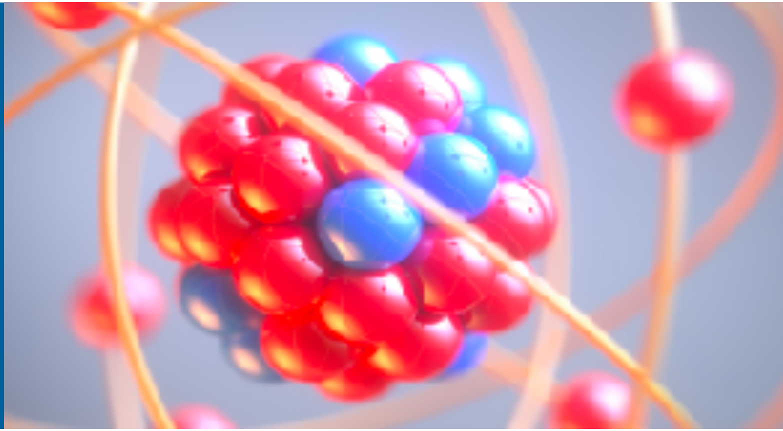
NEURAL NETWORK QUANTUM STATES FOR FEW-BODY NUCLEAR SYSTEMS



ALESSANDRO LOVATO

Trento Institute for Fundamental Physics and Applications

Argonne NATIONAL LABORATORY

Summer school “Light-ion physics in the EIC era”

Jun 26, 2025

ORGANIZATION OF THIS BRIEF COURSE

Scope of the course

- Introduce neural-network quantum states in the continuum (coordinate space)
- Applications to the nuclear quantum few-body problem

Coding goal:

- Solve the deuteron in pionless effective field theory using neural-network quantum states

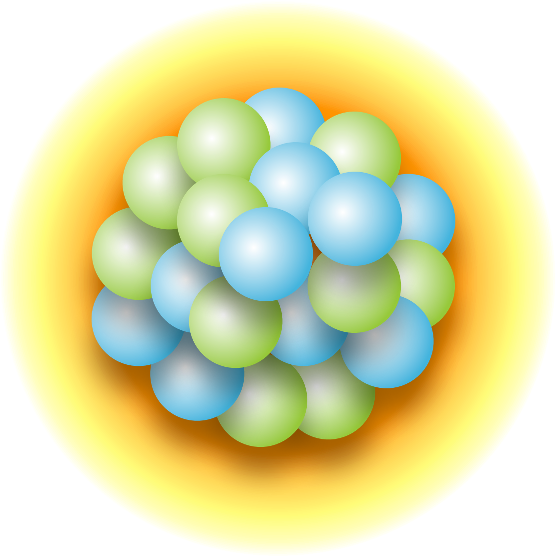
Structure of the lectures:

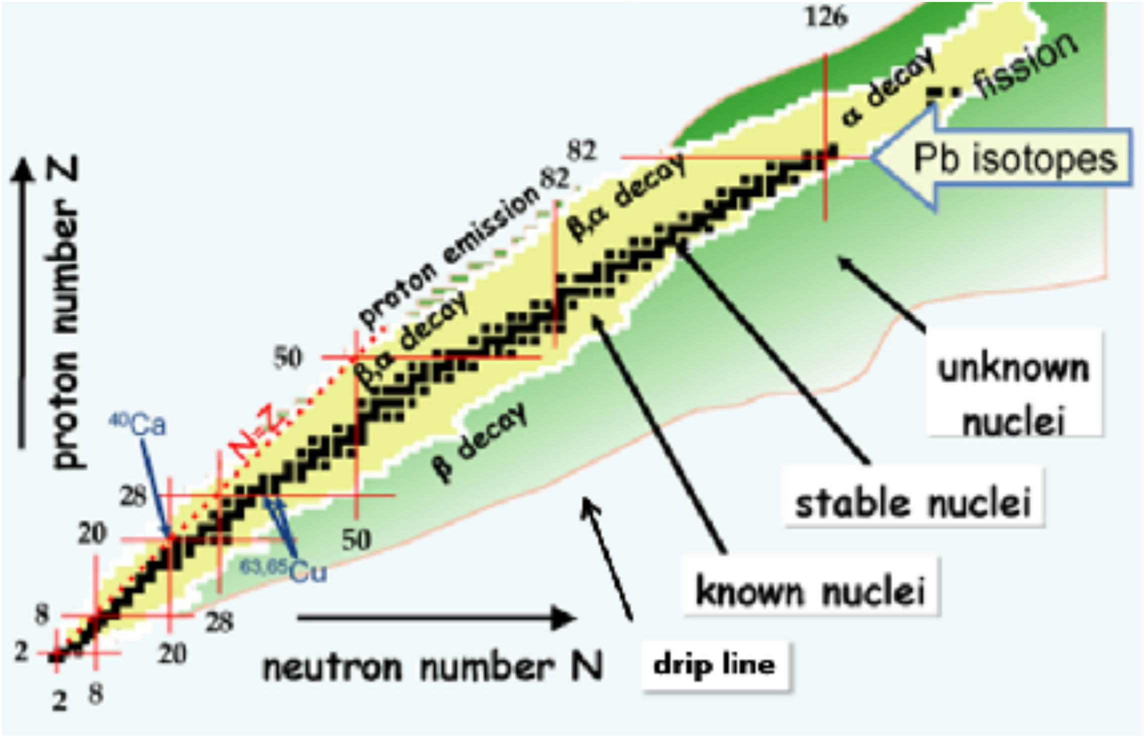
- There will be a single 60-minute lecture plus a 60-minute coding session

Coding requirements

- We will use Jupiter notebooks; required packages are Numpy and Google-JAX (use Google Colab is highly recommended)

NUCLEAR PHYSICS

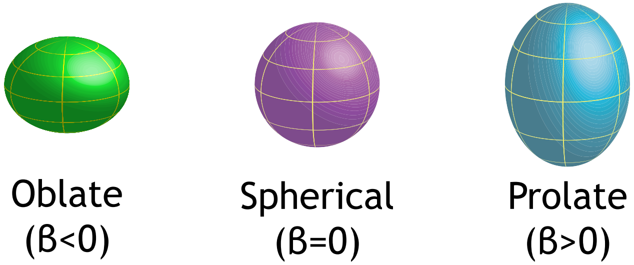




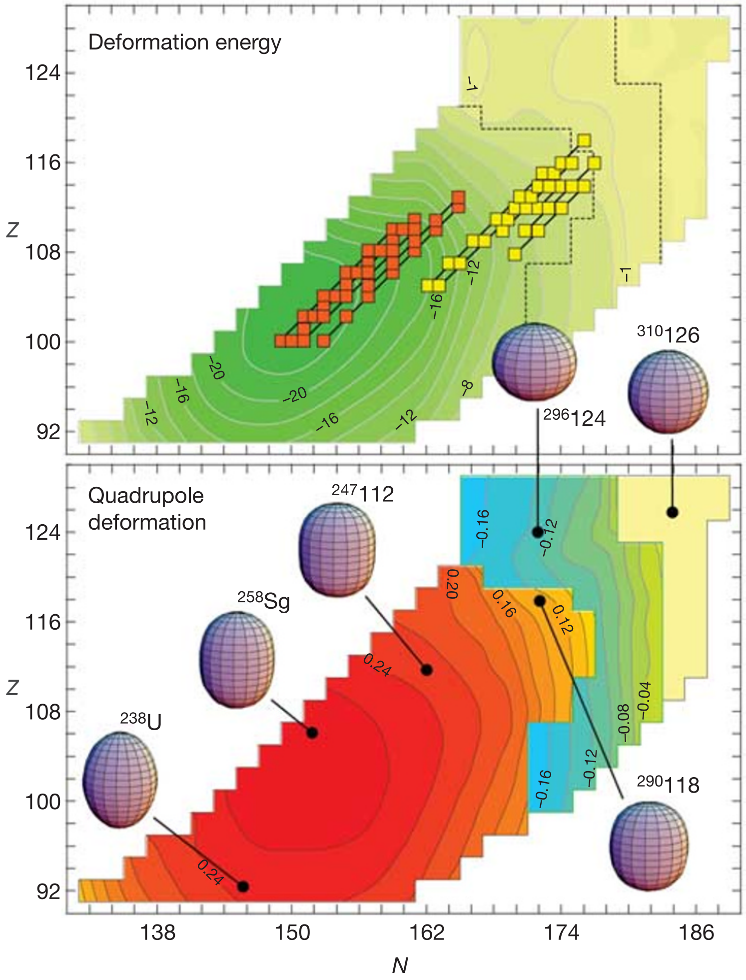
A TALE OF SCALES

- **Long-range: r ~ 5 fm**

Collective nuclear deformation evidenced by the characteristic rotational spectra



T. Naito et al 2021 J. Phys. B ***54*** *165201 (2021)*

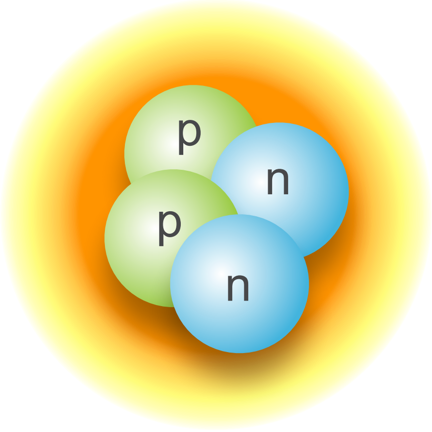


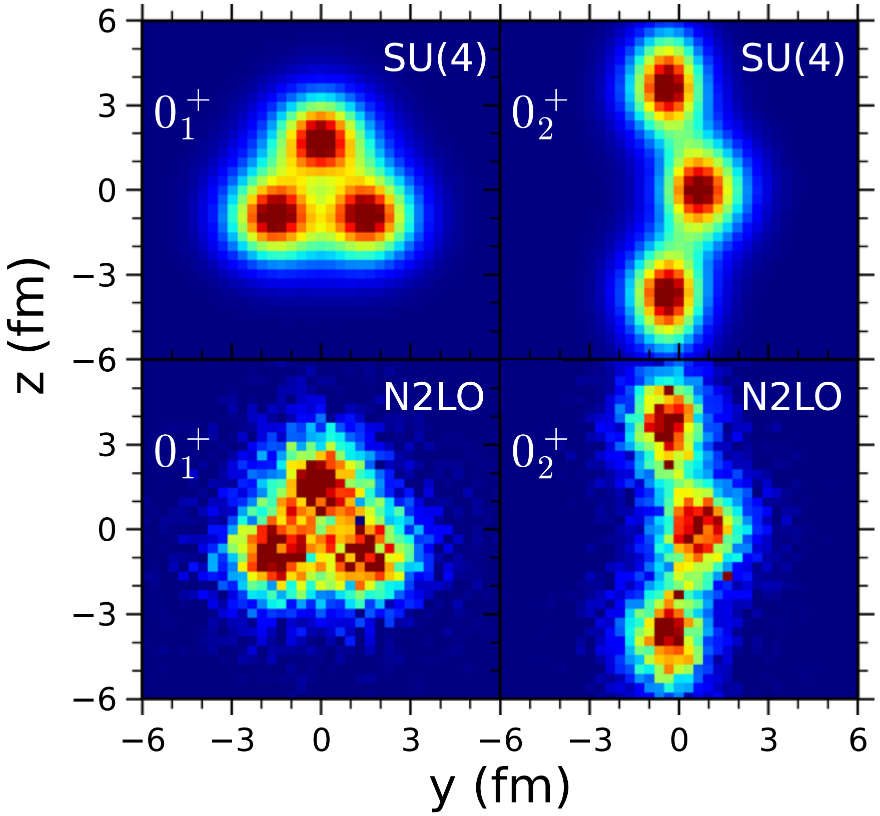
S. Ćwiok, et al., Nature ***433****, 705 (2005)*

