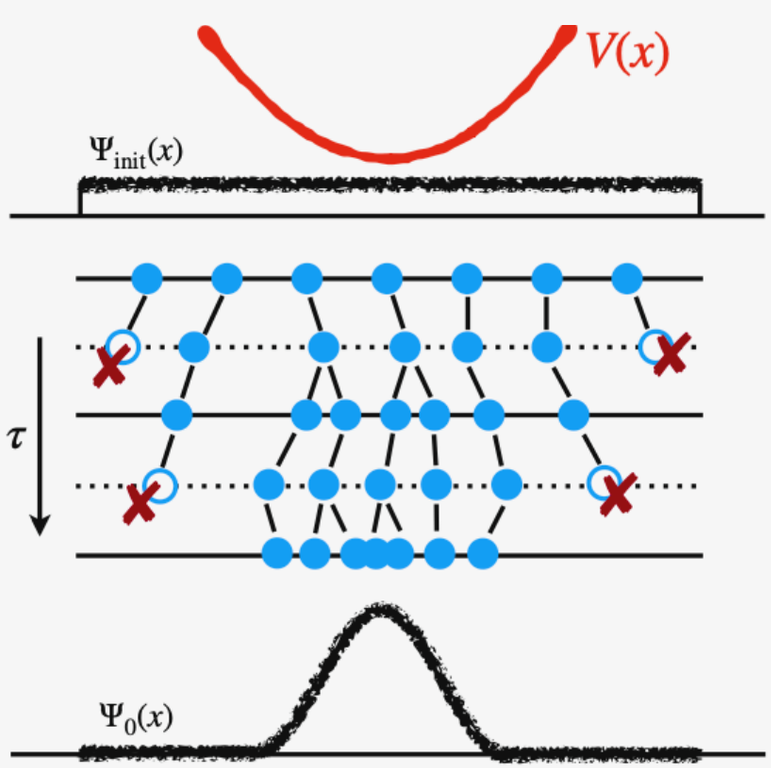
Variational Monte Carlo (VMC)

$$E_0 \leq E_T = \frac{\langle \Psi_T | H | \Psi_T \rangle}{\langle \Psi_T | \Psi_T \rangle}$$



Diffusion Monte Carlo (DMC)

$$\lim_{\tau \to \infty} \mathrm{e}^{-H\tau} |\Psi_T\rangle \propto |\Psi_0\rangle + e^{-E_1^* \tau} |\Psi_1\rangle + \ldots$$

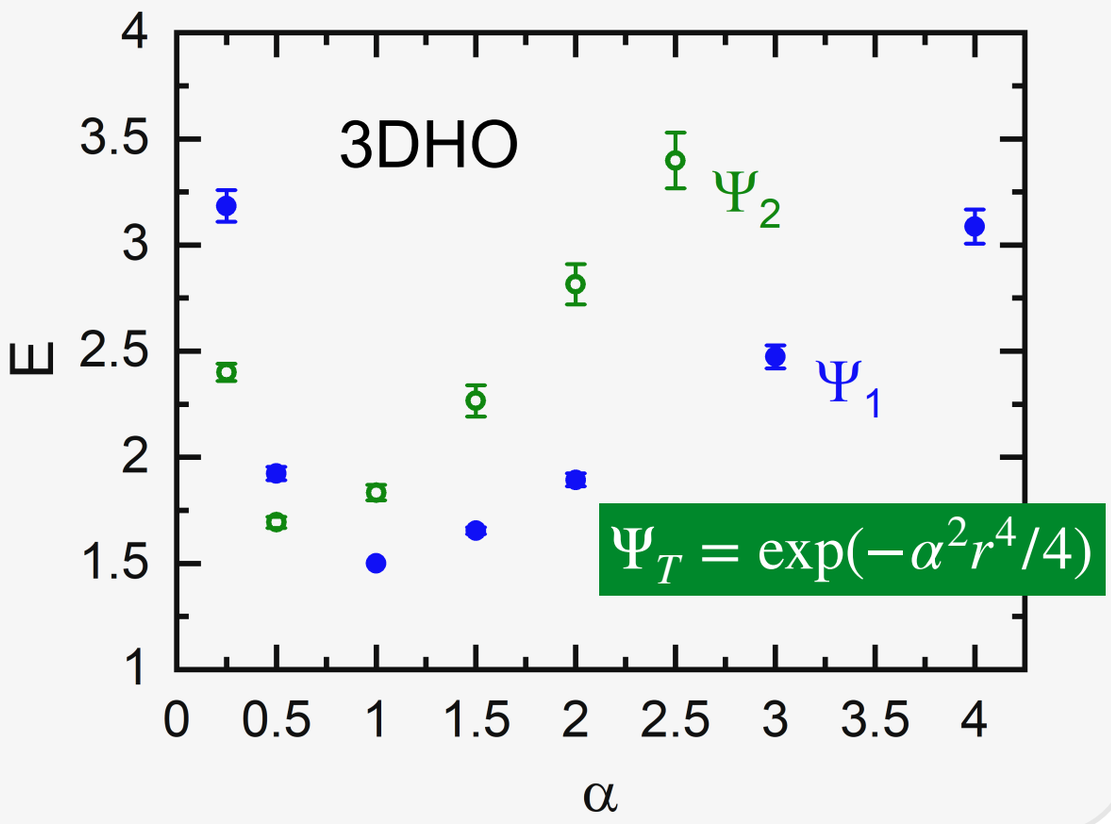


Quantum Monte Carlo methods

- **Monte Carlo**:
  Solve multi-dimensional intergrals by using random numbers
- **Quantum Monte Carlo**:
  Solve quantum mechanical problems using Monte Carlo

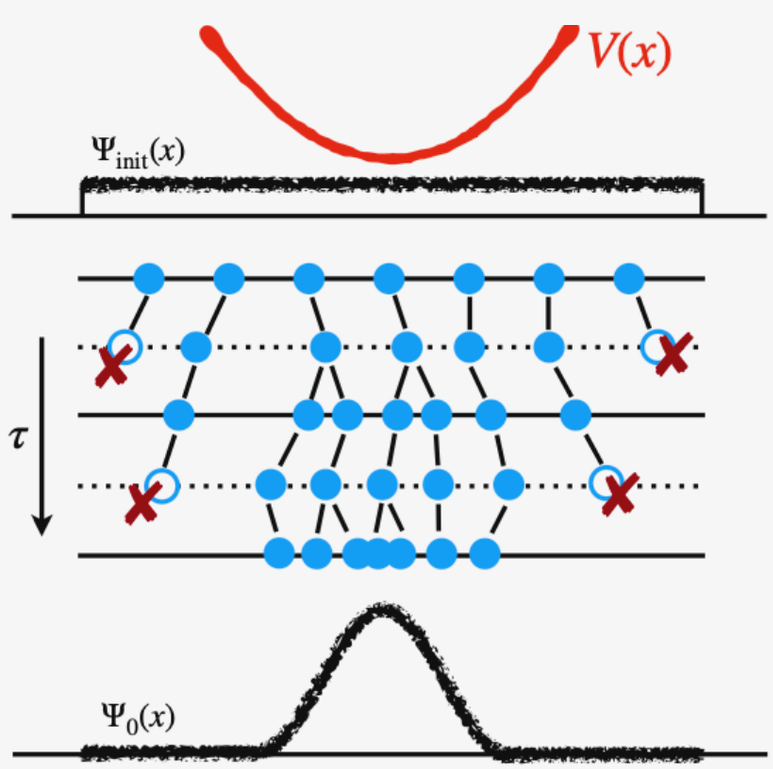
Variational Monte Carlo (VMC)

$$E_0 \leq E_T = \frac{\langle \Psi_T | H | \Psi_T \rangle}{\langle \Psi_T | \Psi_T \rangle}$$



Diffusion Monte Carlo (DMC)

$$\lim_{\tau \to \infty} \mathrm{e}^{-H\tau} |\Psi_T\rangle \propto |\Psi_0\rangle + e^{-E_1^* \tau} |\Psi_1\rangle + \ldots$$



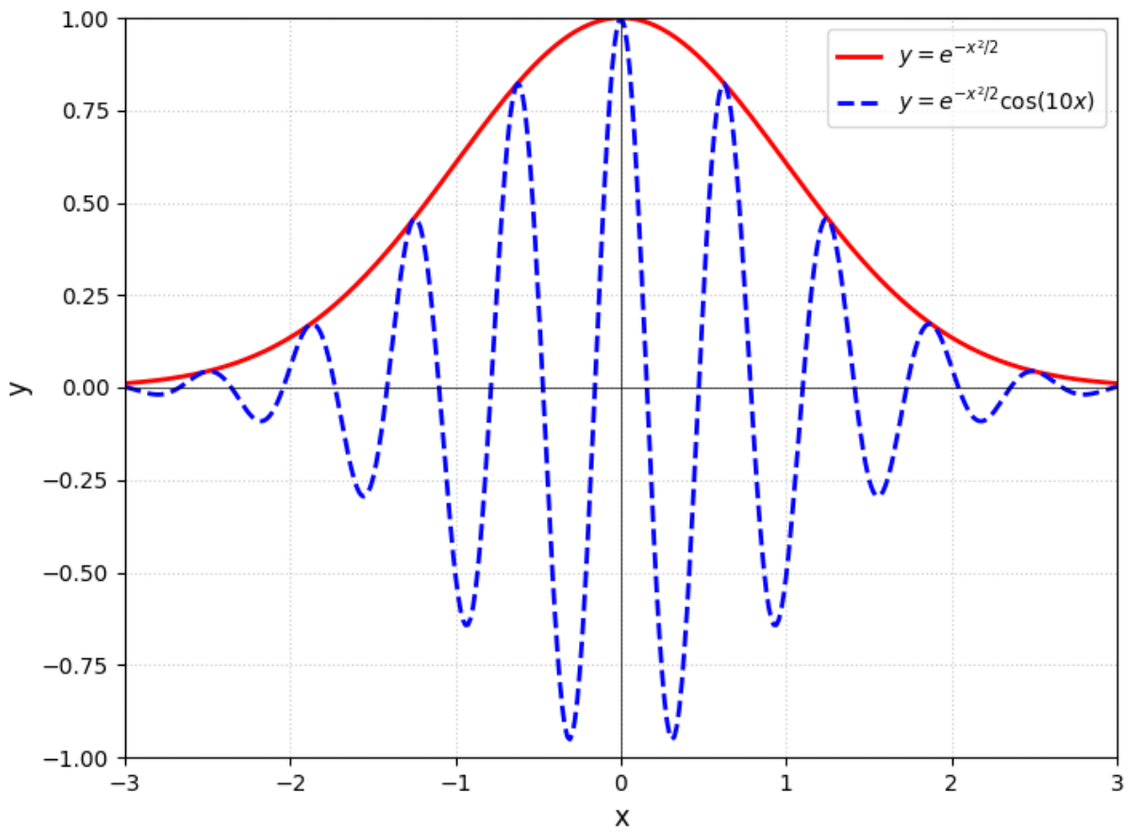
Diffusion Monte Carlo & Sign problem

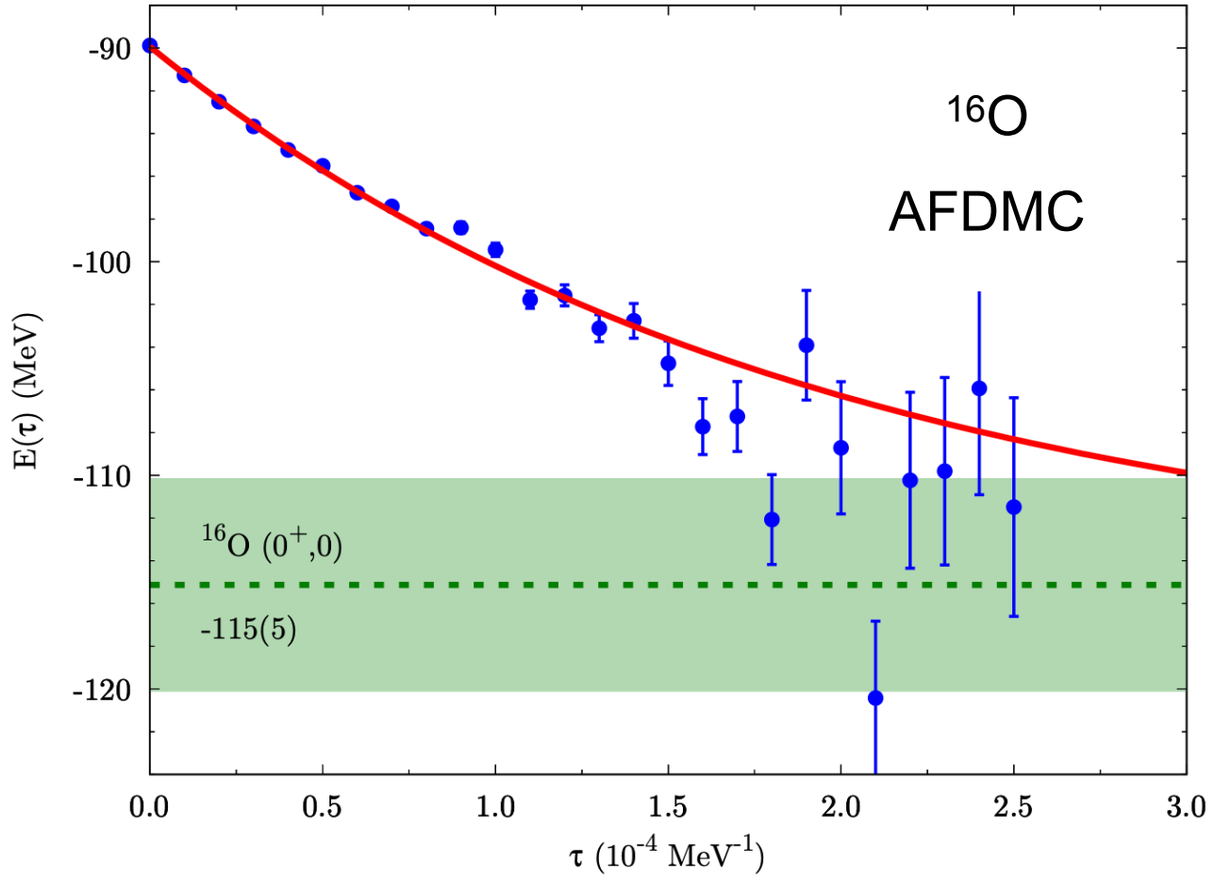
- DMC suffers from the sign problem due to the stochastic realization of $e^{-H\tau}$
- Exponentially increasing noise-tosignal ratio with number of nucleons

$$\langle R'|\, e^{-H\Delta\tau}\,|R\rangle = \mathcal{N}(0,\Delta\tau/M)\, \mathrm{e}^{-V(R)\Delta\tau}\frac{\Psi_T(R')}{\Psi_T(R)}$$

sign oscillation

$$\langle O\rangle_{\mathrm{DMC}} = \frac{\frac{1}{N}\sum_n w_n O_n}{\frac{1}{N}\sum_n w_n}$$



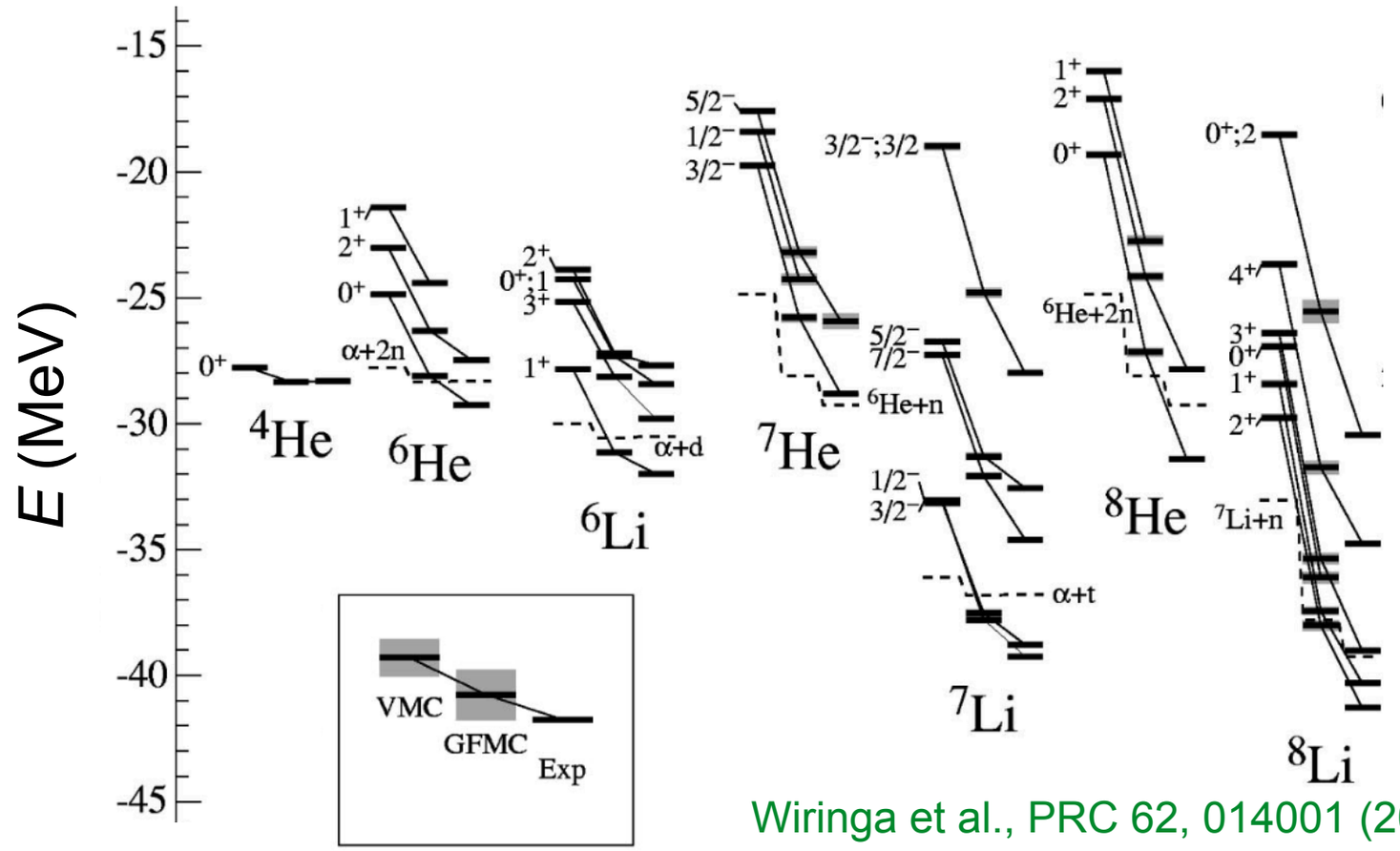


Lonardoni et al., PRC 97, 044318 (2018)

Variational Monte Carlo

- VMC has no sign problem $\quad P(R) = |\Psi_T(R)|^2 \geq 0 \qquad \langle O \rangle_{\mathrm{VMC}} = \frac{1}{N} \sum_n O_n$

- However, conventional wave function ansatz is NOT accurate



Wiringa et al., PRC 62, 014001 (2000)

$$|\Psi_T\rangle = \prod_{i<j} \hat{F}_{ij} |\Phi\rangle$$

$$\frac{\langle \Psi_T | H | \Psi_T \rangle}{\langle \Psi_T | \Psi_T \rangle} > E_0$$

→ Exact wave function ansatz for VMC, exact solution without sign problem

Imaginary-time projection as coordinate transformation (I)

- Consider the Imaginary-time projection on a Slater determinant

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

$$\Psi_0(\boldsymbol{R}) = \lim_{\tau\to\infty} \int_\Omega \mathrm{d}R' \langle \boldsymbol{R}\,|\,e^{-H\tau}\,|\,\boldsymbol{R}'\rangle \det[\varphi_\mu(\boldsymbol{r}_i')] \qquad \boldsymbol{R} = (\boldsymbol{r}_1, \ldots, \boldsymbol{r}_A)$$

Imaginary-time projection as coordinate transformation (II)

$$\Psi_0(\boldsymbol{R}) = \lim_{\tau\to\infty} \int_\Omega \mathrm{d}R' \langle \boldsymbol{R} \,|\, e^{-H\tau} \,|\, \boldsymbol{R}' \rangle \det[\varphi_\mu(\boldsymbol{r}_i')] \qquad \boldsymbol{R} = (\boldsymbol{r}_1, \ldots, \boldsymbol{r}_A)$$

Mean-value theorem

$$= \lim_{\tau\to\infty} V_\Omega \langle \boldsymbol{R} \,|\, e^{-H\tau} \,|\, \boldsymbol{Y}(\boldsymbol{R}) \rangle \det[\varphi_\mu(\boldsymbol{y}_i(\boldsymbol{R}))] \qquad \boldsymbol{Y} = (\boldsymbol{y}_1, \ldots, \boldsymbol{y}_A)$$

Exchange symmetry

$$\boldsymbol{y}_i(\ldots, \boldsymbol{r}_i, \ldots, \boldsymbol{r}_j, \ldots) = \boldsymbol{y}_j(\ldots, \boldsymbol{r}_j, \ldots, \boldsymbol{r}_i, \ldots)$$

Imaginary-time projection as coordinate transformation (III)

$$\Psi_0(\boldsymbol{R}) = \lim_{\tau\to\infty} \int_\Omega \mathrm{d}R' \langle \boldsymbol{R} \,|\, e^{-H\tau} \,|\, \boldsymbol{R}' \rangle \det[\varphi_\mu(\boldsymbol{r}_i')] \qquad \boldsymbol{R} = (\boldsymbol{r}_1, \ldots, \boldsymbol{r}_A)$$

Mean-value theorem

$$= \lim_{\tau\to\infty} V_\Omega \langle \boldsymbol{R} \,|\, e^{-H\tau} \,|\, \boldsymbol{Y}(\boldsymbol{R}) \rangle \det[\varphi_\mu(\boldsymbol{y}_i(\boldsymbol{R}))] \qquad \boldsymbol{Y} = (\boldsymbol{y}_1, \ldots, \boldsymbol{y}_A)$$

Exchange symmetry

$$\boldsymbol{y}_i(\ldots, \boldsymbol{r}_i, \ldots, \boldsymbol{r}_j, \ldots) = \boldsymbol{y}_j(\ldots, \boldsymbol{r}_j, \ldots, \boldsymbol{r}_i, \ldots)$$

→ With transformed coordinates, the g.s. wave function is a Slater determinant

$$\Psi_0(\boldsymbol{R}) = \det[\phi_\mu(\boldsymbol{y}_i(\boldsymbol{R}))]$$

Pescia et al, PRB 110, 035108 (2024)

Imaginary-time projection as coordinate transformation (IV)

$$\Psi_0(\boldsymbol{R}) = \lim_{\tau\to\infty} \int_\Omega \mathrm{d}R' \langle \boldsymbol{R} \,|\, e^{-H\tau} \,|\, \boldsymbol{R}' \rangle \det[\varphi_\mu(\boldsymbol{r}_i')] \qquad \boldsymbol{R} = (\boldsymbol{r}_1, \ldots, \boldsymbol{r}_A)$$

Mean-value theorem

$$= \lim_{\tau\to\infty} V_\Omega \langle \boldsymbol{R} \,|\, e^{-H\tau} \,|\, \boldsymbol{Y}(\boldsymbol{R}) \rangle \det[\varphi_\mu(\boldsymbol{y}_i(\boldsymbol{R}))] \qquad \boldsymbol{Y} = (\boldsymbol{y}_1, \ldots, \boldsymbol{y}_A)$$

Exchange symmetry

$$\boldsymbol{y}_i(\ldots, \boldsymbol{r}_i, \ldots, \boldsymbol{r}_j, \ldots) = \boldsymbol{y}_j(\ldots, \boldsymbol{r}_j, \ldots, \boldsymbol{r}_i, \ldots)$$

→ With transformed coordinates, the g.s. wave function is a Slater determinant

$$\Psi_0(\boldsymbol{R}) = \det[\phi_\mu(\boldsymbol{y}_i(\boldsymbol{R}))]$$

Pescia et al, PRB 110, 035108 (2024)

- Now, the problem turns into finding the many-body transformation $\boldsymbol{R} \to \boldsymbol{Y}$

Parameterizing the transformation **(How?)**

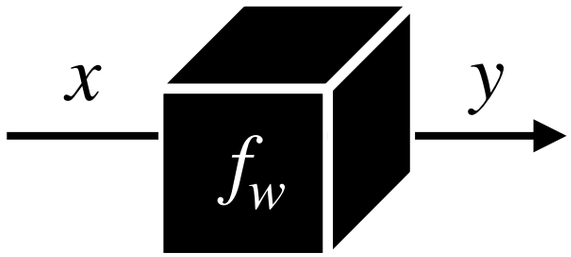
$$(\boldsymbol{r}_1, \ldots, \boldsymbol{r}_A) \to (\boldsymbol{y}_1^\theta(\boldsymbol{R}), \ldots, \boldsymbol{y}_A^\theta(\boldsymbol{R}))$$

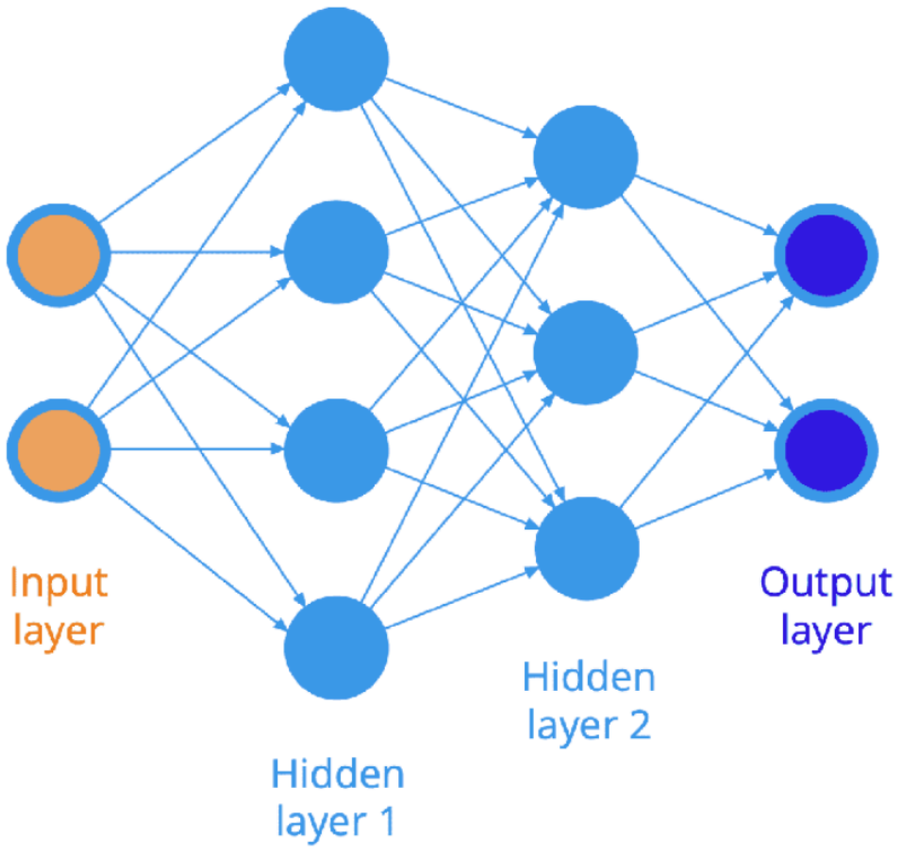
Variational Monte Carlo

$$E_0 = \min_\theta \frac{\langle \Psi_\theta | H | \Psi_\theta \rangle}{\langle \Psi_\theta | \Psi_\theta \rangle}$$

Neural networks

- Function approximator
- Linear affine transformation + Non-linear activation





outputs inputs

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

w, b: adjustable weights

σ: nonlinear functions, e.g. $\tanh(x)$

Universal Approximation Theorem: *existence / limit theorem*

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

Backflow transformation

- Conventional backflow trans. $\boldsymbol{y}_i = \boldsymbol{r}_i + \sum_{j \neq i} \eta(r_{ij})(\boldsymbol{r}_i - \boldsymbol{r}_j)$ $A \times 3$ variables