A TALE OF SCALES

- **Intermediate-range: r ~ 2 fm**

Formation of alpha clusters



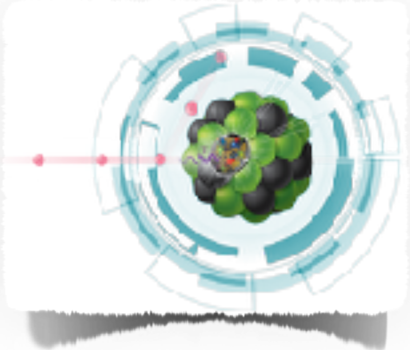


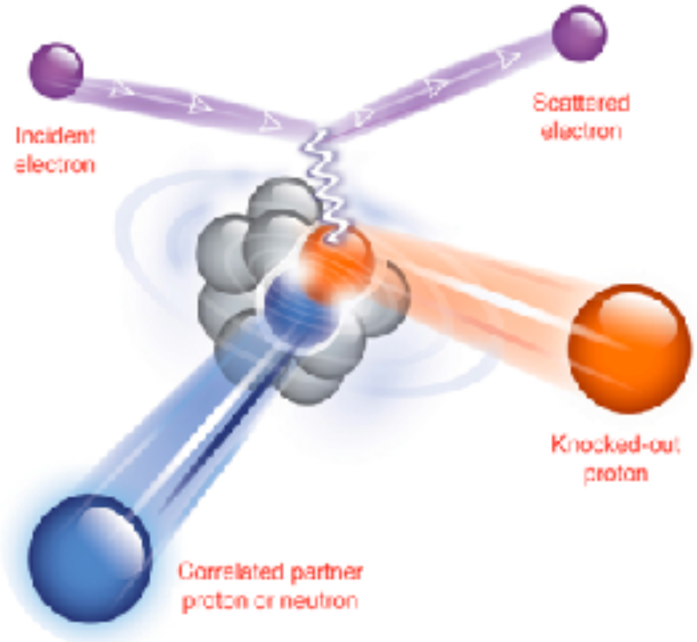
S. Shen, et al., Nat. Comm. **14**, 2777 (2023)

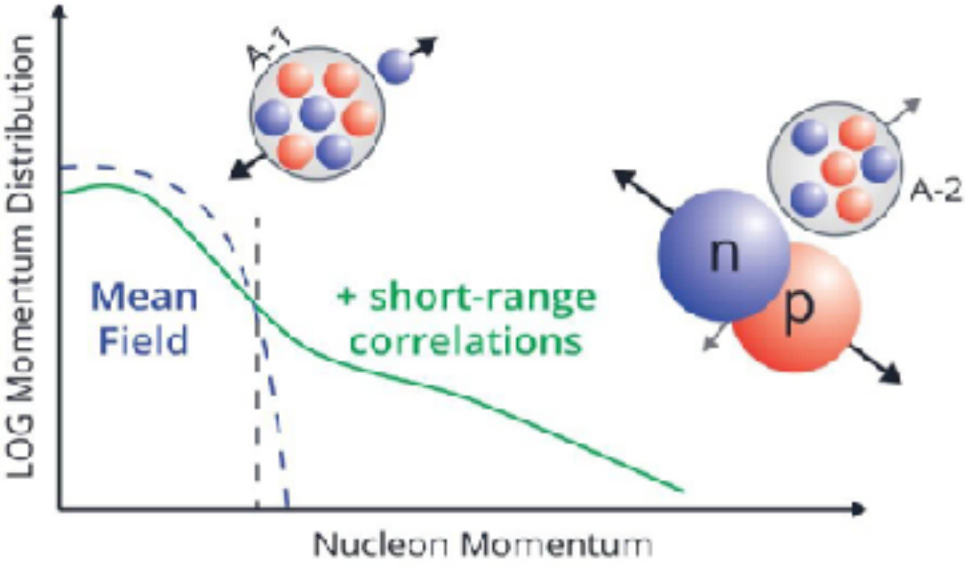
A TALE OF SCALES

- **Short-range: r ~ 1 fm**

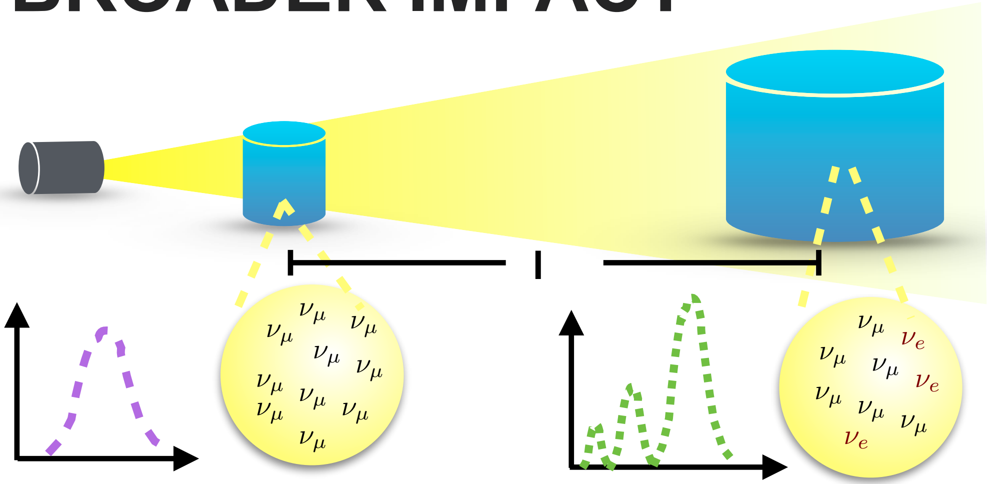
Overlapping nucleons



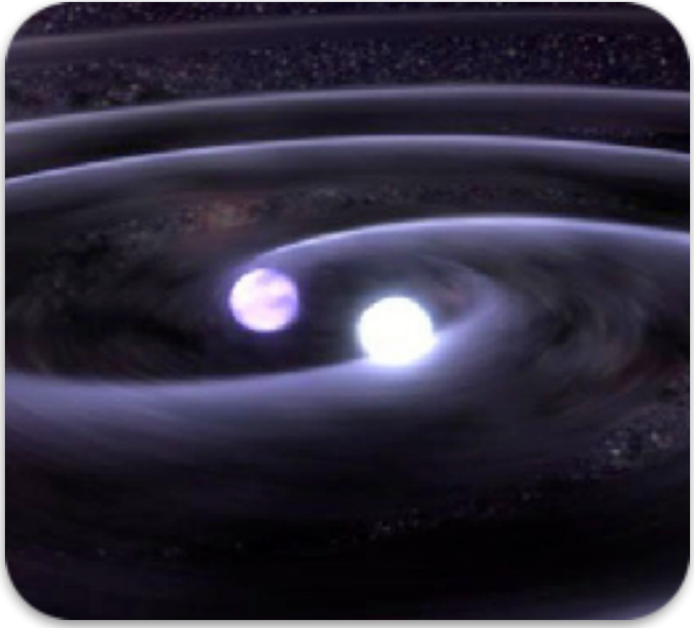




BROADER IMPACT



Credit: N. Rocco



“AB-INITIO” NUCLEAR THEORY

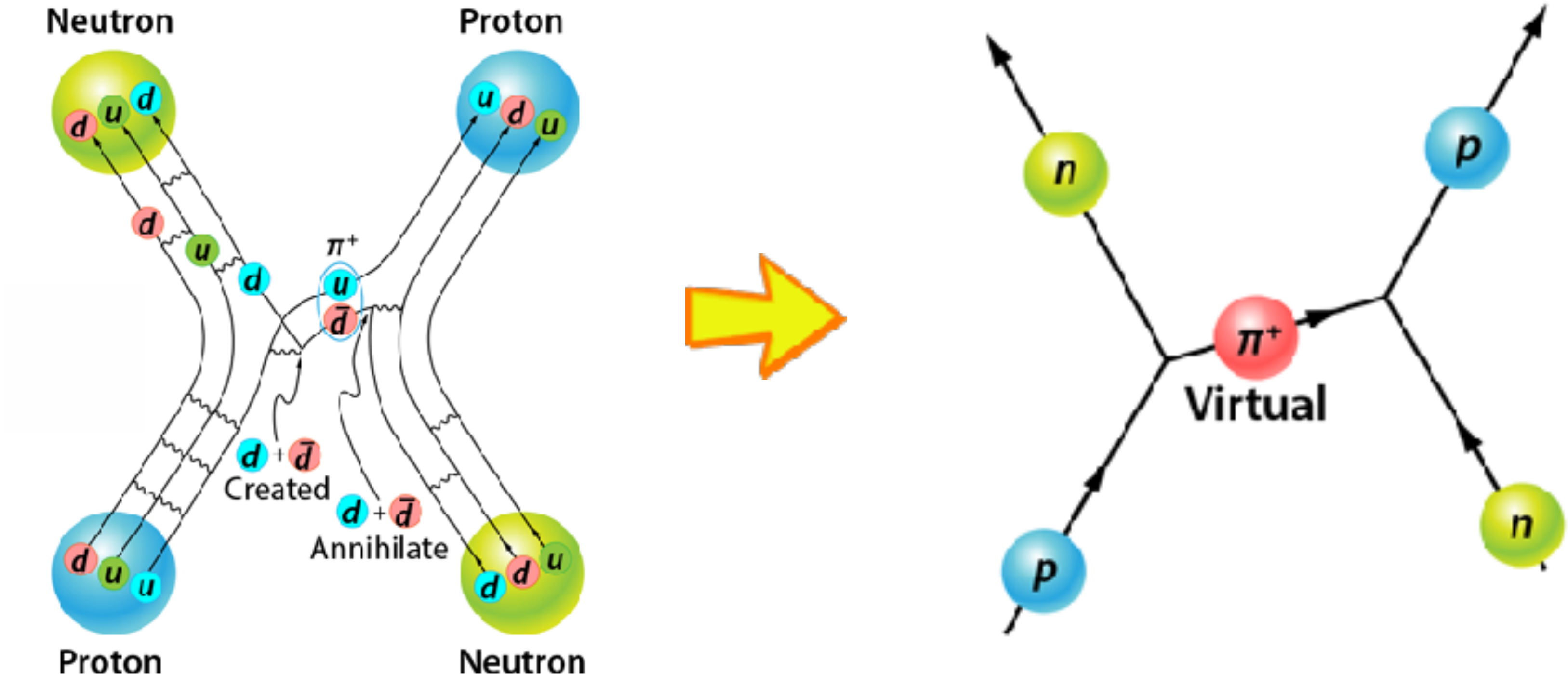
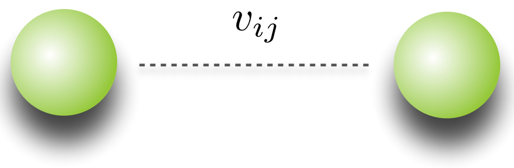