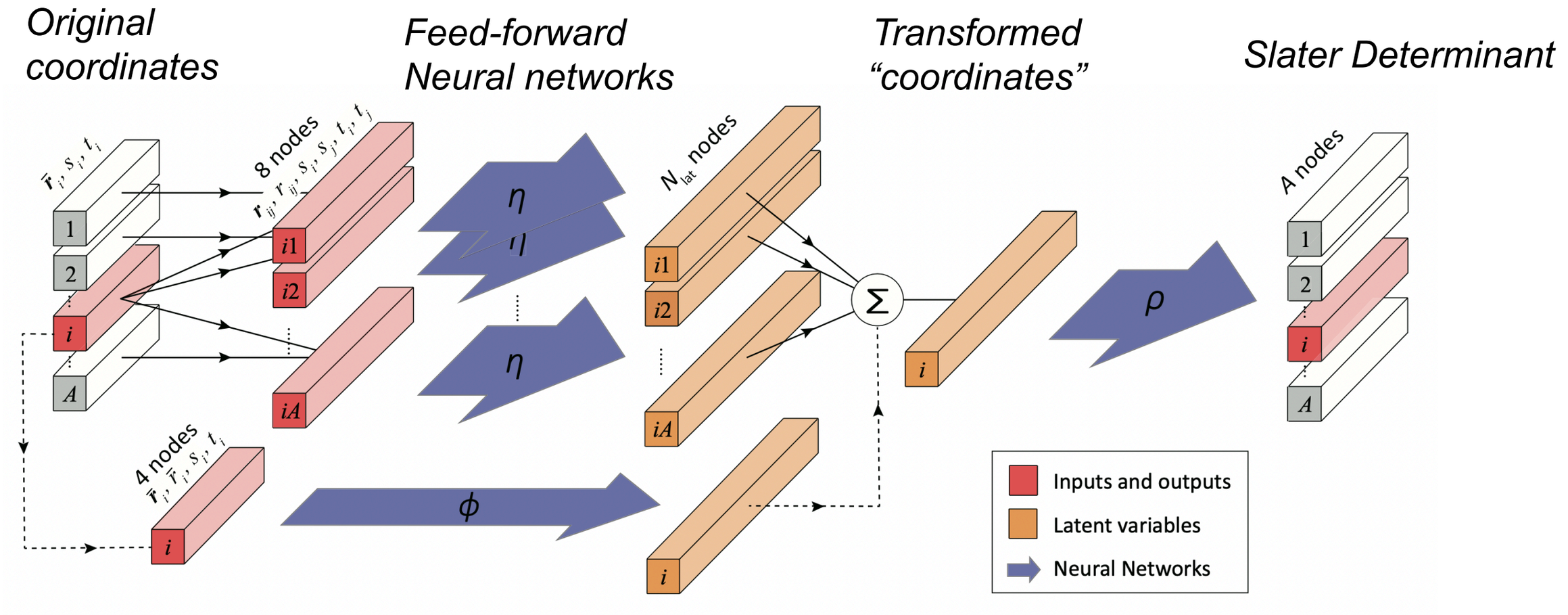
  Feynman and Cohen, Phys. Rev. 102, 1189 (1956)

- Generalized backflow trans.

  Electronic systems: Pfau et al., Phys. Rev. Res. 2, 033429 (2020)
  Hermann et al., Nat. Chem. 12, 891 (2020)
  Nuclear systems: YLY and Pengwei Zhao, PRC 107, 034320 (2023)

$$\vec{\boldsymbol{y}}_i = \vec{\phi}(\bar{\boldsymbol{r}}_i, s_i, t_i) + \sum_{j \neq i} \vec{\eta}(\boldsymbol{r}_{ij}, r_{ij}, s_i, s_j, t_i, t_j)$$

$A \times N_{\text{lat}}$ variables



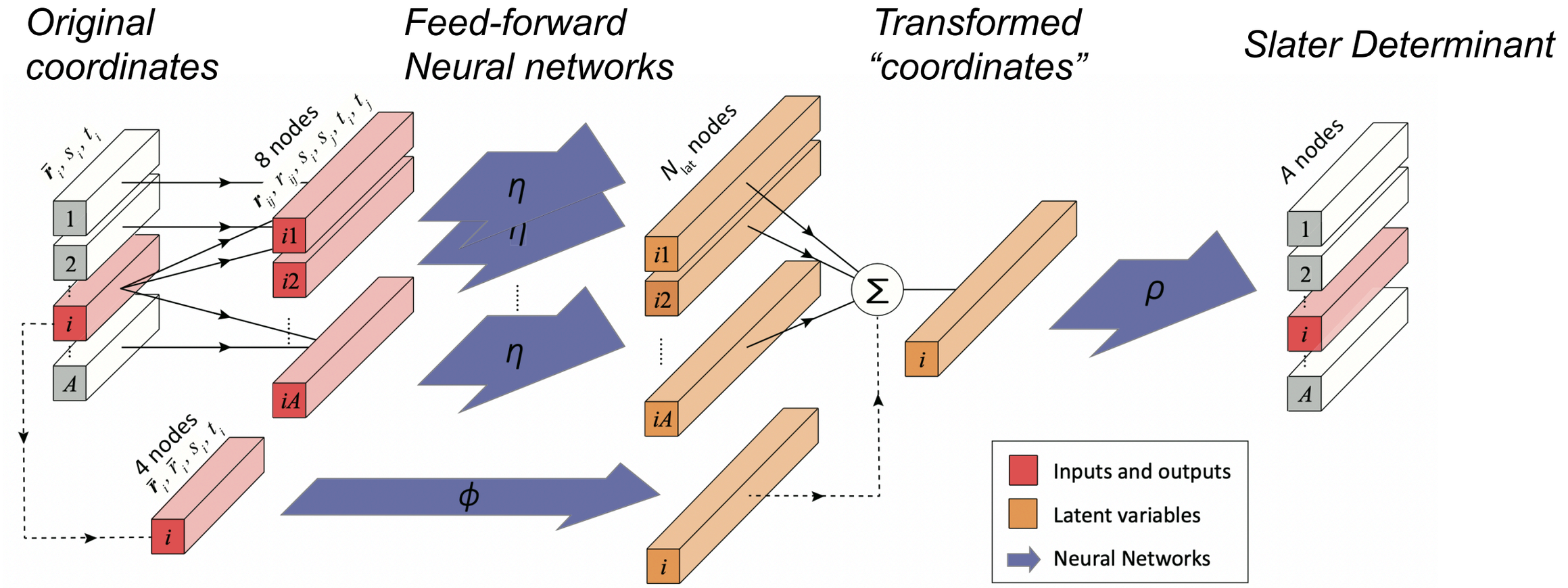
FeynmanNet

- Now, we have a virtually-exact ansatz, *FeynmanNet*, for nuclear VMC calculations

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

$$\Psi(\boldsymbol{x}_1, \ldots, \boldsymbol{x}_A) = \mathrm{e}^{U(\boldsymbol{x}_1,\ldots,\boldsymbol{x}_A)} \sum_n w_n \det[\rho_\mu(\overrightarrow{y}_i)] \qquad \boldsymbol{x}_i = (\boldsymbol{r}_i, s_i, t_i)$$

$$\overrightarrow{\boldsymbol{y}}_i = \overrightarrow{\phi}(\bar{\boldsymbol{r}}_i, s_i, t_i) + \sum_{j\neq i} \overrightarrow{\eta}(\boldsymbol{r}_{ij}, r_{ij}, s_i, s_j, t_i, t_j)$$

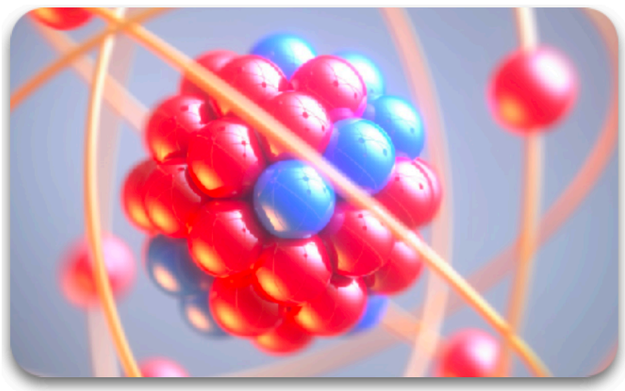


Reinforcement learning vs FeynmanNet-VMC

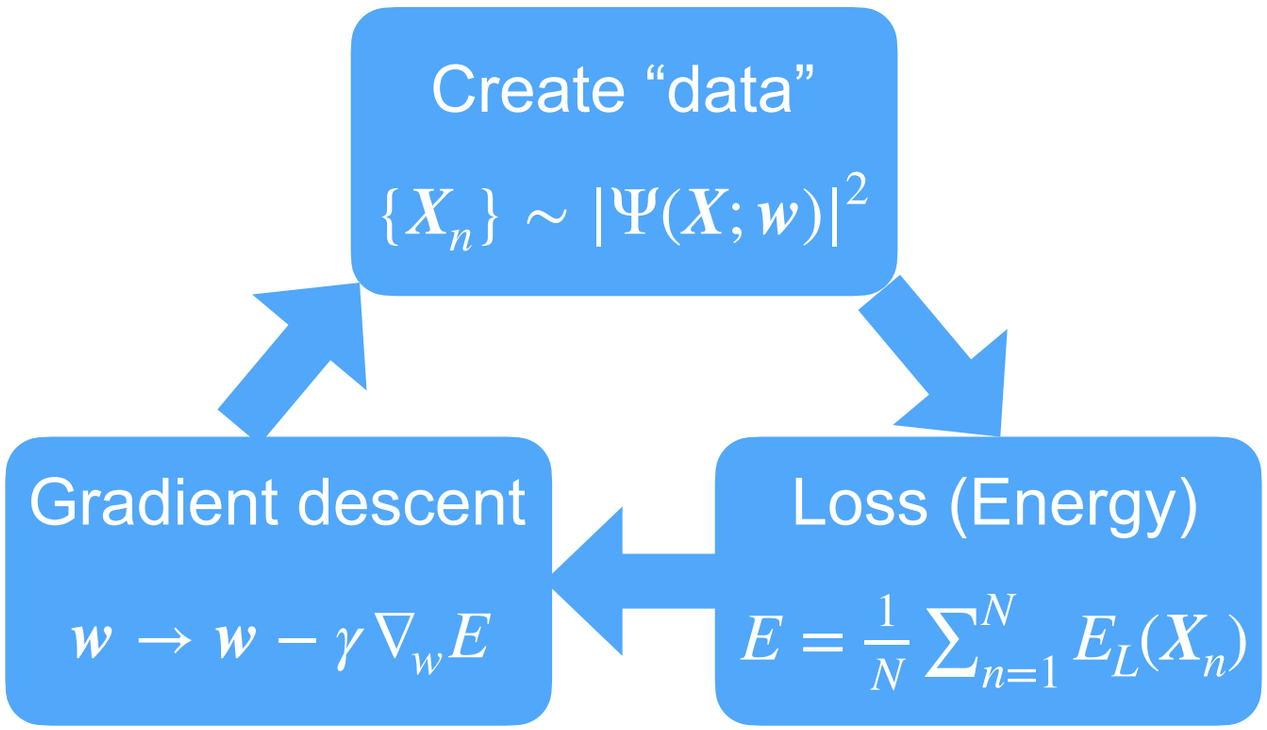
Game rule ⟷ Schrödiner Eq.

Self-play ⟷ VMC iteration

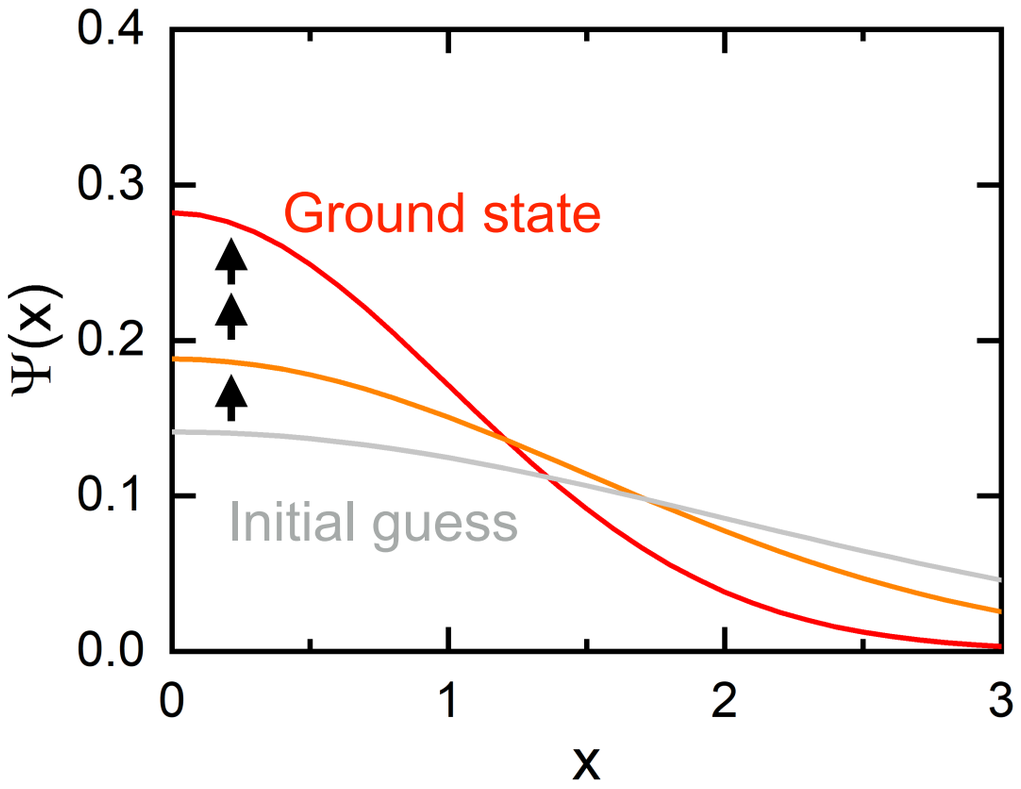
No human data



Variational Monte Carlo



Neural-network wave function



Metropolis-Hastings Monte Carlo

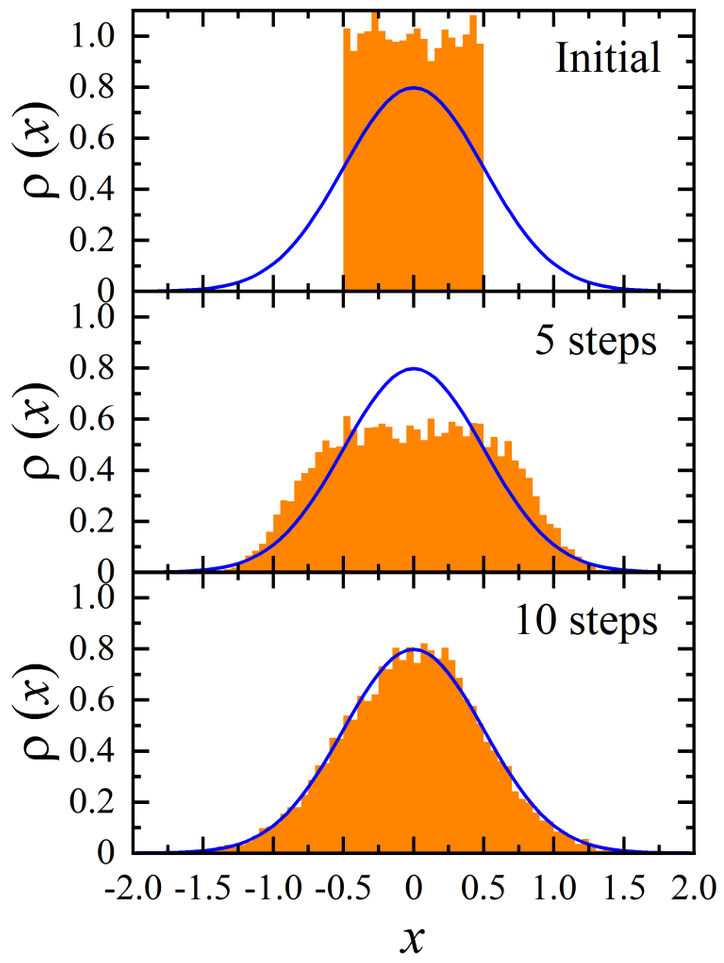
- The energy expectation is calculated stochastically on a set of samples

$$\langle O \rangle = \int \mathrm{d}R P(R) O(R) \simeq \frac{1}{N_{\mathrm{samp}}} \sum_{R \sim P(R)} O(R) \qquad P(R) = \frac{|\Psi(R)|^2}{\int \mathrm{d}R\, |\Psi(R)|^2}$$

- The Metropolis-Hastings algorithm perfoms random walk to obtain samples with the desired distribution $P(R)$.

1. For a given sample R_n, randomly propose a new position R_n', e.g., uniformly in $(R_n - d, R_n + d)$
2. Accept R' with the probability

$$P_{\mathrm{accept}}(R_n \to R_n') = \min\left\{1, \frac{P(R_n')}{P(R_n)}\right\}$$



N. Metropolis et. al., J. Chem. Phys. 21, 1087 (1953)
W. K. Hastings, Biometrika 57, 97 (1970)

Stochastic reconfiguration

- The neural network is trained iteratively by stochastic reconfiguration

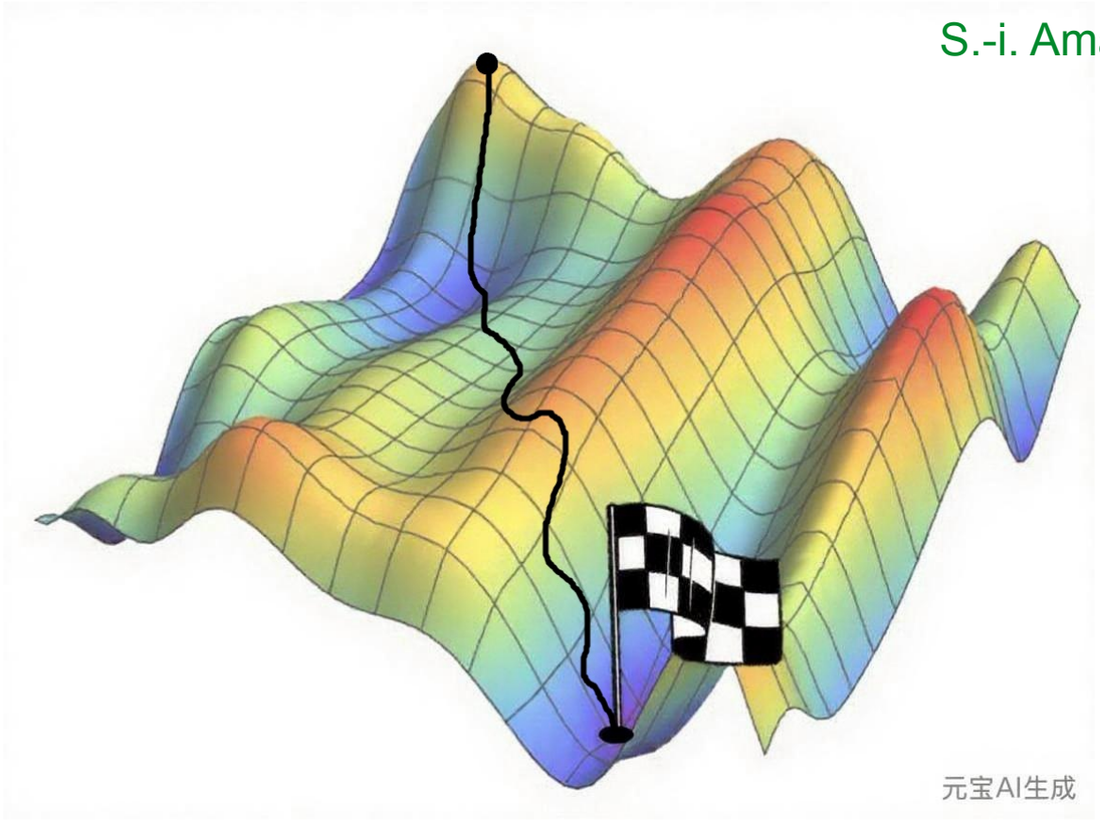
S. Sorella, Phys. Rev. B 71, 241103(R) (2005)

$$\boldsymbol{\theta}^{t+1} = \boldsymbol{\theta}^{t} - \gamma(\mathbf{S} + \epsilon I)^{-1}\boldsymbol{g}$$

$$g_i = \partial_i E = 2\left(\frac{\langle \partial_i \Psi | H | \Psi \rangle}{\langle \Psi | \Psi \rangle} - E\frac{\langle \partial_i \Psi | \Psi \rangle}{\langle \Psi | \Psi \rangle}\right), \quad S_{ij} = \frac{\langle \partial_i \Psi | \partial_j \Psi \rangle}{\langle \Psi | \Psi \rangle} - \frac{\langle \partial_i \Psi | \Psi \rangle}{\langle \Psi | \Psi \rangle}\frac{\langle \Psi | \partial_j \Psi \rangle}{\langle \Psi | \Psi \rangle}$$

- Closely related to natural gradient descent method

S.-i. Amari, Neural Comput. 10, 251 (1998)



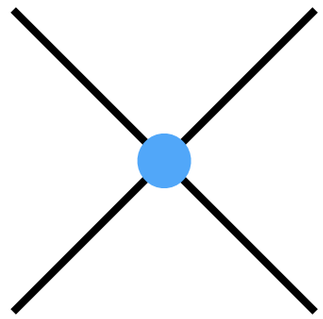
LO pionless Hamiltonian

- Regularized short-range NN+3N potentials

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

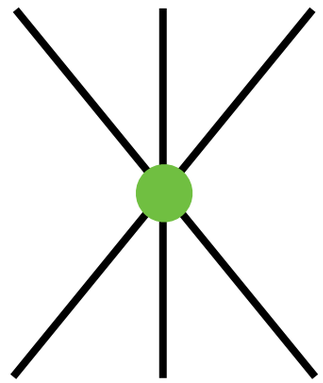
- NN potential: fit to NN S-wave scattering lengths, effective range, and deuteron binding energy

$$v_{ij}^{\mathrm{CI}} = \sum_{p=1}^{4} v_p(r_{ij}) O_{ij}^{p} \qquad O_{ij}^{p=1\text{-}4} = 1,\ \tau_{ij},\ \sigma_{ij},\ \sigma_{ij}\tau_{ij}$$



- 3N potential: adjusted to ^{3}H and ^{16}O binding energy

$$V_{ijk} = D \sum_{\mathrm{cyc}} e^{-(r_{ij}^2 + r_{jk}^2)/R_3^2}$$



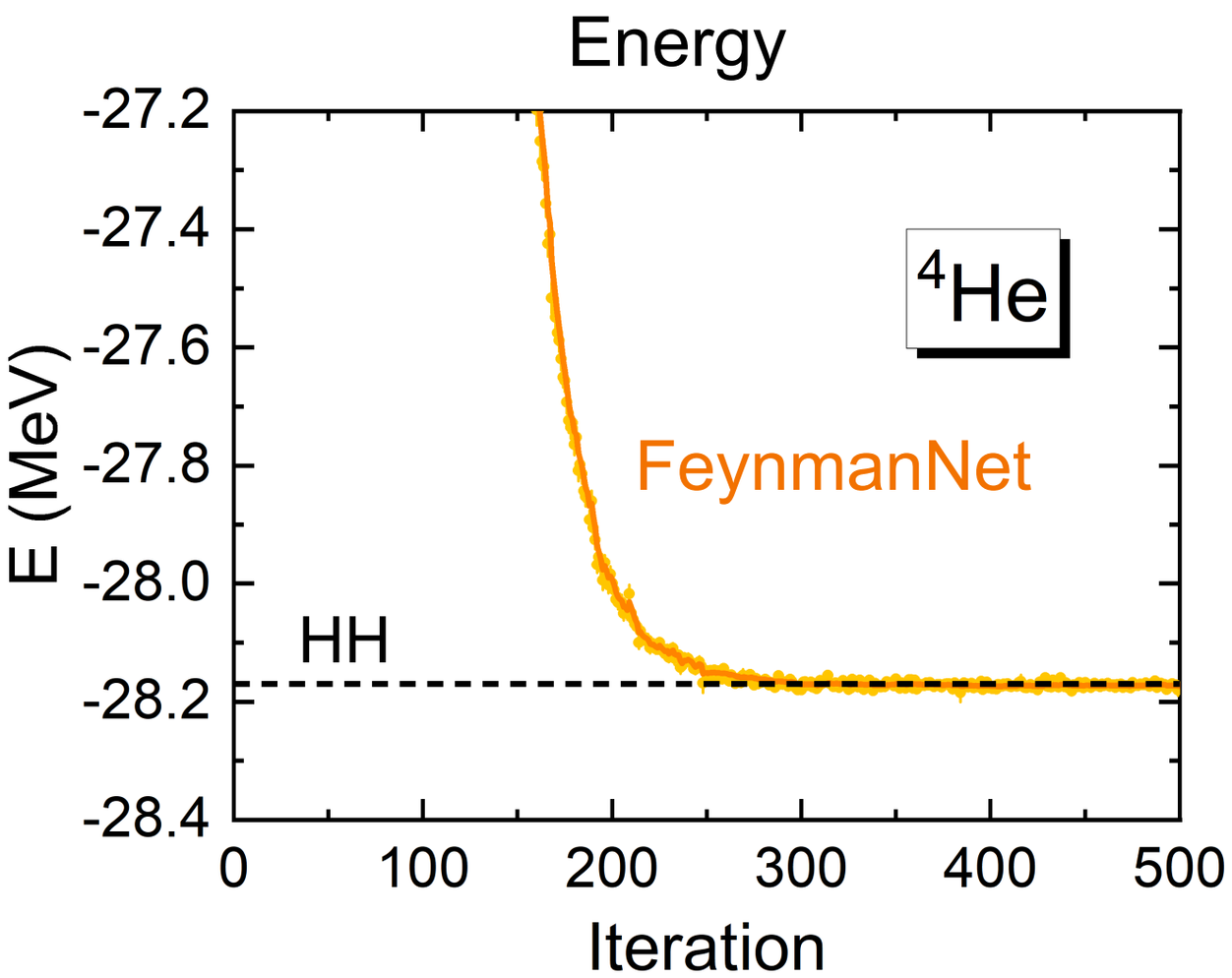
r-space cutoffs: $R_{T=0} \simeq 1.5$ fm, $R_{T=1} \simeq 1.8$ fm, $R_3 = 1.0$ fm