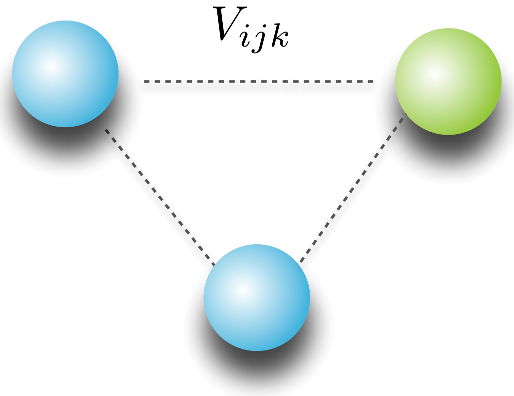
Illustration by APS / Alan Stonebraker

NUCLEAR HAMILTONIAN

Realistic nuclear Hamiltonians include two- and three-body potentials

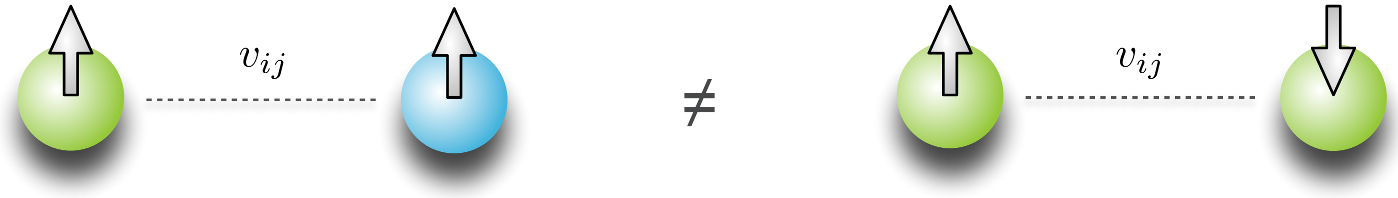
$$H = \sum_i \frac{\mathbf{p}_i^2}{2m} + \sum_{i<j} v_{ij} + \sum_{i<j<k} V_{ijk}$$





NUCLEAR HAMILTONIAN

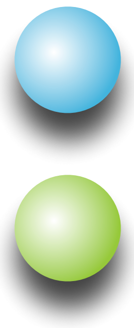
Nuclear potentials depend on the spatial position, spin, and isospin of the nucleons



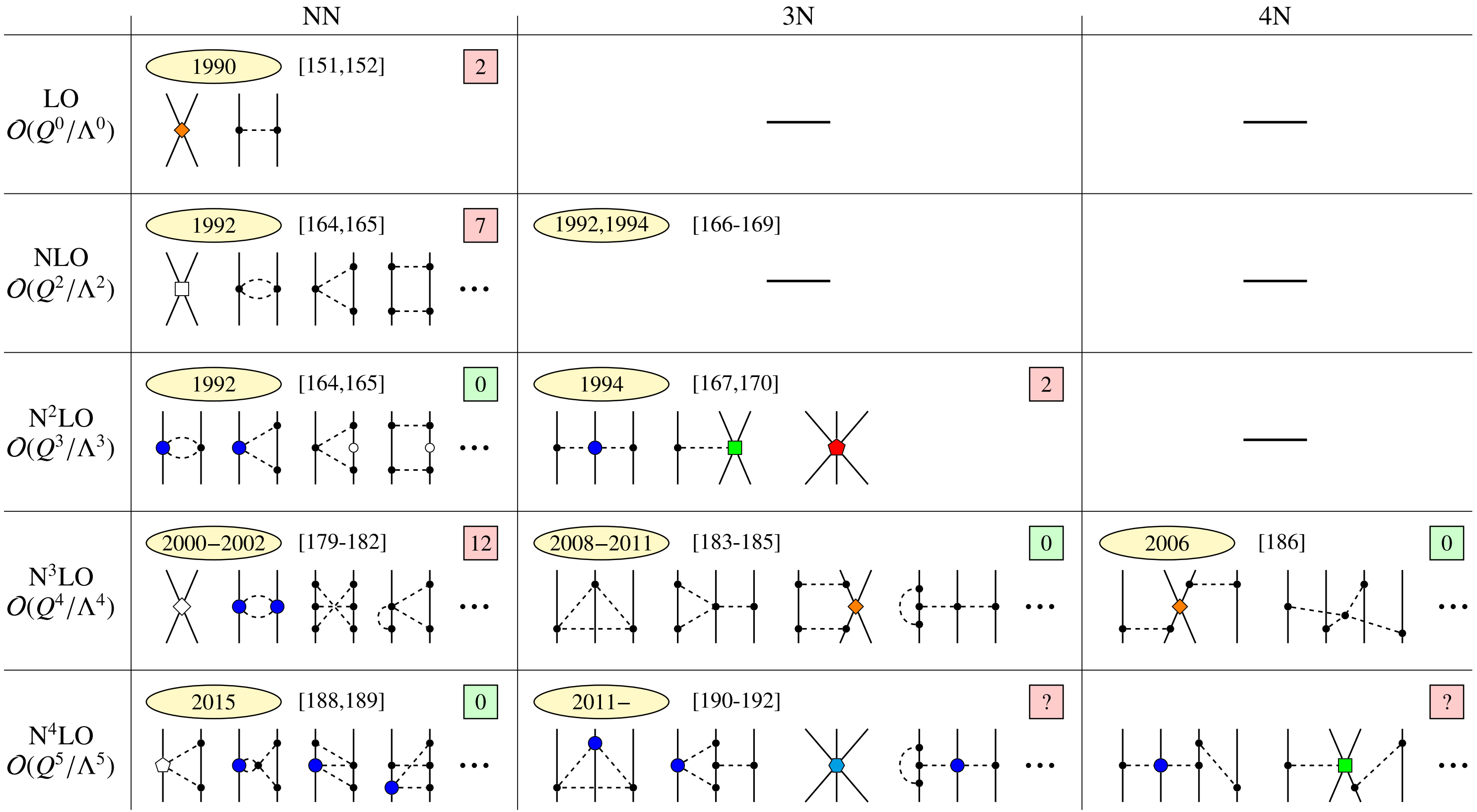
Need to introduce a generalized coordinate $x \equiv \{\mathbf{r}_i, s_z, t_z\}$

$$\begin{cases} s_z = +1/2 \\ s_z = -1/2 \end{cases}$$

$$\begin{cases} t_z = +1/2 \\ t_z = -1/2 \end{cases}$$



NUCLEAR HAMILTONIAN



K. Hebeler et al., *Phys. Rept.* **890** (2021) 1-116

THE QUANTUM MANY-BODY PROBLEM

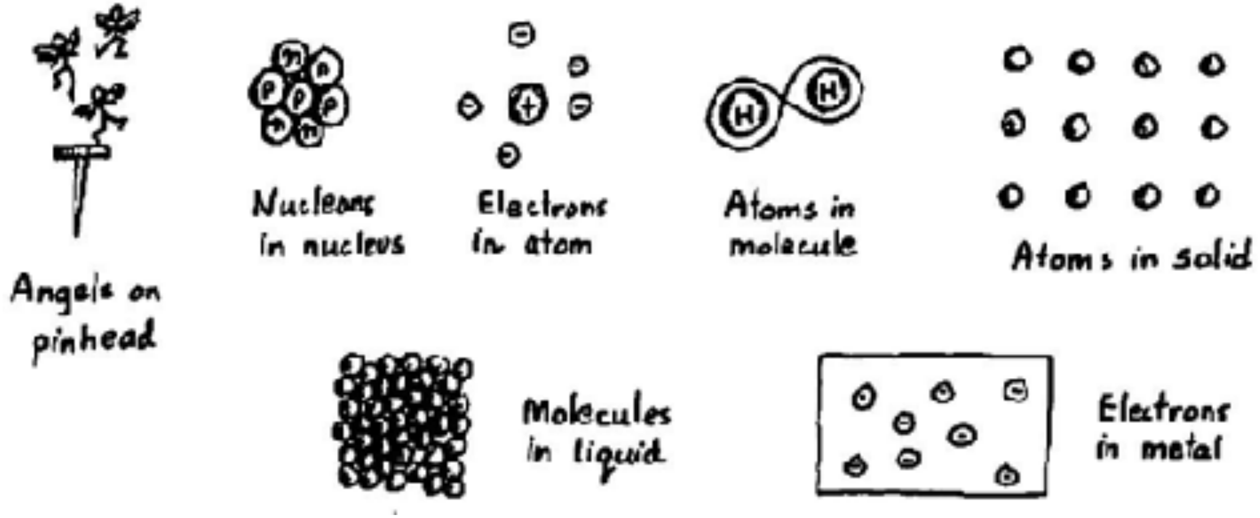
- Non relativistic many body theory aims at solving the many-body Schrödinger equation

$$H\Psi_n(x_1,\dots,x_A) = E_n\Psi_n(x_1,\dots,x_A)$$

- Nucleons are fermions, so the wave function must be anti-symmetric

$$\Psi_n(x_1,\dots x_i,\dots,x_j,\dots,x_A) = -\Psi_n(x_1,\dots x_j,\dots,x_i,\dots,x_A)$$

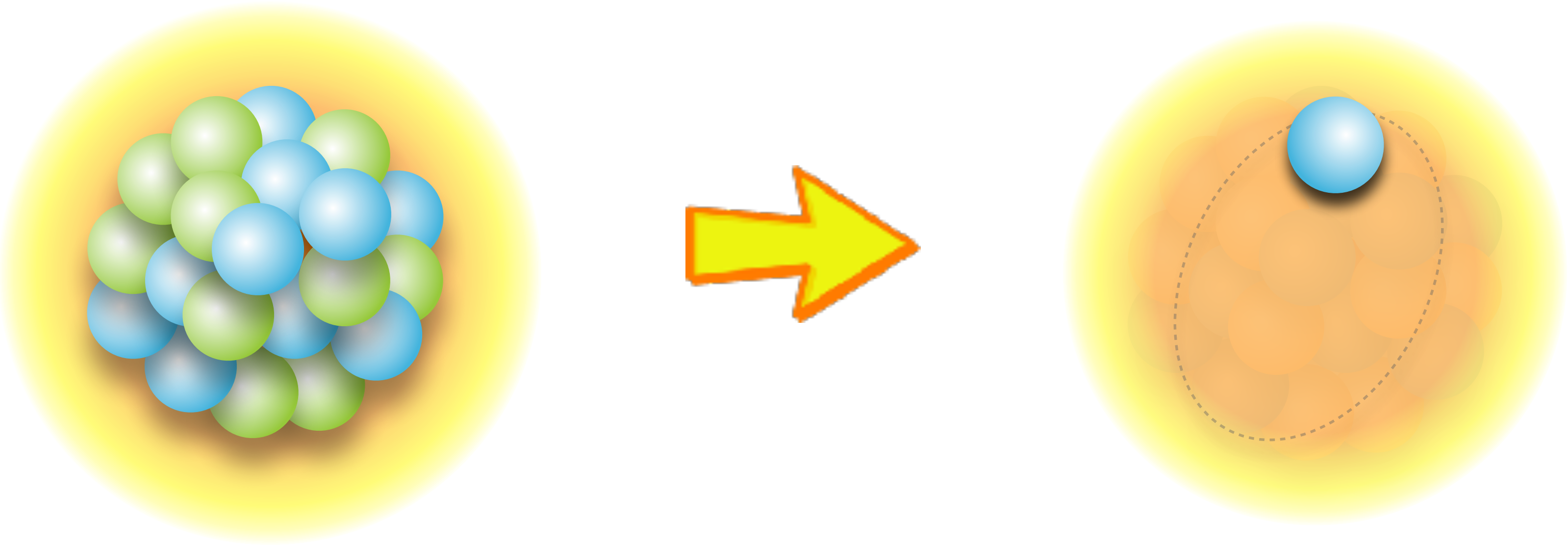
THE QUANTUM MANY-BODY PROBLEM



A guide to Feynman diagrams in the many-body problem

THE MEAN-FIELD APPROXIMATION

Mean field: nucleons are independent particles subject to an average nuclear potential