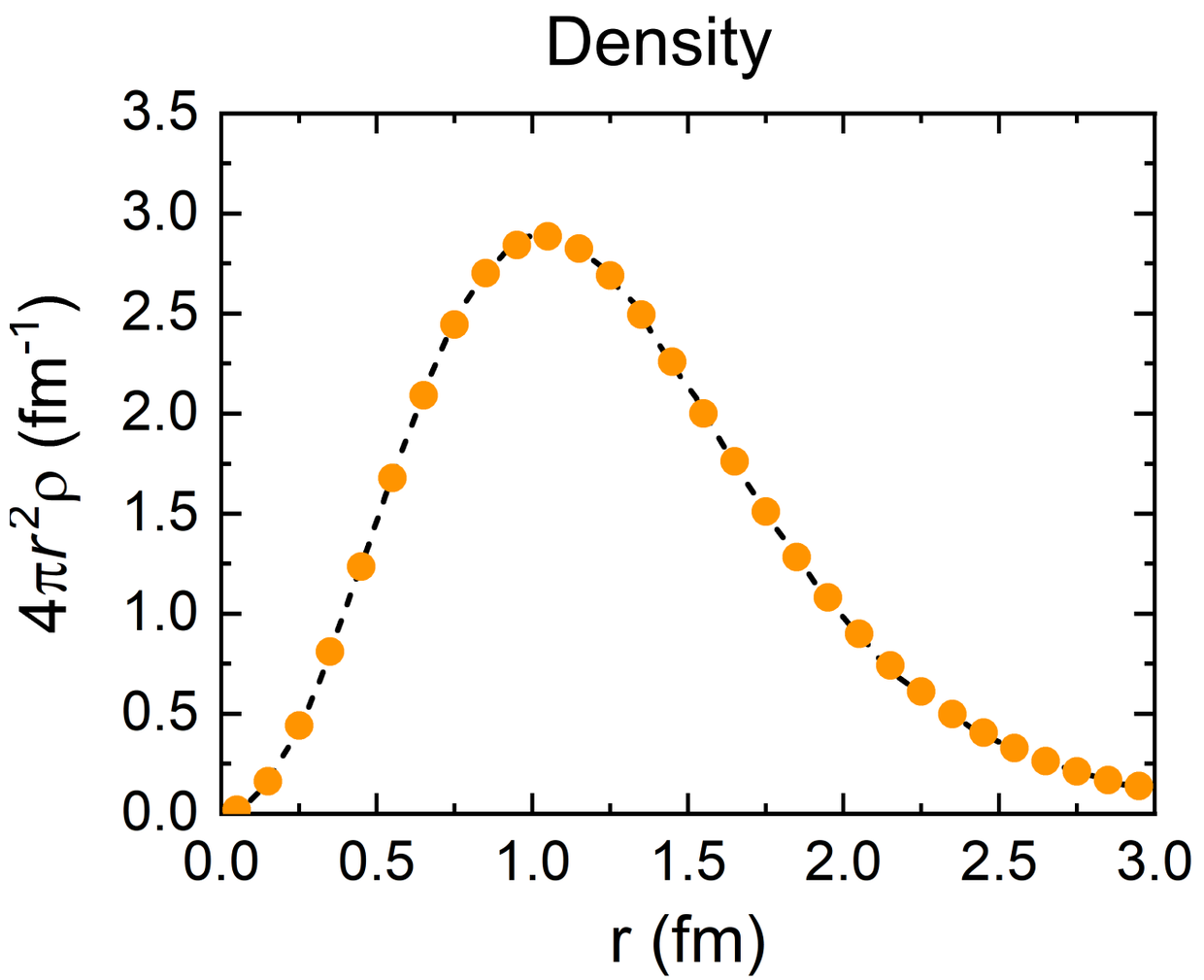
FeynmanNet: ^{4}He ground state

- Perfect agreement with the Hyperspherical Harmonics (HH) method

  Accuracy at the level of ~0.01 MeV for $A \leq 4$ nuclei

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

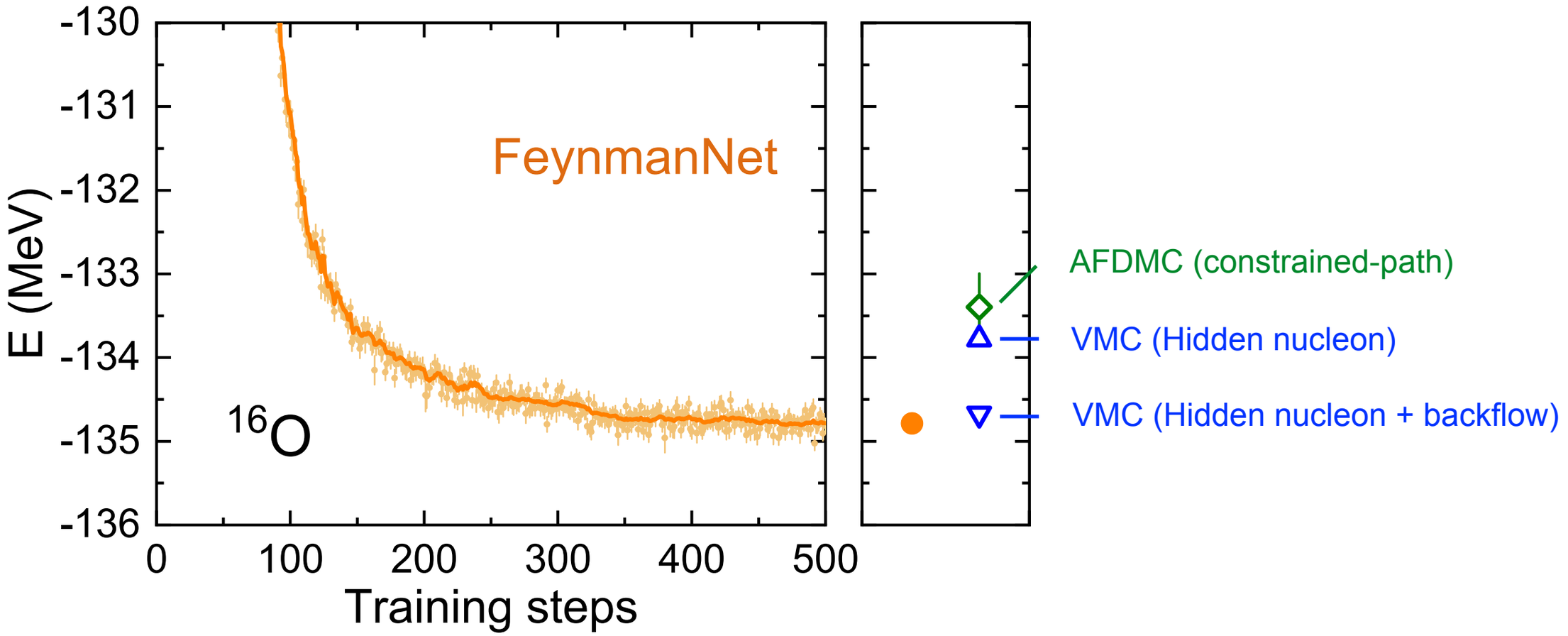




Hyperspherical Harmonics method: Gnech et al., Few-Body Syst. 63, 7 (2022)

FeynmanNet: ^{16}O ground state energy

- FeynmanNet provides the lowest energy among the QMC methods



VMC (FeynmanNet): YLY and Zhao, PRC 107, 034320 (2023)

VMC (Hidden nucleon): *Lovato et al., Phys. Rev. Research 127, 022502 (2022)*

VMC (Hidden nucleon + backflow): *Gnech et al., PRL 133, 142501 (2024)*

AFDMC (constrained-path): *Schiavilla et al., PRC 103, 054003 (2021)*

Chiral Hamiltonians

LO pionless EFT

N²LO chiral EFT

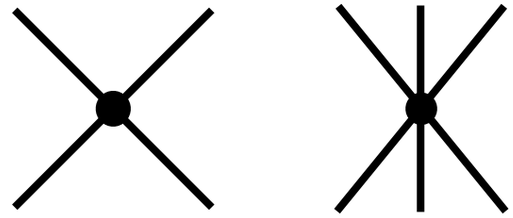
$$O_{ij}^{p=1,14} = \boxed{1, \boldsymbol{\tau}_i\cdot\boldsymbol{\tau}_j,\ \boldsymbol{\sigma}_i\cdot\boldsymbol{\sigma}_j, (\boldsymbol{\sigma}_i\cdot\boldsymbol{\sigma}_j)(\boldsymbol{\tau}_i\cdot\boldsymbol{\tau}_j)}\ \boxed{S_{ij}, S_{ij}(\boldsymbol{\tau}_i\cdot\boldsymbol{\tau}_j),\ \mathbf{L}\cdot\mathbf{S}, \mathbf{L}\cdot\mathbf{S}(\boldsymbol{\tau}_i\cdot\boldsymbol{\tau}_j)},$$
$$L^2, L^2(\boldsymbol{\tau}_i\cdot\boldsymbol{\tau}_j),\ L^2(\boldsymbol{\sigma}_i\cdot\boldsymbol{\sigma}_j), L^2(\boldsymbol{\sigma}_i\cdot\boldsymbol{\sigma}_j)(\boldsymbol{\tau}_i\cdot\boldsymbol{\tau}_j),\ (\mathbf{L}\cdot\mathbf{S})^2, (\mathbf{L}\cdot\mathbf{S})^2(\boldsymbol{\tau}_i\cdot\boldsymbol{\tau}_j)\ .$$

N³LO terms

- LO pionless Hamiltonian: short-range NN+3N potentials

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

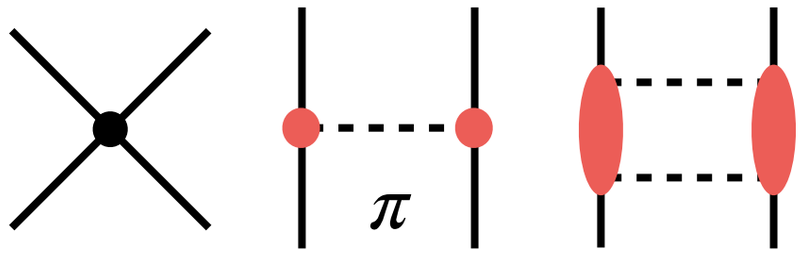
$$v_{ij}^{\mathrm{CI}} = \sum_{p=1}^{4} v_p(r_{ij}) O_{ij}^p$$



- Local N²LO chiral Hamiltonian: short-range and pion-exchange NN+3N potentials

Lynn et al. PRL 116, 062501 (2016)

$$v_{ij}^{\mathrm{CI}} = \sum_{p=1}^{8} v_p(r_{ij}) O_{ij}^p$$



Tensor forces

Iterative correlator ansatz

- When tensor force is present, the transformation $\boldsymbol{R} \to \boldsymbol{Y}(\boldsymbol{R}, \boldsymbol{S})$ exists but may be hard to find; thus, we treat spin-isospin operators explicitly in the transformation.

$$
\begin{aligned}
\mathrm{e}^{-H\Delta\tau}|\Phi(\boldsymbol{R})\rangle &= \langle \boldsymbol{R}|e^{-H\Delta\tau}|\boldsymbol{Y}(\boldsymbol{R})\rangle|\Phi(\boldsymbol{Y}(\boldsymbol{R}))\rangle \\
(\mathrm{e}^{-H\Delta\tau} \simeq 1 - \hat{T}\Delta\tau - \hat{V}\Delta\tau) &\Rightarrow \sum_{i<j}\sum_{p} g^p(\boldsymbol{r}_{ij}, \boldsymbol{y}_{ij}(\boldsymbol{R}))O^p_{ij}|\Phi(\boldsymbol{Y}(\boldsymbol{R}))\rangle
\end{aligned}
$$

O^p_{ij}: spin-isospin dependent operators in the NN force

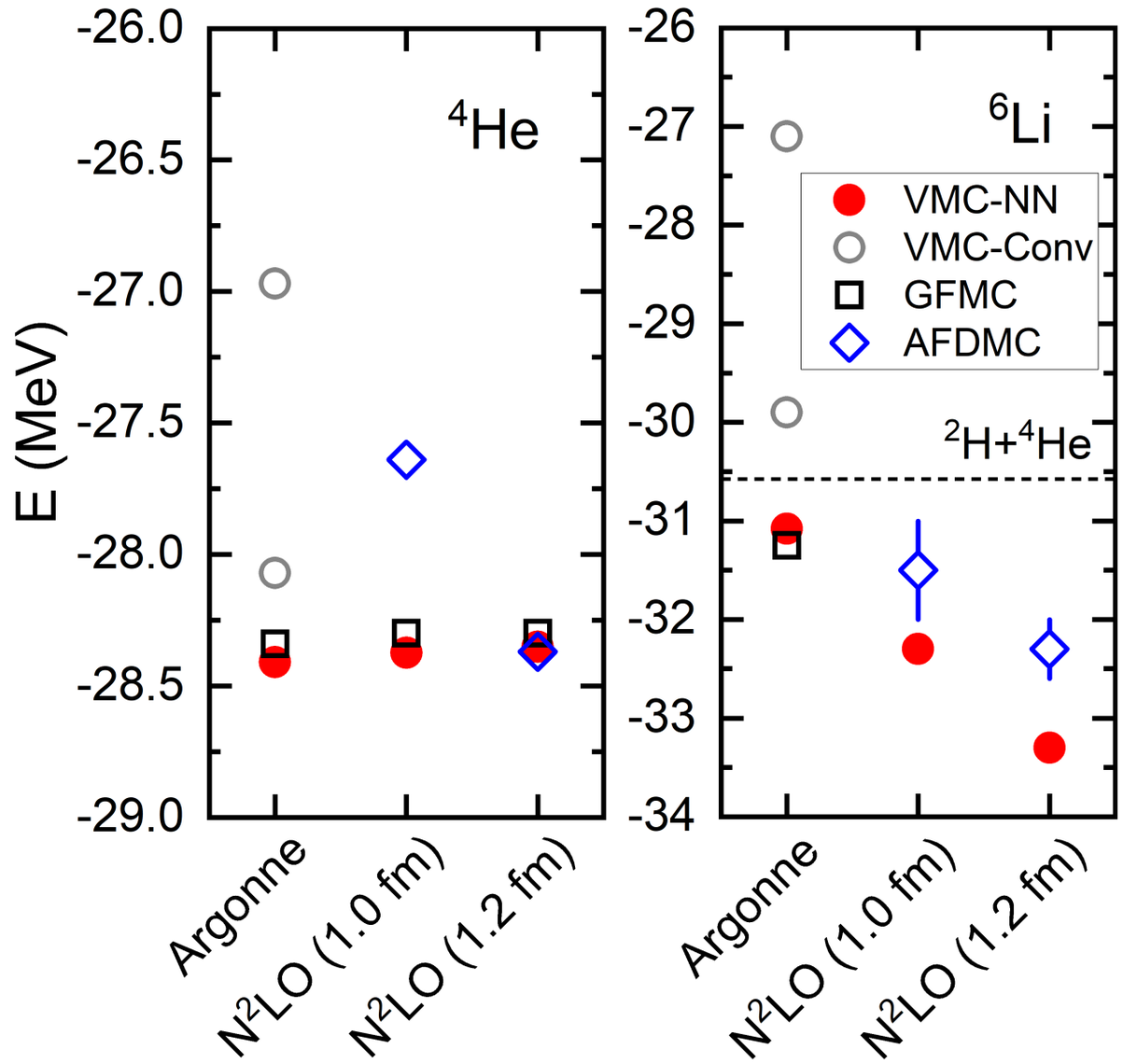
- Neural-network iterative correlator ansatz:

$$
|\Psi(\boldsymbol{R})\rangle = \prod_{n=1}^{n_J}\left[1 + \sum_{i<j}\mathcal{U}^{(n)}_{ij}(\boldsymbol{R}) + \sum_{i<j<k}\mathcal{V}^{(n)}_{ijk}(\boldsymbol{R})\right]|\Phi(\boldsymbol{R})\rangle
$$

$$
\mathcal{U}^{(n)}_{ij}(\boldsymbol{R}) = \sum_{p=2}^{6} u^{(n)}_p(y_{ij})O^p_{ij}, \quad \mathcal{V}^{(n)}_{ijk}(\boldsymbol{R}) = \sum_{q=1}^{8} v^{(n)}_q(\boldsymbol{y}_i, \boldsymbol{y}_j, \boldsymbol{y}_k)\tilde{O}^q_{ijk} \qquad \boldsymbol{Y} = \boldsymbol{Y}(\boldsymbol{R})
$$

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

Accurate NN wave function for solving realistic forces



VMC-NN: VMC with neural-network ansatz (this work)

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

VMC-Conv: VMC with conventional ansatz

Wiringa et al., PRC 62, 014001 (2000); Usmani et al., PRC 86, 034323 (2012)

GFMC: Green's function Monte Carlo (a nuclear DMC method)

Lynn et al., PRC 96, 054007 (2017)

AFDMC: Auxiliary-field Diffusion Monte Carlo

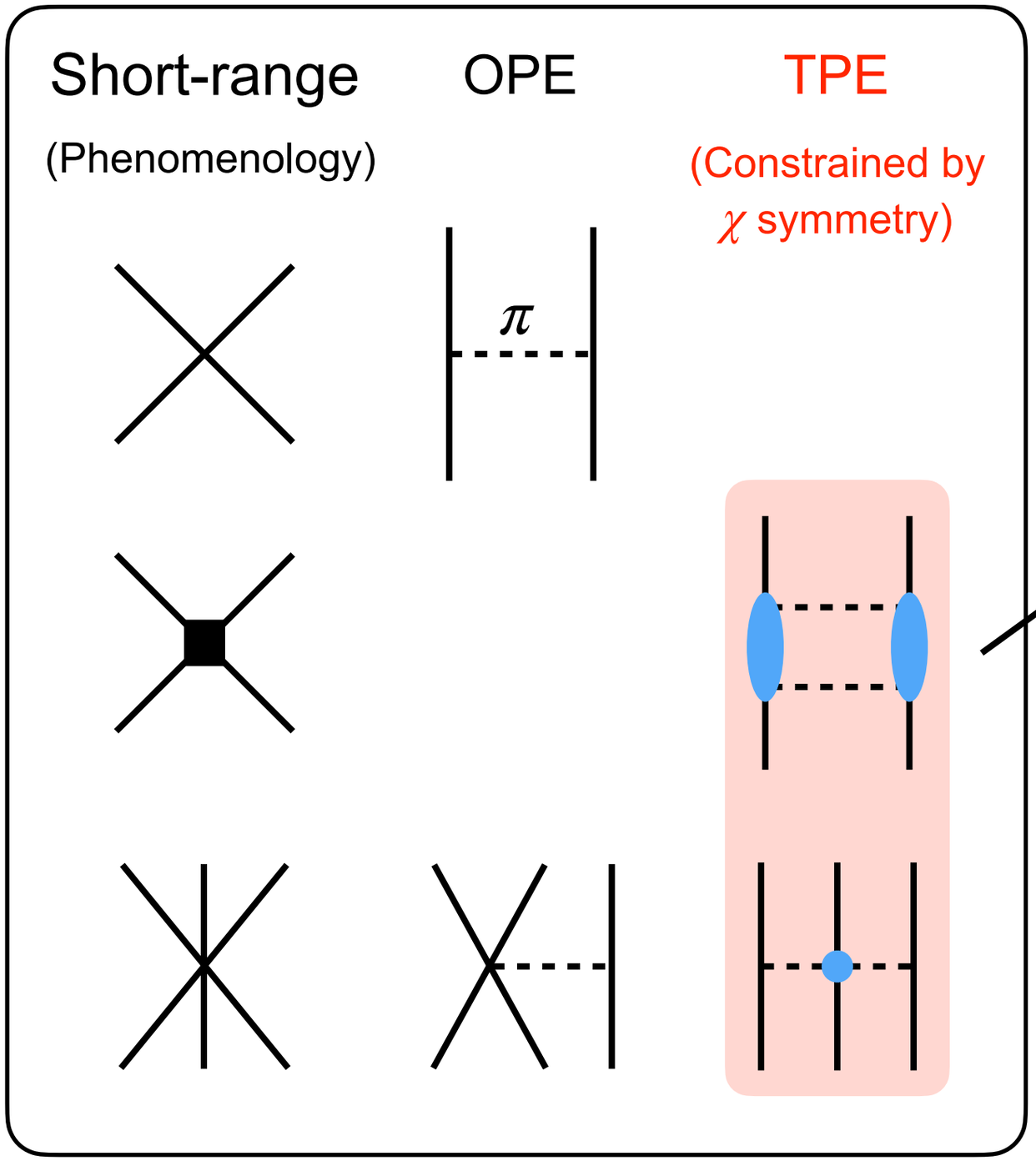
Lonardoni et al., PRC 97, 044318 (2018)

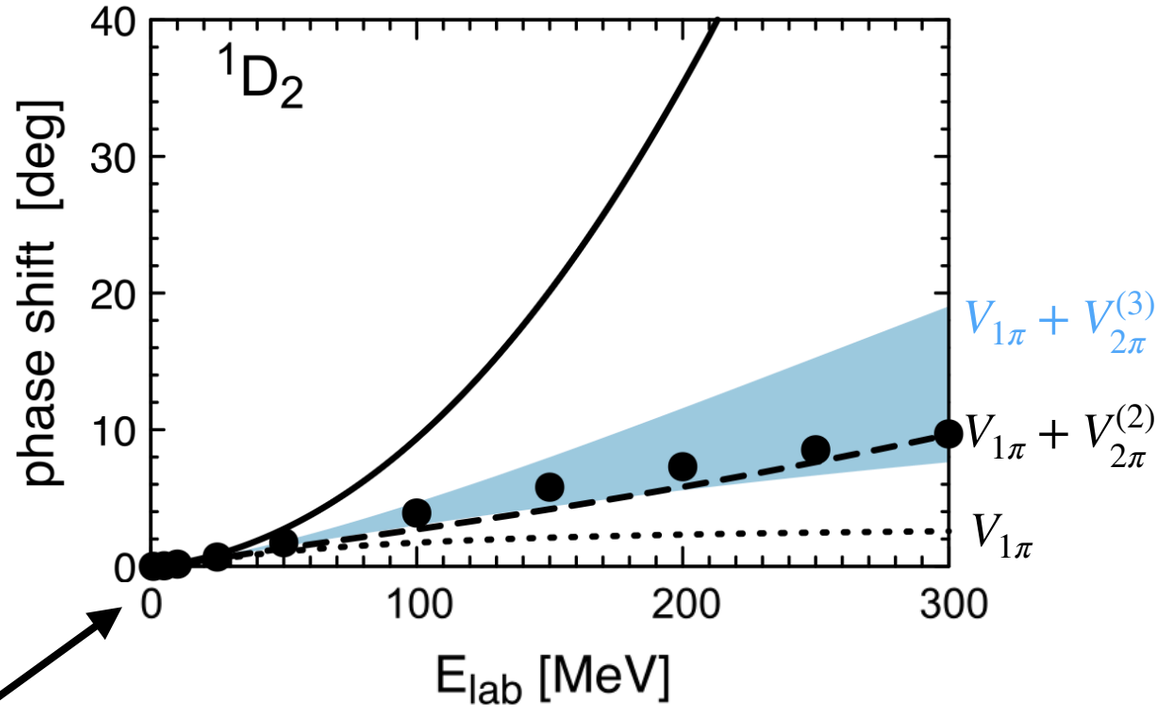
Outline

- *Ab initio* nuclear theory
- Neural-network quantum Monte Carlo
- **Probing long-range 3NF in peripheral neutron-α scattering**
- Summary and outlook

Motivation

- How to test the chiral EFT prediction of long-range part of nuclear force?





Testing TPE NN force in peripheral NN scattering

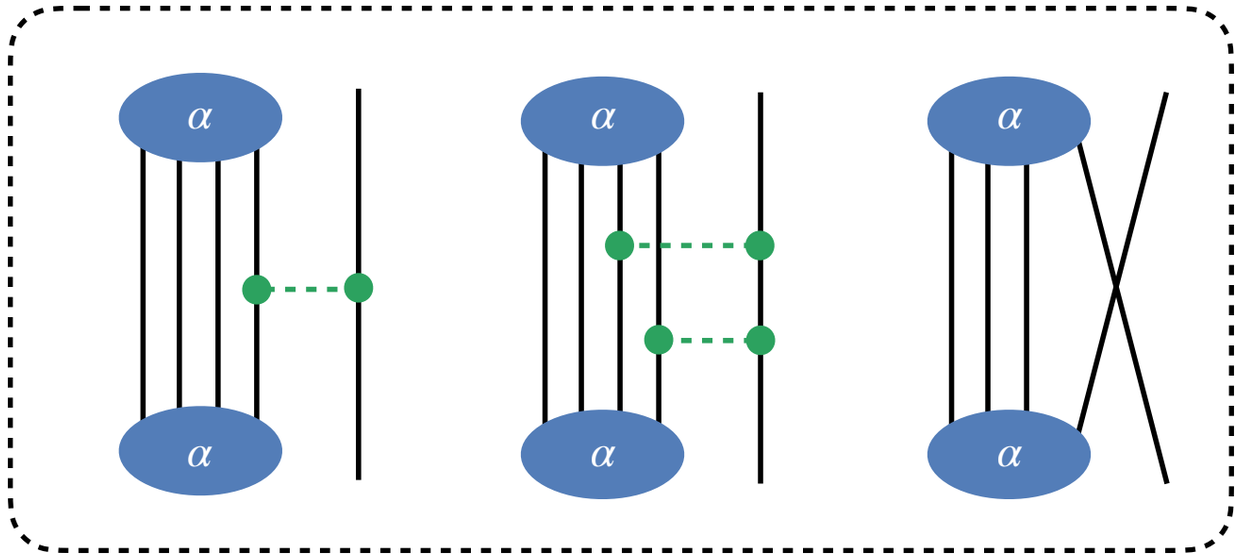
Kaiser, Brockmann, and Weise, NPA 625, 758 (1997)

1. Can one find more direct probe for TPE, without OPE interfering?
2. How to probe TPE 3NF?

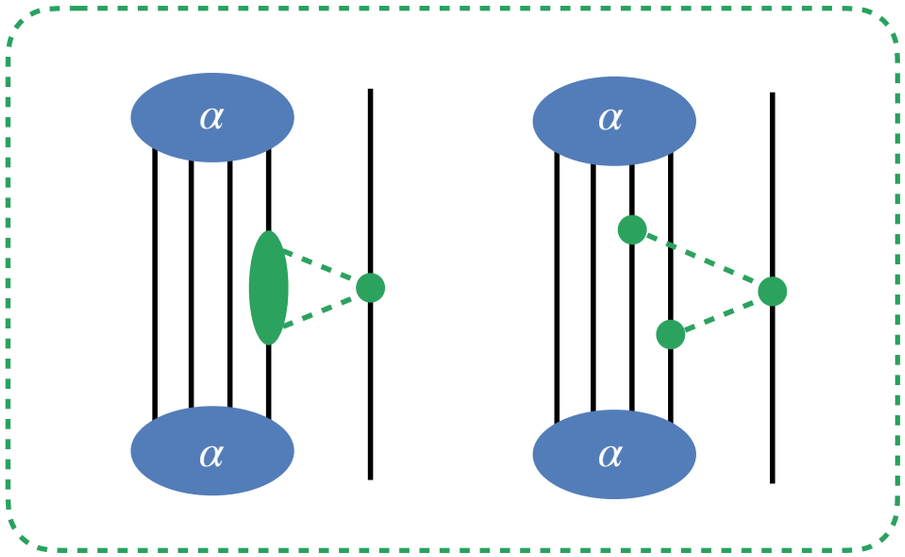
Peripheral $n\alpha$ scattering

- Peripheral $n\alpha$ scattering might be suitable!

Suggested in Higa and Robilotta, arXiv:nucl-th/9908062 (1999)



Suppressed



Allowed

- The existing studies have focused on *S*- and *P*-waves, where short-range mechanisms dominate, while **no *ab initio* studies of peripheral $n\alpha$ scattering are available yet to probe long-range TPE three-nucleon forces.**

QMC: Carslon1987PRC, Lynn2016PRL, …

Faddeev-Yakubovsky: Lazauskas2018PRC, …

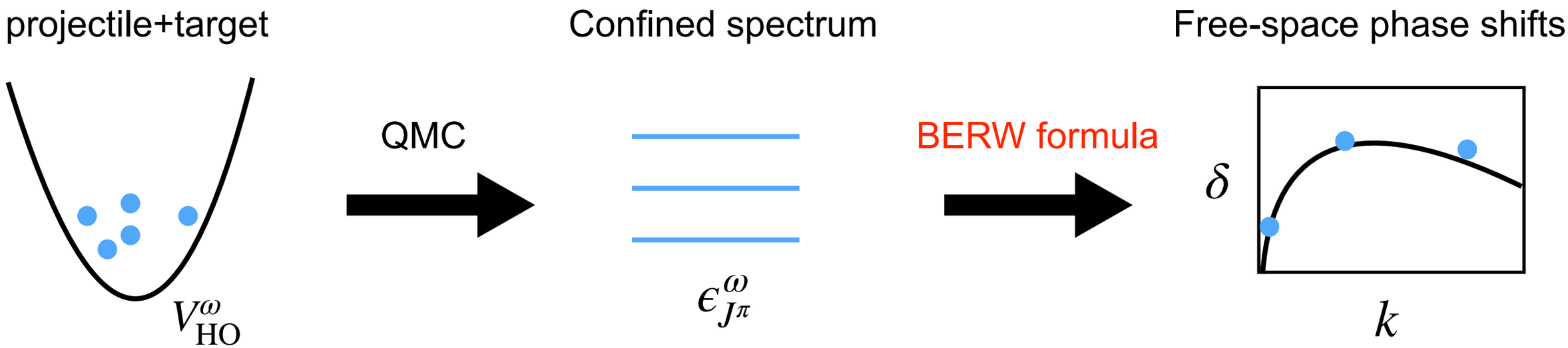
NCSM: Navrátil2016PS, Shirokov2018PRC, …

SVM: Bagnarol2023PLB, …

Harmonic potential trap approach

- Bridging the bound-state techinques and scattering observables

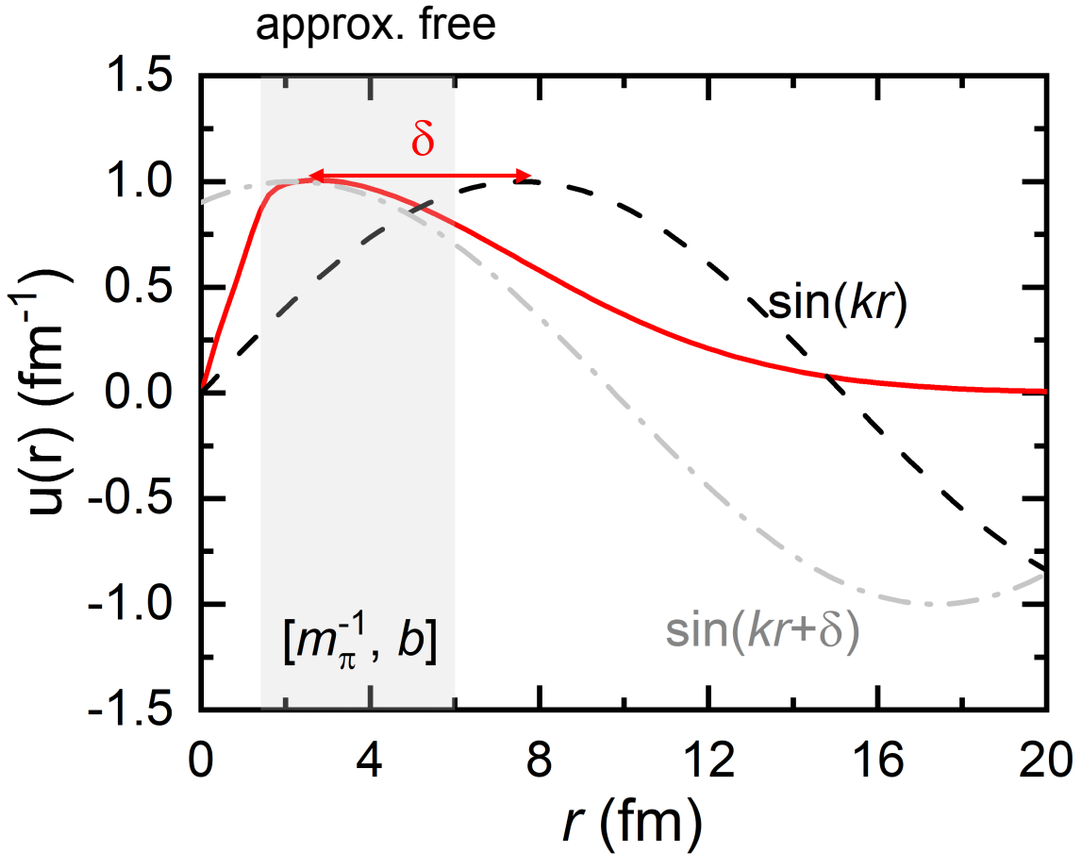
T. Busch, B.-G. Englert, K. Rzazewski, and M. Wilkens, Foundations of Physics 28, 549 (1998)