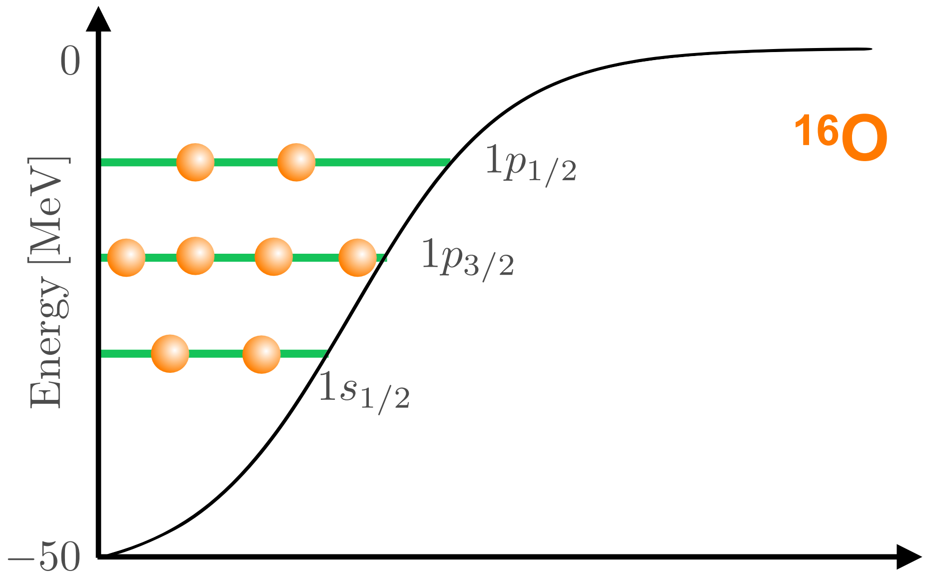
$$\sum_{i<j} v_{ij} + \sum_{i<j<k} V_{ijk} \longrightarrow \sum_i U_i$$

THE MEAN-FIELD APPROXIMATION

The mean-field ground-state wave function is a Slater determinant

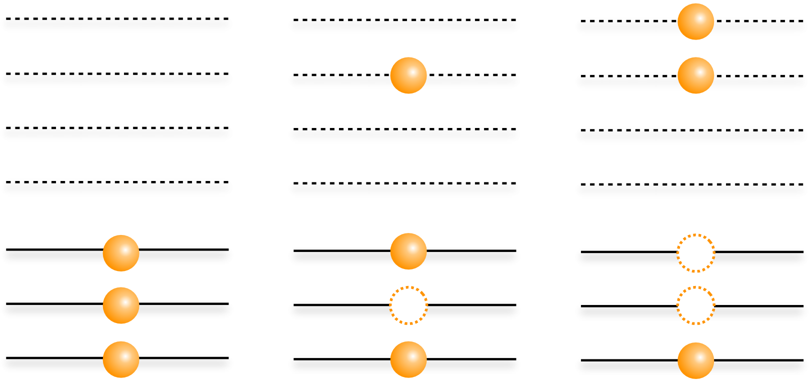
$$\Phi_0(x_1, \ldots, x_A) = \mathcal{A}[\phi_{n_1}(x_1), \ldots, \phi_{n_A}(x_A)]$$

$$\Phi_0(x_1, x_2) = \phi_1(x_1)\phi_2(x_2) - \phi_2(x_1)\phi_1(x_2)$$



CONFIGURATION-INTERACTION METHODS

$$\Psi_0(x_1, \ldots, x_A) = \sum_n c_n \Phi_n(x_1, \ldots, x_A)$$



$|\Phi_0\rangle$ $|\Phi_{h_2}^{p_3}\rangle$ $|\Phi_{h_2 h_3}^{p_3 p_4}\rangle$

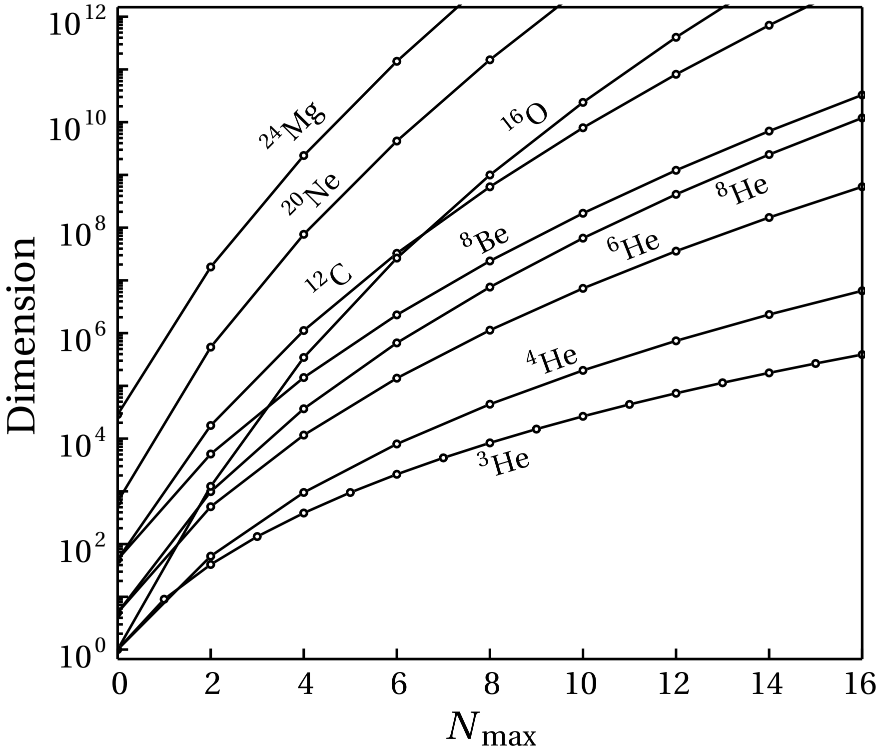
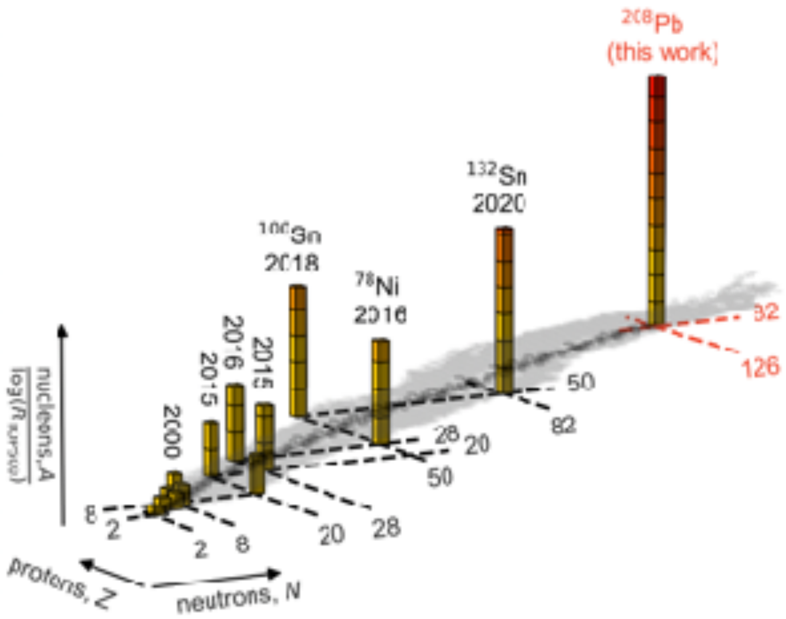


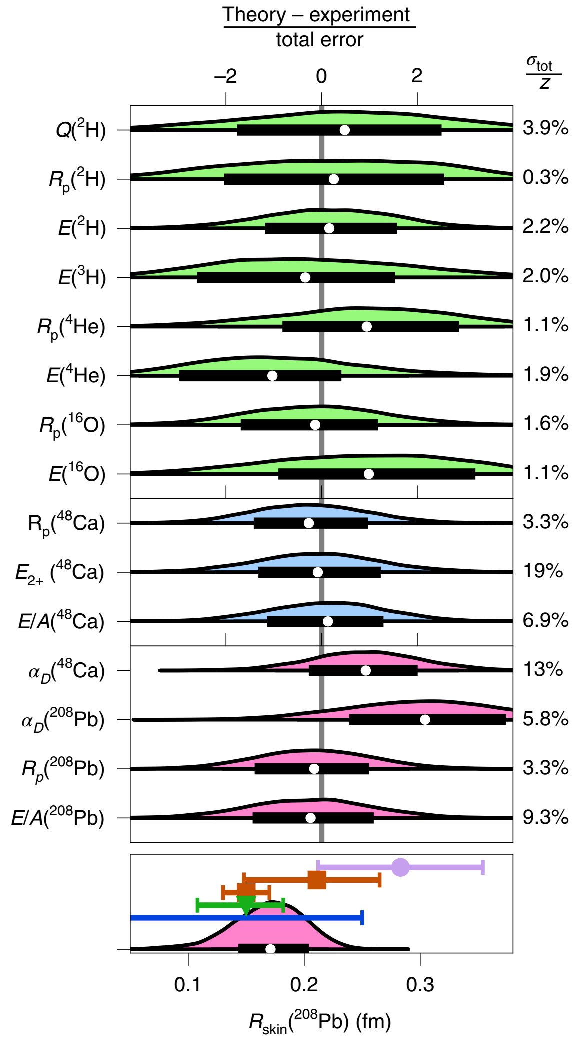
Image courtesy of Patrick Fasano

TACKLE LARGE SYSTEMS

Polynomially-scaling methods reach (much) larger systems with some approximations



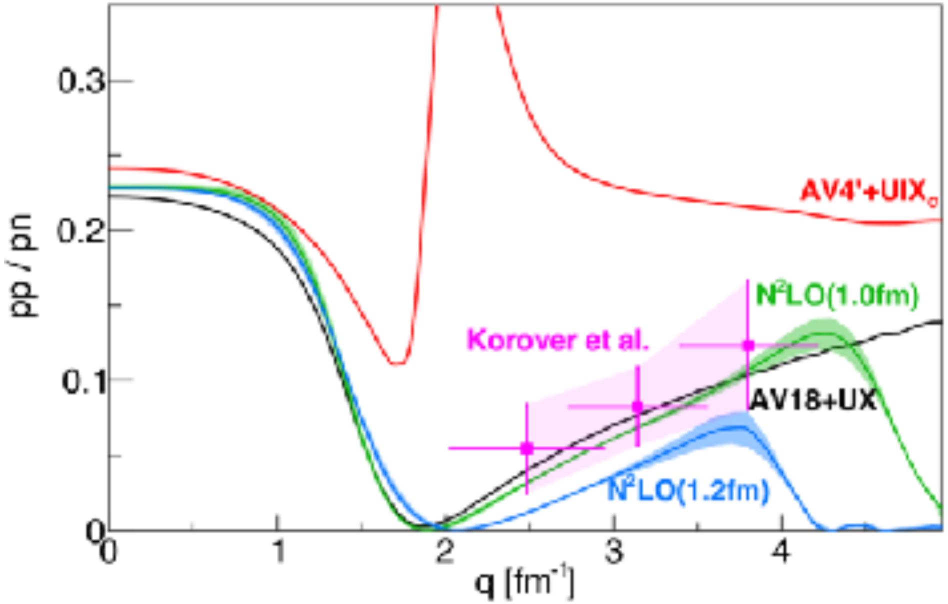
B. S. Hu et al., Nature Phys. (2022)



NEED FOR HIGH RESOLUTION

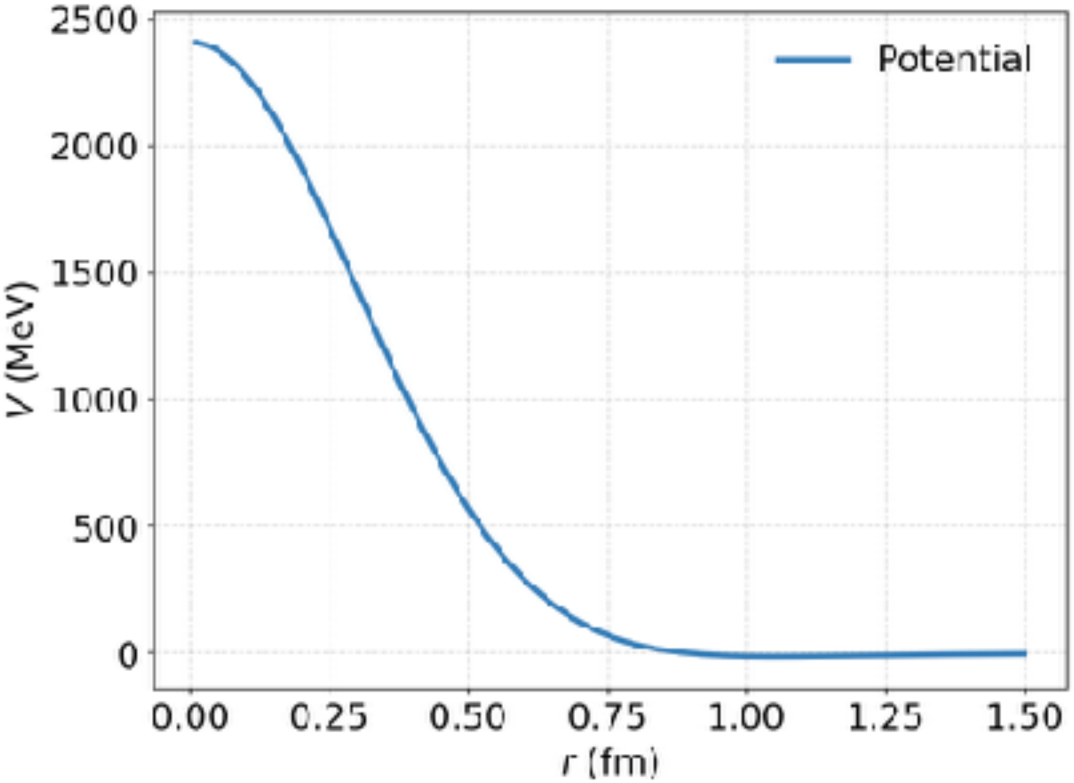
Continuum nuclear quantum Monte Carlo use a coordinate-space representation of many-body wave functions.

- They have no difficulties in treating “stiff” nuclear forces: test the convergence of nuclear EFTs;
- Access to high-momentum components of the nuclear wave functions;
- Limited to relatively light nuclear systems

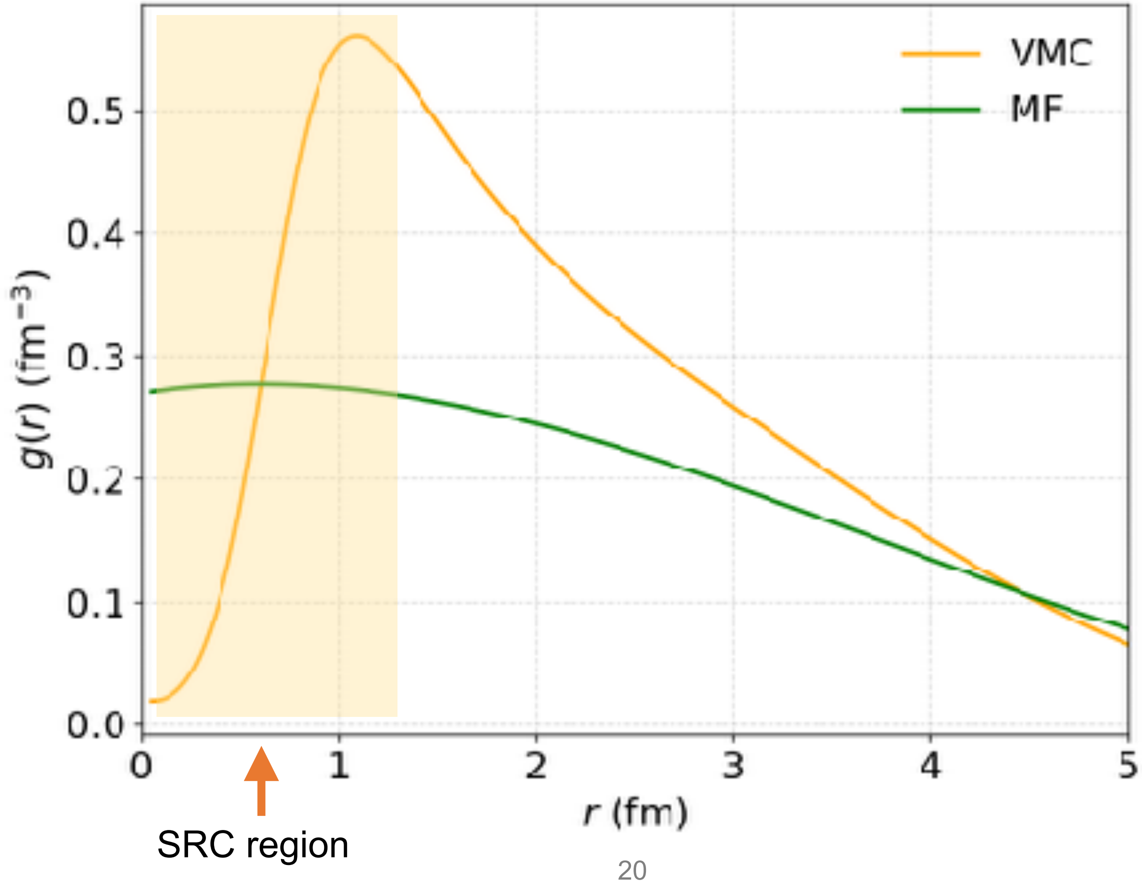


R. Cruz-Torres et al., *Nature Phys.* **17** (2021) 3, 306

INCLUDING CORRELATIONS



INCLUDING CORRELATIONS



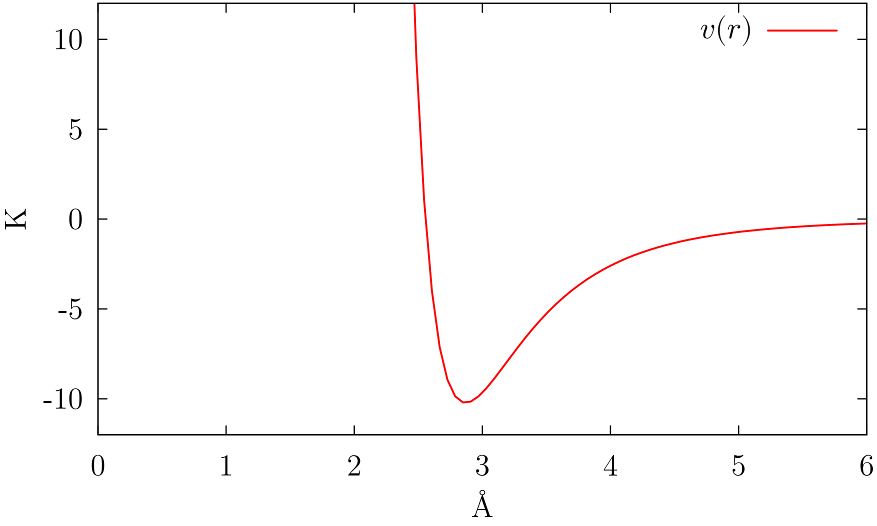
VARIATIONAL MONTE CARLO

Argonne NATIONAL LABORATORY

VARIATIONAL MONTE CARLO

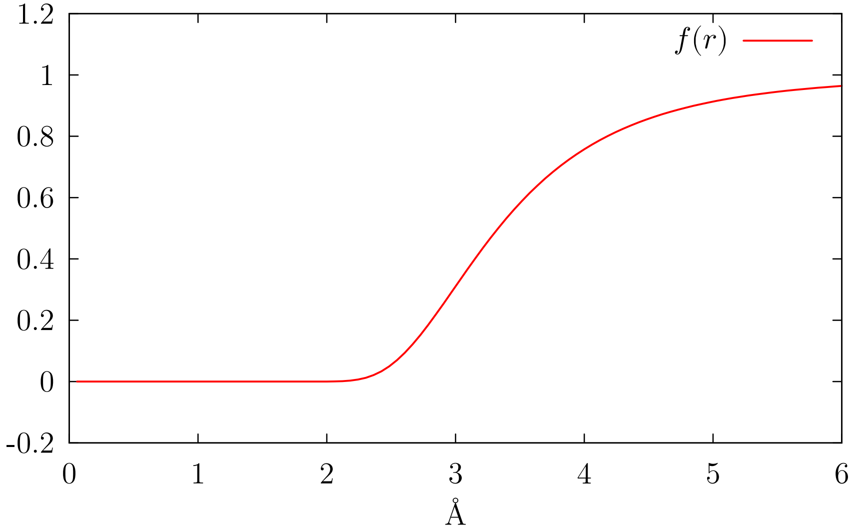
Homogeneous liquid of ^{4}He atoms; interaction parametrized by the Lennard Jones potential

$$v(r) = 4\epsilon \left[\left(\frac{\sigma}{r} \right)^{12} - \left(\frac{\sigma}{r} \right)^{6} \right]$$



The wave function must be small (large) where the potential is repulsive (attractive)

$$\Psi_V(R) = \prod_{i<j} f(r_{ij}) \;;\quad f(r) = \exp\left[-\frac{1}{2} \left(\frac{b}{r} \right)^{5} \right]$$



VARIATIONAL MONTE CARLO

The **variational principle** guarantees the variational energy to be larger greater than or equal to the ground-state energy with the same quantum numbers

$$E_V \equiv \frac{\langle \Psi_V | H | \Psi_V \rangle}{\langle \Psi_V | \Psi_V \rangle} \geq E_0$$

Computing the variational energy requires evaluating a **high-dimensional integral**

$$E_V = \frac{\langle \Psi_V | H | \Psi_V \rangle}{\langle \Psi_V | \Psi_V \rangle} = \frac{\sum_S \int dR \langle \Psi_V | RS \rangle \langle RS | H | \Psi_V \rangle}{\sum_S \int dR \langle \Psi_V | RS \rangle \langle RS | \Psi_V \rangle} = \frac{\sum_S \int dR |\Psi_V(R,S)|^2 \frac{\langle RS | H | \Psi_V \rangle}{\langle RS | \Psi_V \rangle}}{\sum_S \int dR |\Psi_V(R,S)|^2} \,.$$

$$R = \{\mathbf{r}_1, \ldots, \mathbf{r}_A\} \quad \longleftrightarrow \quad S = \{(s_1^z, t_1^z), \ldots, (s_A^z, t_A^z)\}$$

ESTIMATING OBSERVABLES

$$E_V = \frac{\sum_S \int dR |\Psi_V(R,S)|^2 \frac{\langle RS|H|\Psi_V\rangle}{\langle RS|\Psi_V\rangle}}{\sum_S \int dR |\Psi_V(R,S)|^2} \, .$$

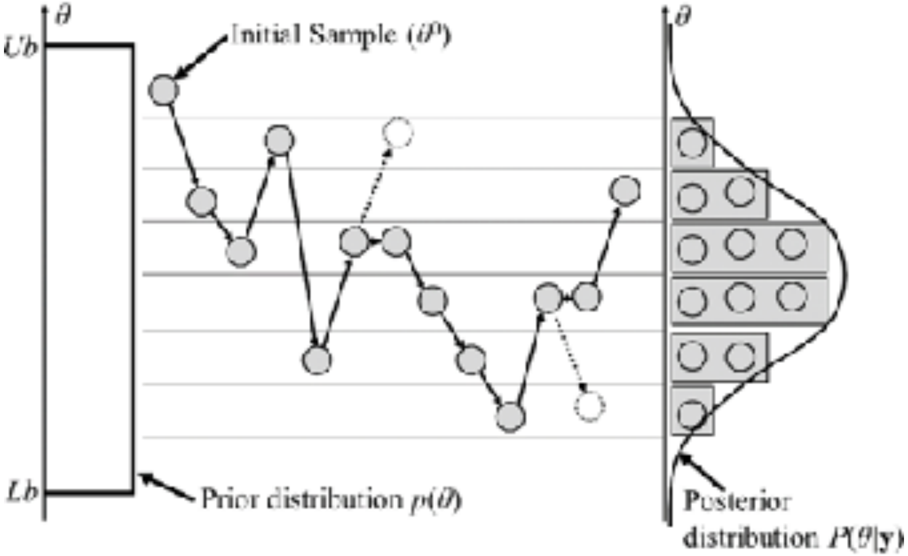
Leverage the central limit theorem, we can estimate the above integral as

$$E_V \simeq \frac{1}{N} \sum_{(R_i,S_i)\sim\pi_V} \frac{\langle R_i S_i|H|\Psi_V\rangle}{\langle R_i S_i|\Psi_V\rangle} \quad \longleftrightarrow \quad \pi_V(R,S) = \frac{|\Psi_V(R,S)|^2}{\sum_S \int dR |\Psi_V(R,S)|^2}$$