- The BERW formula connects the confined spectrum with free-space phase shifts

$$k^{2l+1}\cot\delta_l(k) = (-)^{l+1}\,(4\mu\omega)^{l+\frac{1}{2}}\,\frac{\Gamma\left(\frac{3+2l}{4}-\frac{\epsilon_{J\pi}^{\omega}}{2\omega}\right)}{\Gamma\left(\frac{1-2l}{4}-\frac{\epsilon_{J\pi}^{\omega}}{2\omega}\right)}$$

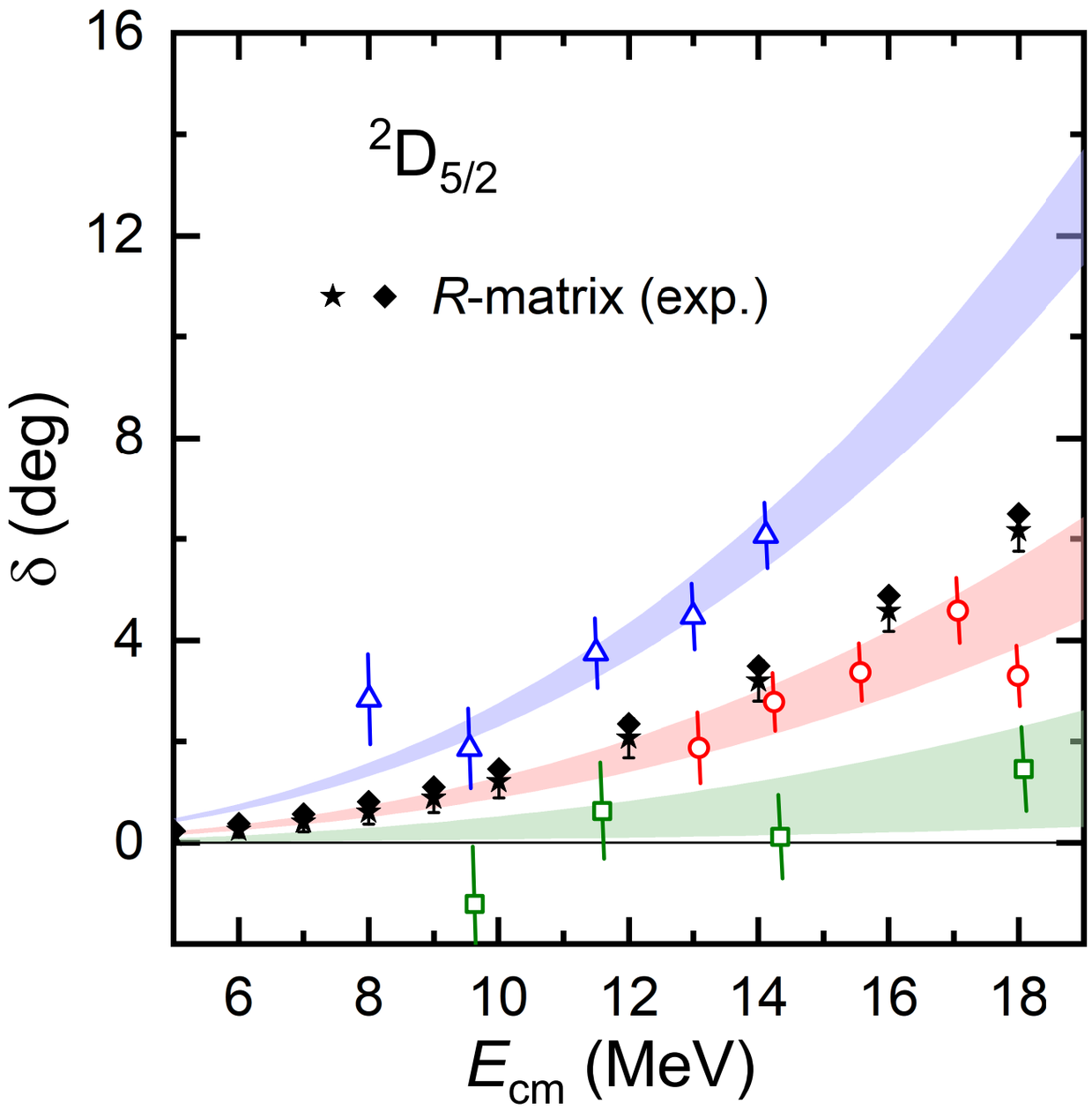
ω : harmonic oscillator (HO) frequency

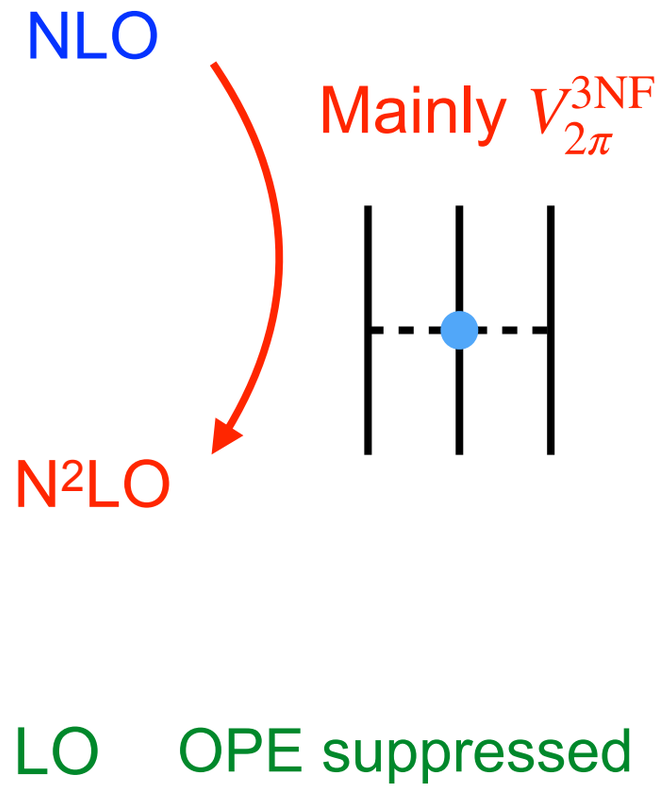


Impact of leading TPE 3NF

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

- Leading chiral TPE 3NF at N²LO provides a large repulsive contribution that improves the agreement with empirical D-wave $n\alpha$ phase shifts.

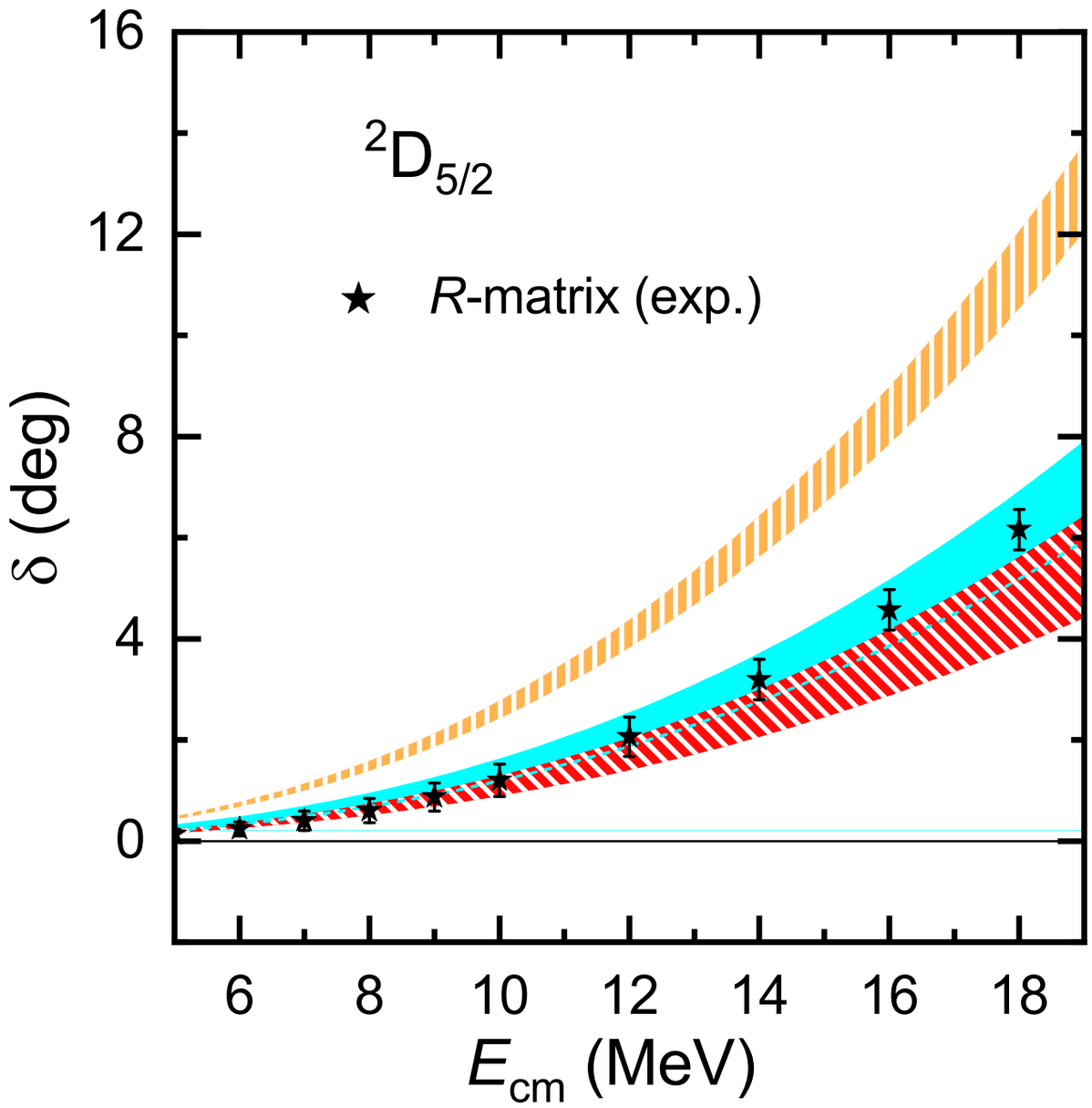




Impact of subleading TPE 3NF

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

- Peripheral $n\alpha$ scattering provides a clean & sensitive probe to long-range 3NFs governed by χ symmetry



N²LO NN only

N²LO NN+3NF(effective c_i s)

$c_1 = -0.87,\ c_3 = -2.71,\ c_4 = 1.41$

N²LO NN+3NF

$c_1 = -0.81,\ c_3 = -3.40,\ c_4 = 3.40$

The N³LO and N⁴LO corrections effectively mimicked by reducing c_is

Krebs, Gasparyan, and Epelbaum PRC 85, 054006 (2012)

Summary and outlooks

- **Neural-network variational Monte Carlo: a novel nuclear *ab initio* method**

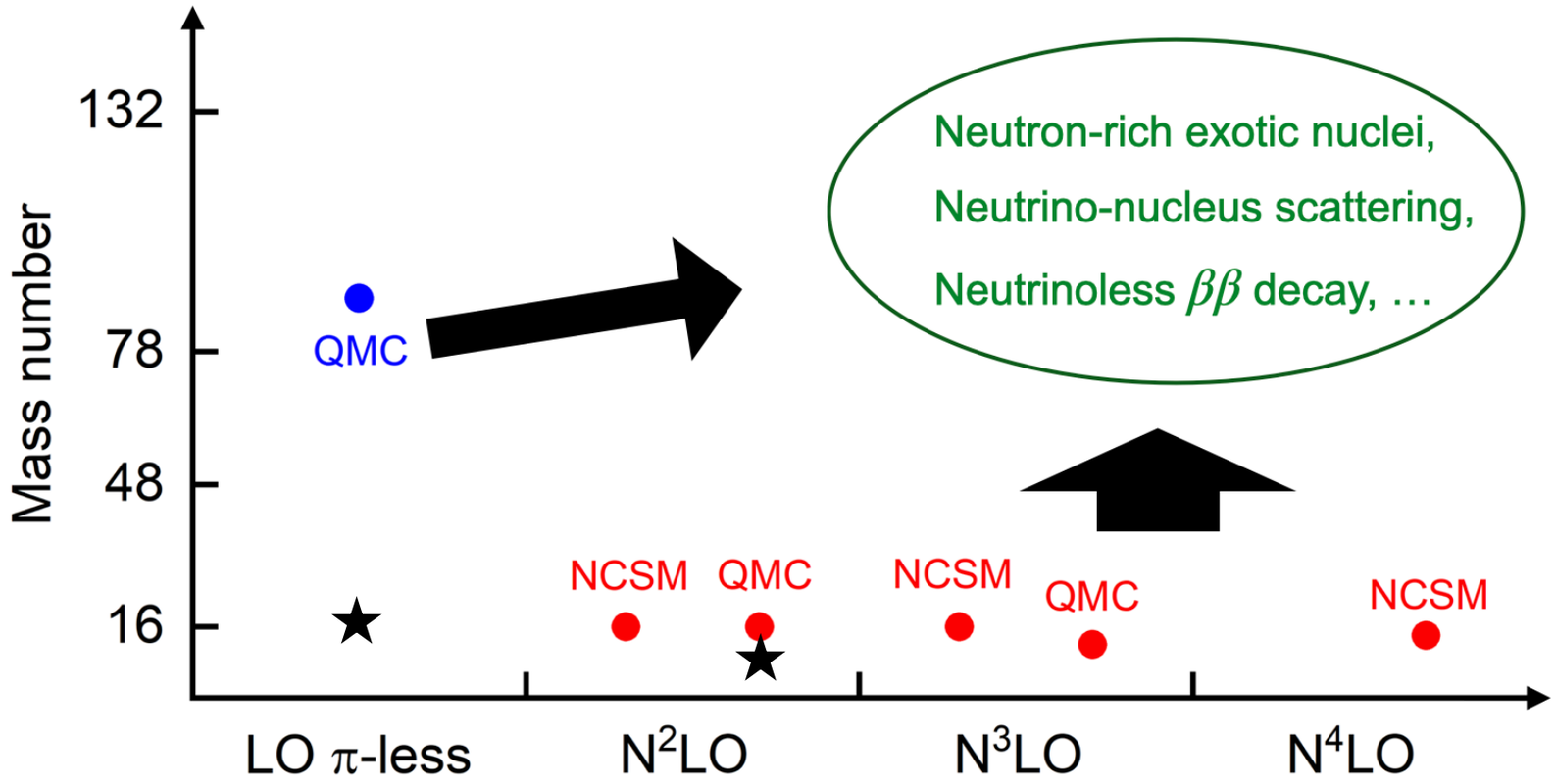
Present: Benchmark calculations in light nuclei

Rivaling/being superior than conventional diffusion Monte Carlo

Future: Heavier nuclei with more realistic nuclear forces

Excited states, resonances, …

Nuclear response, nuclear matrix elements, …



Acknowledgement

Thank you for your attention!

Appendix

Chiral perturbation theory

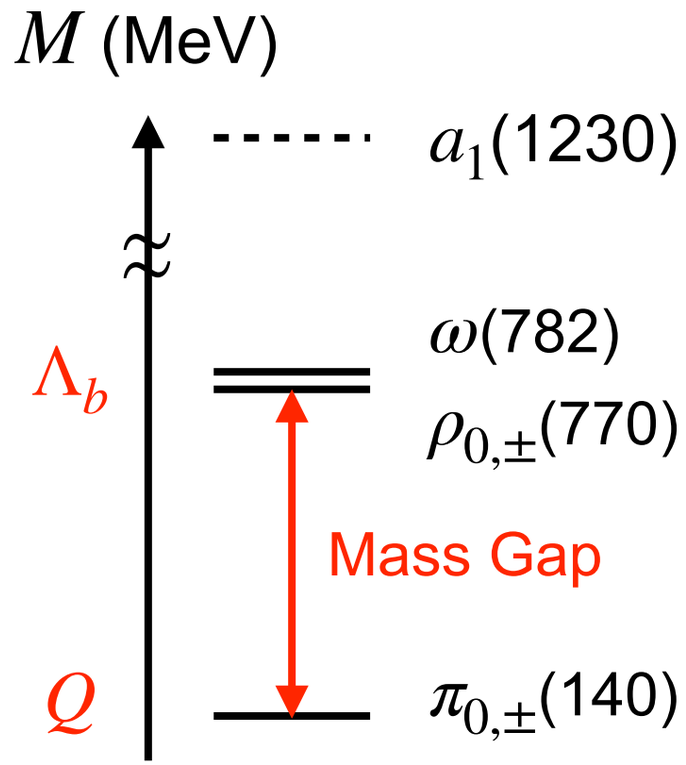
- QCD and chiral symmetry

$$\mathscr{L}_{\text{QCD}} = -\frac{1}{4} G_{\mu\nu} G^{\mu\nu} + \overbrace{\bar{q}_L i \not{D} q_L + \bar{q}_R i \not{D} q_R}^{\chi \text{ sym}} - \overbrace{\bar{q}_L \mathscr{M} q_R - \bar{q}_R \mathscr{M} q_L}^{\chi \text{ sym breaking}}$$

m_u, m_d small $\Rightarrow \mathscr{L}_{\text{QCD}}$ is approximately chiral invariant

Spontaneous symmetry breaking $SU(2)_L \times SU(2)_R \to SU(2)_V$

Leads to (almost massless) Goldstone bosons → pions



- Chiral perturbation theory

$$\mathscr{L}_{\text{eff}}[N,\pi] = \sum_{n=1}^{\infty} \mathscr{L}_{\pi}^{(2n)} + \sum_{n=1}^{\infty} \mathscr{L}_{\pi\text{N}}^{(n)} + \ldots \qquad \mathscr{A} = \sum_{n=1}^{\infty} \mathscr{A}_n$$

Most general $\mathscr{L}_{\text{eff}}$ consistent with the χ symmetry of QCD

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

Generates the most general amplitudes via perturbation expansion in $Q = \{p, m_\pi, \mu \sim m_\pi\}$

over $\Lambda_b \sim m_\rho$ (power counting)

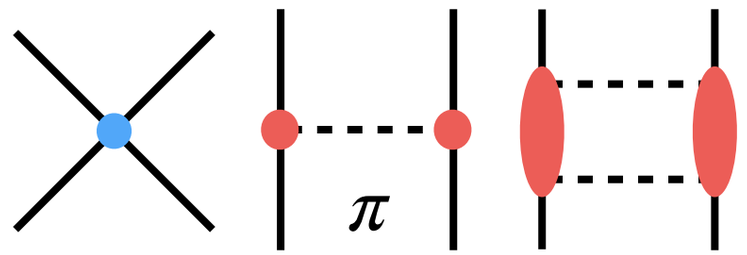
Chiral Hamiltonians

- Regularized short-range and pion-exchange NN+3N potentials

Lynn et al. PRL 116, 062501 (2016)

- NN potential: fit to NN S- and P- wave phase shifts

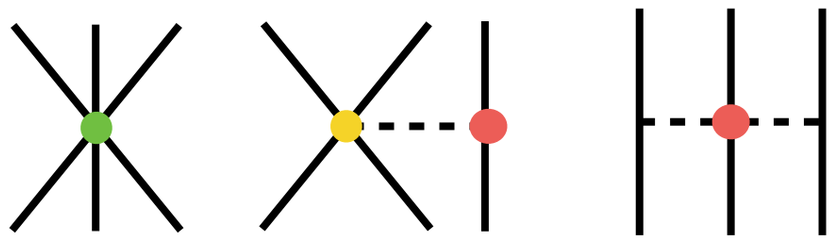
$$v_{ij}^{\mathrm{CI}} = \sum_{p=1}^{8} v_p(r_{ij}) O_{ij}^{p} \qquad O_{ij}^{p=5\text{-}8} = S_{ij},\ \tau_{ij},\ \boldsymbol{L}\cdot\boldsymbol{S},\ \boldsymbol{L}\cdot\boldsymbol{S}\tau_{ij}$$



Tensor forces

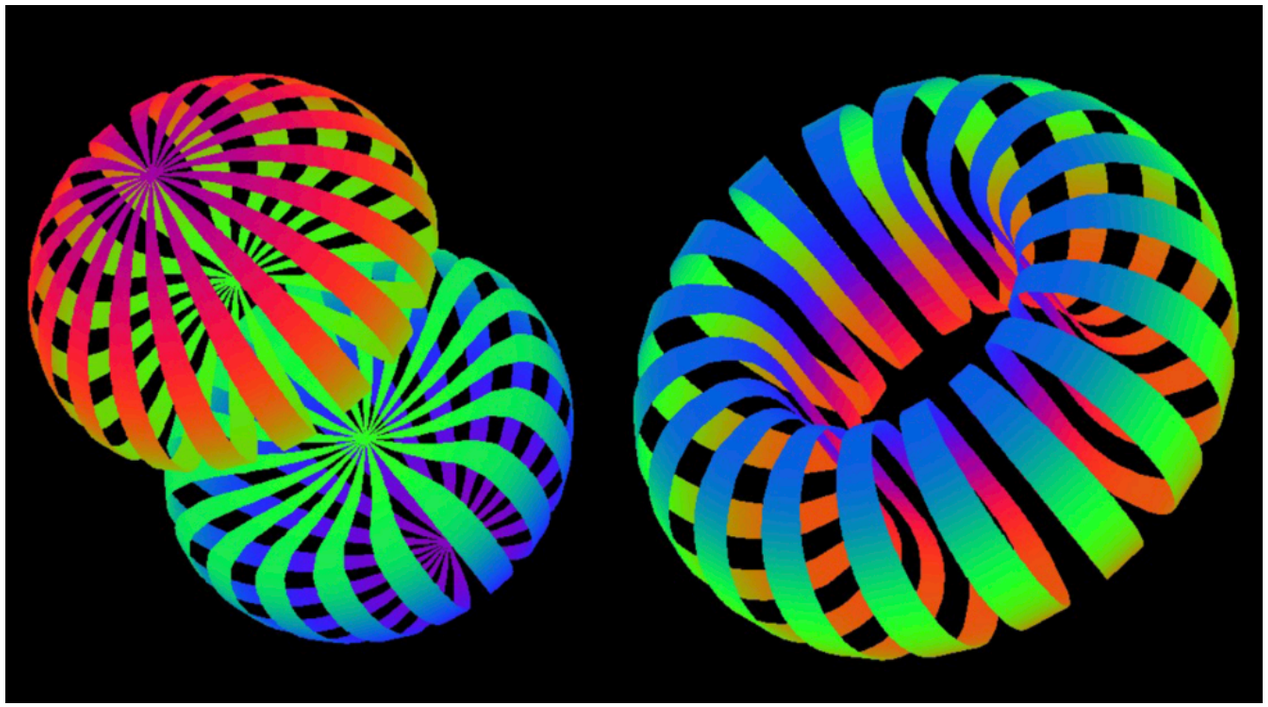
- 3N potential: fit to ^{3}H binding energy and neutron-α *P*-wave phase shifts

$$V_{ijk} = V_{2\pi} + c_D V_{1\pi-\mathrm{cont}} + c_E V_{\mathrm{cont}}$$



r-space cutoffs: $R = 1.0, 1.2$ fm

Deutron and tensor force

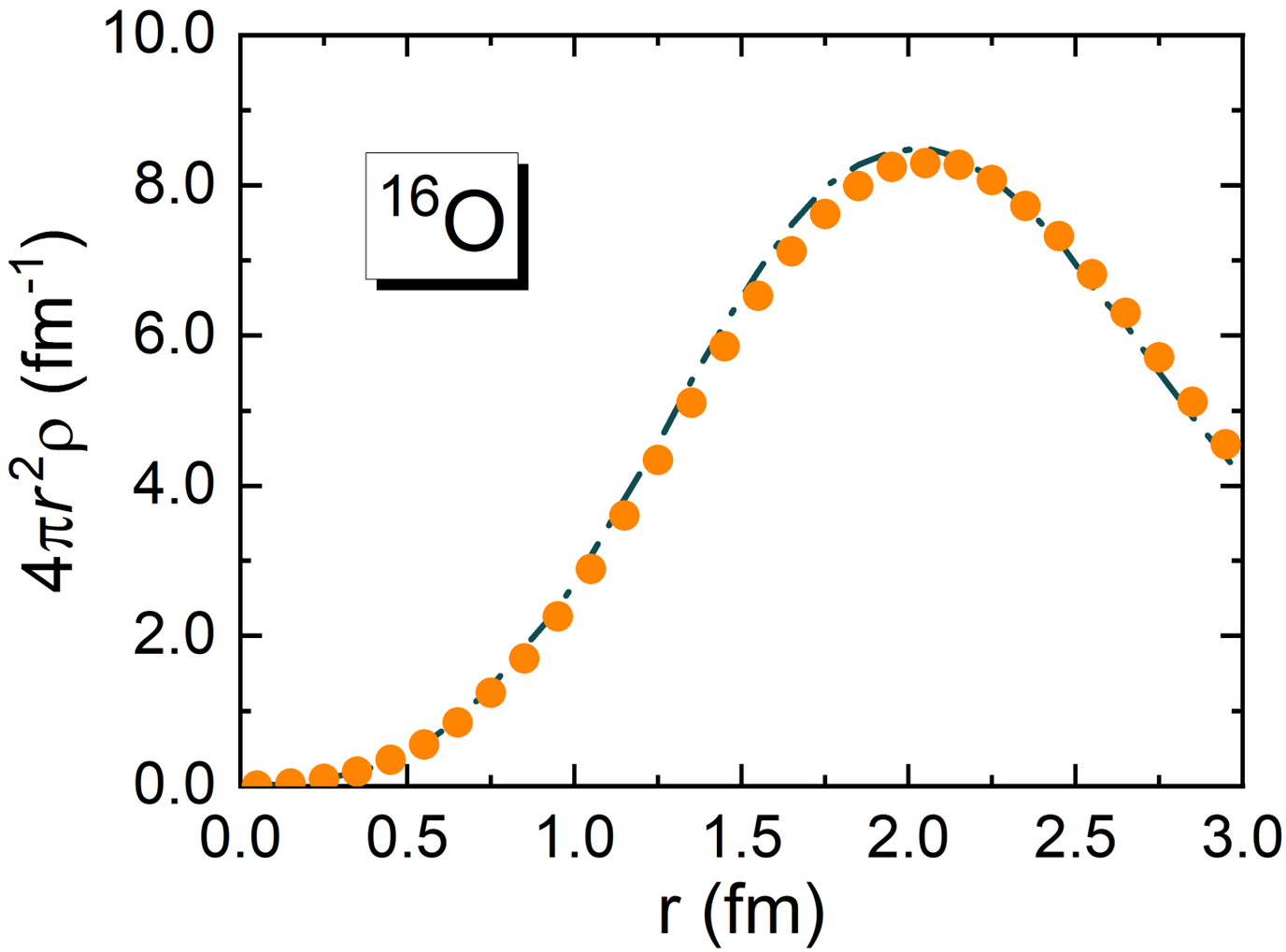


Constant density surfaces of the deuteron in its spin-1 (left) and spin-0 (right) projections, as computed using the realistic Argonne v18 nucleon-nucleon potential.

Taken from ANL theory group page.

FeynmanNet: ^{16}O ground state density

- FeynmanNet and AFDMC provide similar density distributions.



VMC (FeynmanNet): YLY and Zhao, PRC 107, 034320 (2023)

AFDMC (constrained-path): *Schiavilla et al., PRC 103, 054003 (2021)*

Towards excited states

- 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.

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

Science

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)