We use Metropolis Hastings to sample $\pi_V(R,S)$

$$P_{\text{acc}} = \min\left(1, \frac{|\Psi_V(R',S')|^2}{|\Psi_V(R,S)|^2}\right)$$

THE M(RT)^2 ALGORITHM



THE M(RT)^2 ALGORITHM

Goal: sample the probability distribution

$$R_n \sim P(R) = \frac{|\Psi_V(R)|^2}{\int dR |\Psi_V(R)|^2}$$

The M(RT)^2 algorithm is **based on the idea of random walk**. A set of random configurations are generated by applying the transformation.

$$P_{i+1}(R_{i+1}) = \int dR_i P_i(R_i) T(R_i \to R_{i+1})$$

By recursively applying the same transformation we get

$$P_n(R_n) = \int dR_1 \dots dR_{n-1} P_1(R_1) T(R_1 \to R_2) \dots T(R_{n-1} \to R_n)$$

Under some very general conditions it can be proven that

$\lim_{n \to \infty} P_n(R_n) = P(R)$ ⟶ $P(R)$ only depends on $T(R_i \to R_{i+1})$

THE M(RT)^2 ALGORITHM

Let us impose the asymptotic distribution to be in an “equilibrium” state, which translates into **detailed balance condition:** that point by point there is no net flux of probability

$$P(R)T(R \to R') = P(R')T(R' \to R)$$

We can arbitrarily split the transition probability in two terms

$$T(R \to R') = G(R \to R')A(R \to R')$$

Proposal probability ← G · A → Acceptance probability

The detailed balance implies:

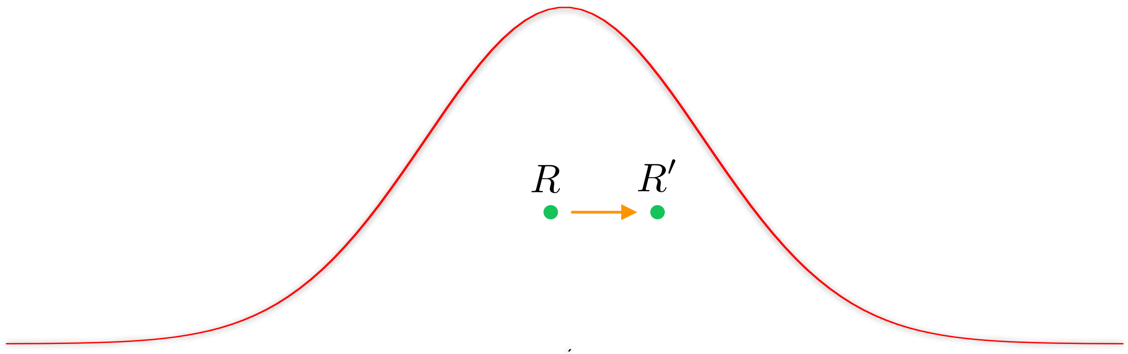
$$\frac{A(R' \to R)}{A(R \to R')} = \frac{P(R)G(R \to R')}{P(R')G(R' \to R)}$$

It can be easily checked that the following acceptance probability satisfies the above requirement

$$A(R \to R') = \min\left(1, \frac{P(R')G(R' \to R)}{P(R)G(R \to R')}\right)$$

THE M(RT)^2 ALGORITHM

A common choice for $G(R \to R')$ is a Gaussian distribution centered in zero. In this case, at each step of the propagations, the walkers are moved by $R' = R + \Delta$



- In the multiple-particle case, we need to consider a three-dimensional Gaussian for each particle.
- Since the Gaussian probability is symmetric, the acceptance probability simplifies to

$$A(R \to R') = \min\left(1, \frac{P(R')}{P(R)}\right)$$

M(RT)² APPLIED TO VMC

At this point, we can describe the Metropolis algorithm for a VMC calculation

Step 0 - Start from an arbitrary distribution of configurations on the coordinate R

Step 1 - Move the walkers according to G(R→R'), such as R' = R + Δ

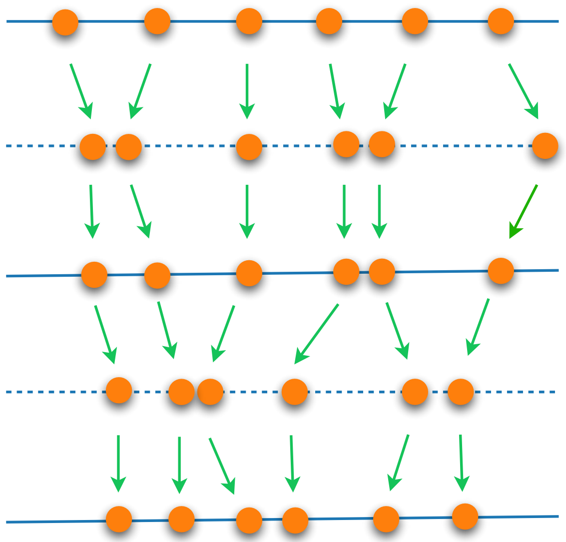
Step 2 - Compute the acceptance probability

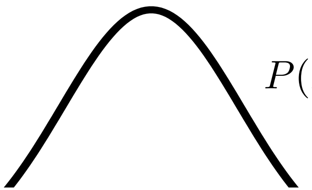
$$A(R \to R') = \min\left(1, \frac{|\Psi_V(R')|^2}{|\Psi_V(R)|}\right)$$

Step 3 - Accept or reject the proposed move comparing with ξ~U(0,1]

$\frac{|\Psi_V(R')|^2}{|\Psi_V(R)|^2} \geq \xi$ → Accept: $R = R'$; $\frac{|\Psi_V(R')|^2}{|\Psi_V(R)|^2} < \xi$ → Reject $R = R$

M(RT)^2 APPLIED TO VMC





$$P(R) \propto |\Psi_V(R)|^2$$

- Sample from an initial distribution
- Random Gaussian move
- Acceptance/rejection of the move
- Random Gaussian move
- Acceptance/rejection of the move
- Iterate until convergence

ESTIMATING OBSERVABLES

$$E_V = \frac{\sum_S \int dR |\Psi_V(R,S)|^2 \frac{\langle RS|H|\Psi_V\rangle}{\langle RS|\Psi_V\rangle}}{\sum_S \int dR |\Psi_V(R,S)|^2} .$$

Leverage the central limit theorem, we can estimate the above integral as

$$E_V \simeq \frac{1}{N} \sum_{(R_i,S_i)\sim\pi_V} \frac{\langle R_i S_i|H|\Psi_V\rangle}{\langle R_i S_i|\Psi_V\rangle} \quad \longleftrightarrow \quad \pi_V(R,S) = \frac{|\Psi_V(R,S)|^2}{\sum_S \int dR |\Psi_V(R,S)|^2}$$

We use Metropolis Hastings to sample $\pi_V(R,S)$

$$P_{\mathrm{acc}} = \min\left(1, \frac{|\Psi_V(R',S')|^2}{|\Psi_V(R,S)|^2}\right)$$

ENERGY MINIMIZATION

The variational wave function depends on a set of variational parameters

$$|\Psi_V\rangle \longrightarrow |\Psi_V(\mathbf{p})\rangle$$

It is convenient to introduce the derivative operator

$$O^i|\Psi_V(\mathbf{p})\rangle \equiv \frac{\partial}{\partial p_i}|\Psi_V(\mathbf{p})\rangle$$

Recall:

$$E_V = \frac{\langle\Psi_V|H|\Psi_V\rangle}{\langle\Psi_V|\Psi_V\rangle}$$

The gradient of the energy reads

$$g_i \equiv \frac{\partial E_V}{\partial p_i} = 2\left(\frac{\langle\Psi_V|O^i H|\Psi_V\rangle}{\langle\Psi_V|\Psi_V\rangle} - \frac{\langle\Psi_V|H|\Psi_V\rangle}{\langle\Psi_V|\Psi_V\rangle}\frac{\langle\Psi_V|O^i|\Psi_V\rangle}{\langle\Psi_V|\Psi_V\rangle}\right) = \langle HO^i\rangle - \langle H\rangle\langle O^i\rangle \longleftrightarrow O^i = \frac{\partial}{\partial p_i}$$

FIRST-ORDER UPDATES

Since the gradient is known, we can use stochastic gradient descent to update the parameters

$$\mathbf{p}^{n+1} = \mathbf{p}^n - \eta\,\mathbf{g}^n \longrightarrow \eta \simeq 0.001$$

Inspired by machine-learning application, we can consider RMS, Adam, or any other improved first-order algorithm

$$\mathbf{p}^{n+1} = \mathbf{p}^n - \eta\,\frac{\mathbf{m}^n}{\sqrt{\mathbf{v}^n} + \epsilon}$$

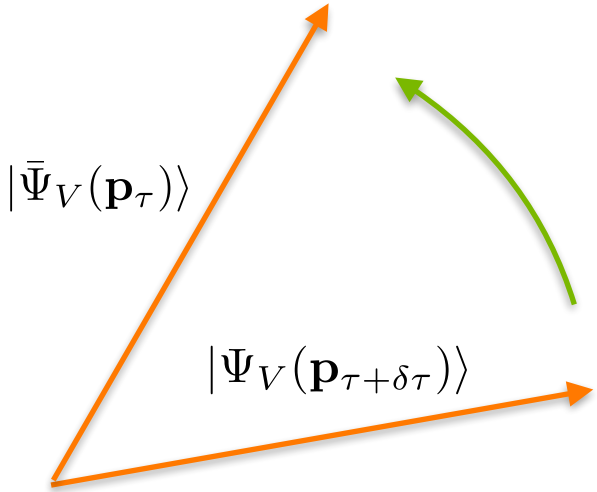
$$\begin{cases} \mathbf{m}^n = \beta_1 \mathbf{m}^{n-1} + (1-\beta_1)\mathbf{g}^n \\ \mathbf{v}^n = \beta_2 \mathbf{v}^{n-1} + (1-\beta_2)(\mathbf{g}^n)^2 \end{cases}$$

First-order algorithms are commonly used within the NQS community, but typically require many iterations to converge

NATURAL GRADIENT

A more powerful method consists in performing an imaginary-time evolution in the variational manifold

$$\begin{cases} |\bar{\Psi}_V(\mathbf{p}_\tau\rangle \equiv (1 - H\delta\tau)|\Psi_V(\mathbf{p}_\tau)\rangle \\ \mathbf{p}_{\tau+\delta\tau} = \underset{\mathbf{p}\in R^d}{\arg\max} \left(\left| \langle \bar{\Psi}_V(\mathbf{p}_\tau) | \Psi_V(\mathbf{p}_{\tau+\delta\tau}) \rangle \right|^2 \right) \end{cases}$$



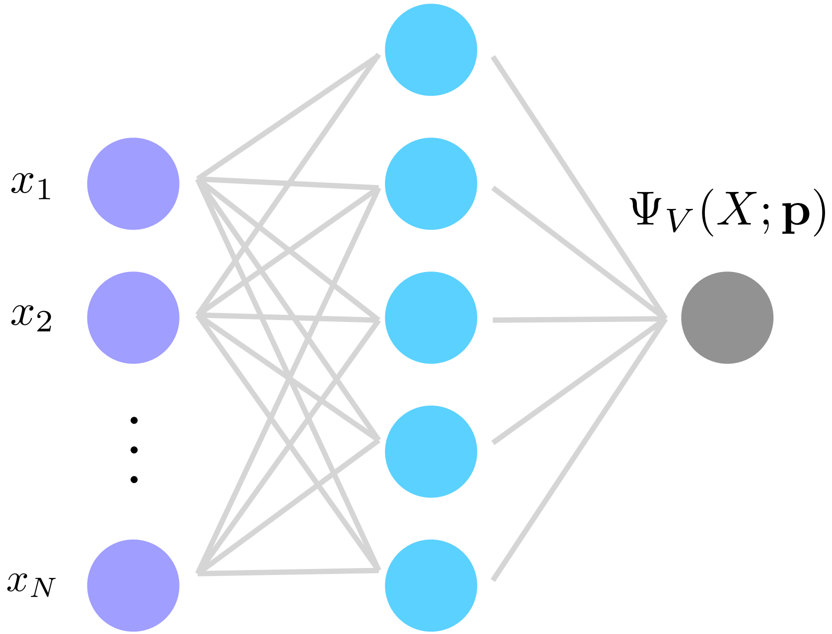
The parameters are updated as

$$\mathbf{p}_{\tau+\delta\tau} = \mathbf{p}_\tau - \delta\tau S^{-1}\mathbf{g}_\tau \longrightarrow S_{ij} = \frac{\langle \Psi_V | O^i O^j | \Psi_V \rangle}{\langle \Psi_V | \Psi_V \rangle} - \frac{\langle \Psi_V | O^i | \Psi_V \rangle}{\langle \Psi_V | \Psi_V \rangle} \frac{\langle \Psi_V | O^j | \Psi_V \rangle}{\langle \Psi_V | \Psi_V \rangle}$$

J. Stokes, at al., Quantum 4, 269 (2020).

S. Sorella, Phys. Rev. B 64, 024512 (2001)

NEURAL-NETWORK QUANTUM STATES



$$E_V \equiv \frac{\langle \Psi_V | H | \Psi_V \rangle}{\langle \Psi_V | \Psi_V \rangle} > E_0$$

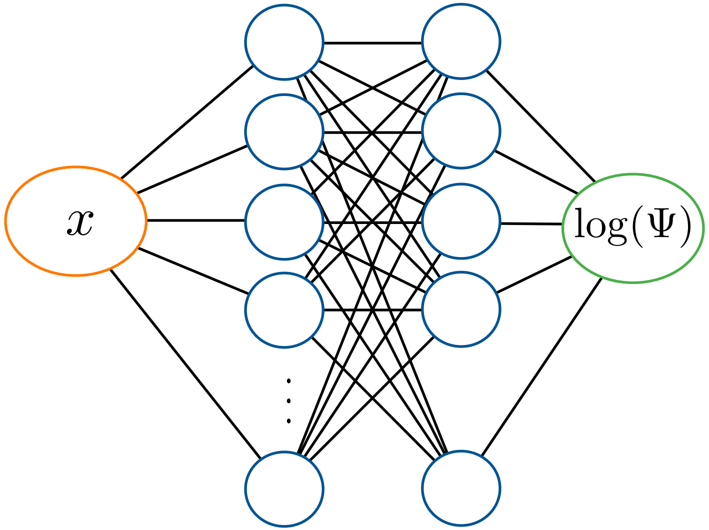
$$E_V \simeq \frac{1}{N} \sum_{X \in |\Psi_V(X)|^2} \frac{\langle X | H | \Psi_V \rangle}{\langle X | \Psi_V \rangle}$$

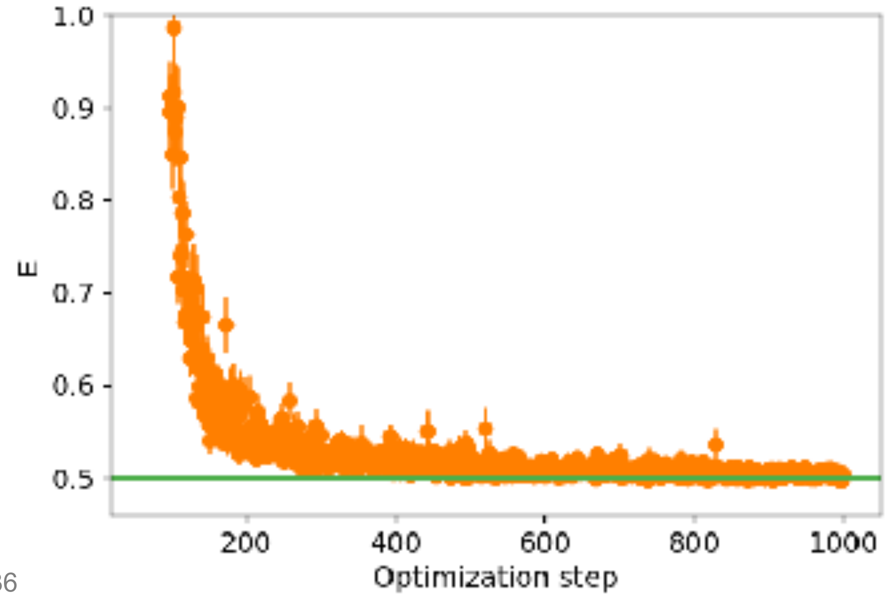
1D QUANTUM HARMONIC OSCILLATOR

To begin with, let us consider a prototypal problem: the 1d quantum harmonic oscillator

$$H = -\frac{\partial^2}{\partial x^2} + \frac{x^2}{2} \longrightarrow \Psi_0(x) = e^{-x^2/2} \quad ; \quad E_0 = 1/2$$

We represent the ground-state wave function with a feed-forward neural network



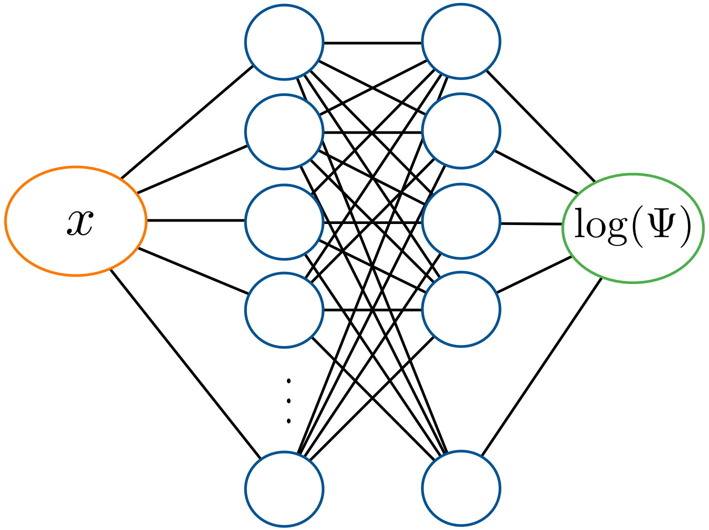


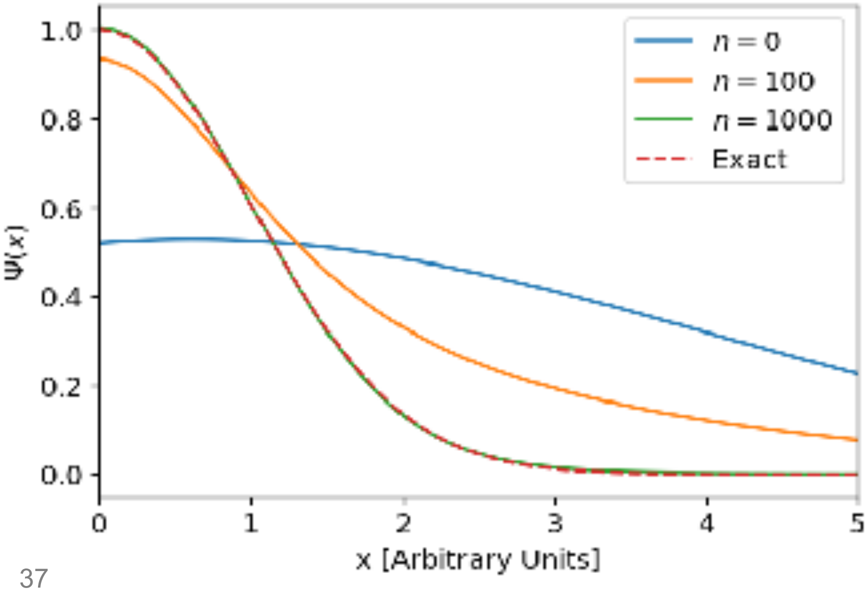
1D QUANTUM HARMONIC OSCILLATOR

To begin with, let us consider a prototypal problem: the 1d quantum harmonic oscillator

$$H = -\frac{\partial^2}{\partial x^2} + \frac{x^2}{2} \longrightarrow \Psi_0(x) = e^{-x^2/2} \quad ; \quad E_0 = 1/2$$

We represent the ground-state wave function with a feed-forward neural network





FERMION MANY-BODY WAVE FUNCTIONS

The fermion antisymmetry must be built in the wave function

$$\Psi_n(x_1, \dots x_i, \dots, x_j, \dots, x_A) = -\Psi_n(x_1, \dots x_j, \dots, x_i, \dots, x_A)$$

Different ansatzë have been put forward

- Slater-Jastrow: $\Psi_V(X) = e^{U(X)}\Phi_S(X) \rightarrow \Psi_V(X) = e^{U(X)}\Phi_S(Y_{\rm bf}(X))$
- Hidden Fermions: $\Psi_V(X) = \Phi_{HF}(X)$
- Neural Pfaffian: $\Psi_V(X) = e^{U(X)}\Phi_P(X) \rightarrow \Psi_V(X) = e^{U(X)}\Phi_P(Y_{\rm bf}(X))$

*Hermann et al., Nature Chemistry, **12**, 891 (2020)*

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

*J. Stokes et al., PRB, **102**, 205122 (2020)*

*J. R. Moreno, et al., PRL **125**, 076402 (2022)*

SLATER JASTROW ANSATZ

$$\Psi_V(X) = e^{J(X)} \times \det \begin{bmatrix} \phi_1(x_1) & \phi_1(x_2) & \cdots & \phi_1(x_N) \\ \phi_2(x_1) & \phi_2(x_2) & \cdots & \phi_2(x_N) \\ \vdots & \vdots & \ddots & \vdots \\ \phi_N(x_1) & \phi_N(x_2) & \cdots & \phi_N(x_N) \end{bmatrix}$$

*J. Stokes et al., Physical Review B **102**, 205122 (2020)*

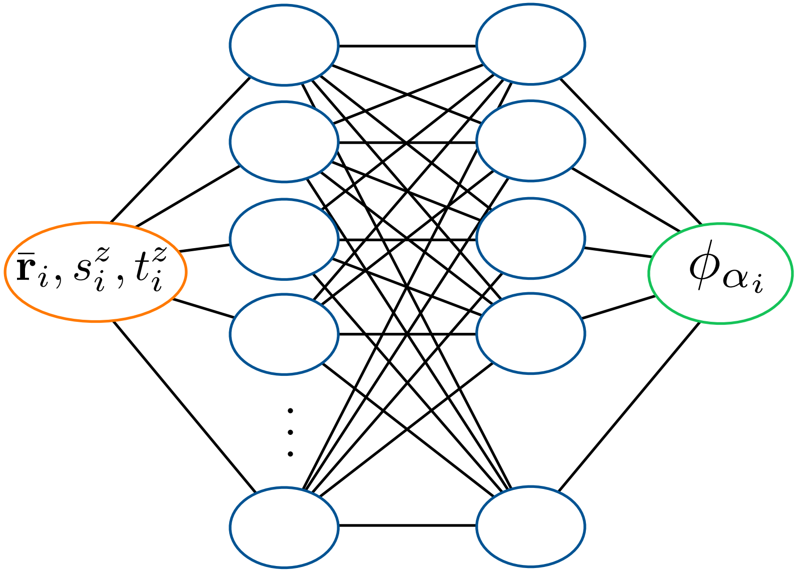
*Pfau et al., Physical Review Research **2**, 033429 (2020)*

*Hermann et al., Nature Chemistry **12**, 891 (2020)*

SLATER JASTROW ANSATZ

Mean-field component: Slater determinant of single-particle orbitals

$$\Phi(X) = \begin{bmatrix} \phi_1(x_1) & \phi_1(x_2) & \cdots & \phi_1(x_N) \\ \phi_2(x_1) & \phi_2(x_2) & \cdots & \phi_2(x_N) \\ \vdots & \vdots & \ddots & \vdots \\ \phi_N(x_1) & \phi_N(x_2) & \cdots & \phi_N(x_N) \end{bmatrix}$$



(If needed) The center of mass motion is automatically removed by

$$\bar{\mathbf{r}}_i = \mathbf{r}_i - \mathbf{R}_{CM}$$

SLATER JASTROW ANSATZ

"Manually" imposing permutation-invariance scales factorially with A

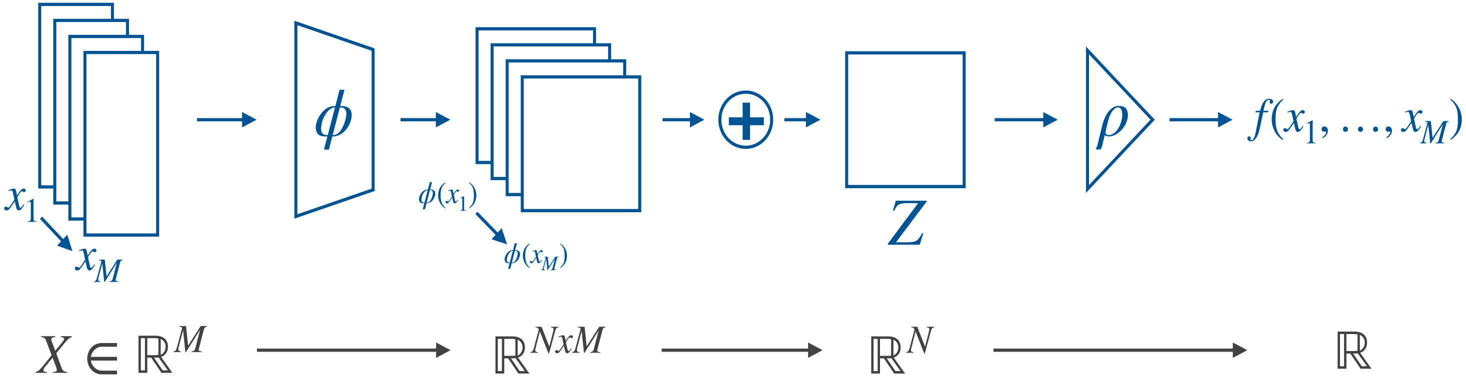
$$J(X) = j(x_1, x_2, x_3) + j(x_1, x_3, x_2) + j(x_2, x_1, x_3) + j(x_2, x_3, x_1) + j(x_3, x_1, x_2) + j(x_3, x_2, x_1)$$

SLATER JASTROW ANSATZ

"Manually" imposing permutation-invariance scales factorially with A

$$J(X) = j(x_1, x_2, x_3) + j(x_1, x_3, x_2) + j(x_2, x_1, x_3) + j(x_2, x_3, x_1) + j(x_3, x_1, x_2) + j(x_3, x_2, x_1)$$

Solution: "deep-sets" → $J(X) = \rho_F \left[\sum_i \vec{\phi}_{\mathcal{F}}(\bar{\mathbf{r}}_i, \mathbf{s}_i) \right]$



Wagstaff et al., arXiv:1901.09006 (2019)

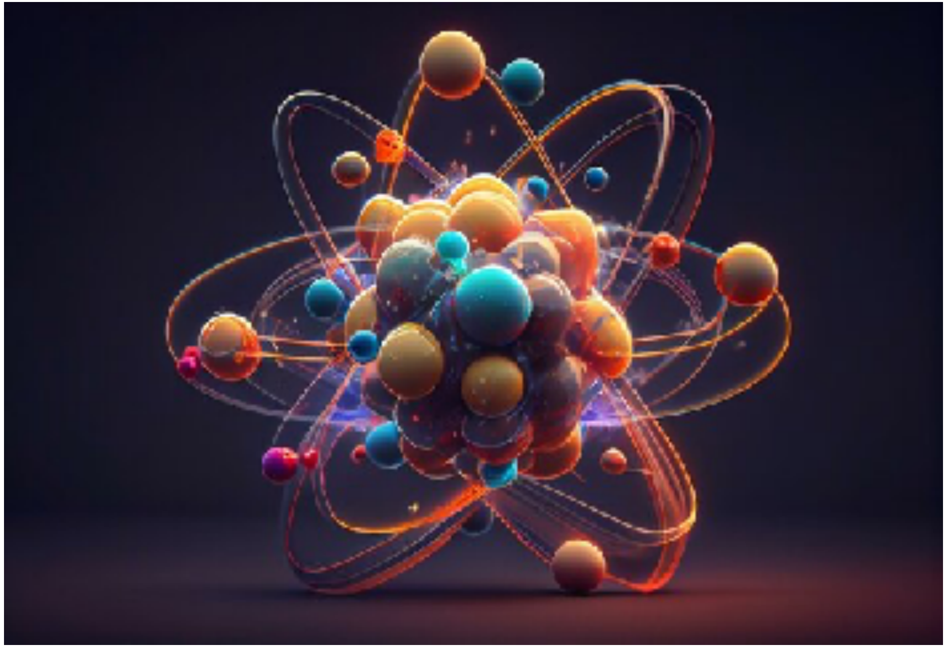
Zaheer et al., arXiv:1703.06114 (2017)

NEURAL BACKFLOW CORRELATIONS

The nodal structure is improved with neural back-flow transformations $\mathbf{x}_i \rightarrow \phi(\mathbf{x}_i; \mathbf{x}_{j \neq i})$

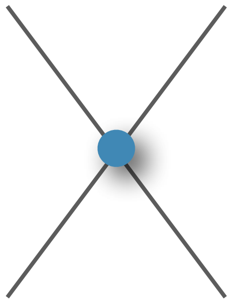
Di Luo and B. K. Clark, Phys. Rev. Lett. ***122****, 226401 (2019)*

BACK TO NUCLEAR PHYSICS



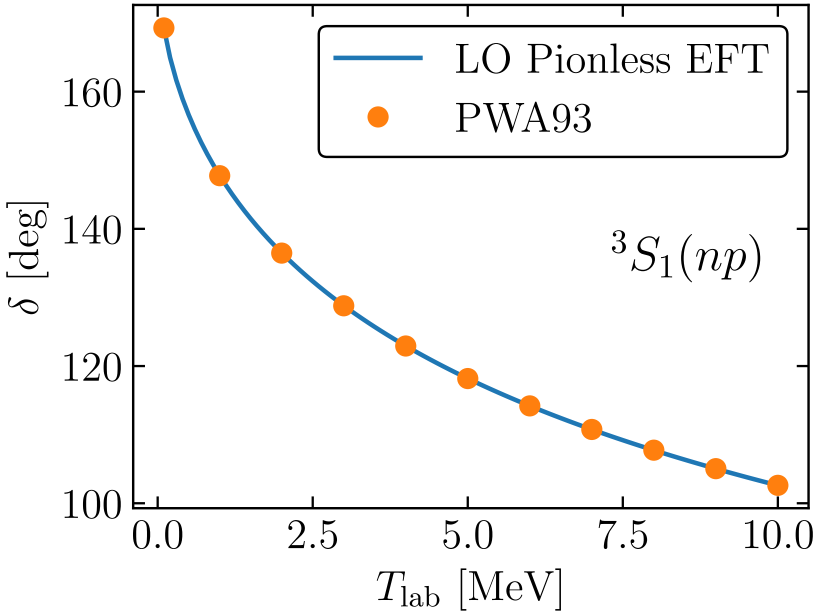
NUCLEAR HAMILTONIAN

- Nucleon-nucleon potential fit to s-wave np scattering lengths and effective ranges



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

$$O_{ij}^{p=1,4} = (1, \tau_{ij}, \sigma_{ij}, \sigma_{ij}\tau_{ij})$$



R. Schiavilla, AL, PRC **103**, 054003 (2021)

NUCLEAR HAMILTONIAN

Let us examine the different spin-isospin operators

$$\tau_{ij} = \boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_j = 2P^{\tau}_{ij} - 1 \quad \rightarrow \quad \tau_{ij}|t^z_i t^z_j\rangle = 2|t^z_j t^z_i\rangle - |t^z_i t^z_j\rangle$$

$$\sigma_{ij} = \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j = 2P^{\sigma}_{ij} - 1 \quad \rightarrow \quad \sigma_{ij}|s^z_i s^z_j\rangle = 2|s^z_j s^z_i\rangle - |s^z_i s^z_j\rangle$$

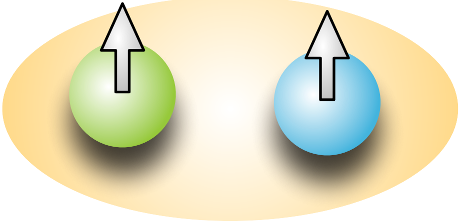
The spin-isospin operator is just the combination of the above two

$$\sigma_{ij}\tau_{ij} = 4P^{\sigma}_{ij}P^{\tau}_{ij} - 2P^{\sigma}_{ij} - 2P^{\tau}_{ij} + 1$$

$$\sigma_{ij}\tau_{ij}|s^z_i t^z_i s^z_j t^z_j\rangle = 4|s^z_j t^z_j s^z_i t^z_i\rangle - 2|s^z_j t^z_i s^z_i t^z_j\rangle - 2|s^z_i t^z_j s^z_j t^z_i\rangle + |s^z_i t^z_i s^z_j t^z_j\rangle$$

LET'S SOLVE THE DEUTERON

The deuteron is the lightest nucleus, composed of a proton and a neutron



The total spin is $S = 1$, the total isospin is $T = 0$

$$|\Phi\rangle = |\uparrow\uparrow\rangle \otimes \frac{1}{\sqrt{2}} \left(|pn\rangle - |np\rangle\right)$$

$$\Phi(S) \equiv \langle s_1^z t_1^z s_2^z t_2^z | \Phi\rangle = \langle s_1^z s_2^z | \uparrow\uparrow\rangle \frac{1}{\sqrt{2}} \left(\langle t_1^z t_2^z | pn\rangle - \langle t_1^z t_2^z | np\rangle\right)$$

LET'S SOLVE THE DEUTERON

Taking into account the spatial dependencies, the most general wave function can be parameterized as

$$\Psi(R, S) = e^{U(r_{12})}\Phi(S)$$

- Since $U(r_{12})$ only depends on the distance $r_{12} = |\mathbf{r}_{12}|$, the wave function is symmetric under the exchange of spatial coordinates

- However, $\Phi(S)$ is antisymmetric under the exchange of spin-isospin coordinates

- Hence, the total wave function $\Psi(R, S)$ is antisymmetric under the exchange of two particles

LOCAL ENERGY

Reminder: the energy can be estimated as

$$E_V \simeq \frac{1}{N} \sum_{(R_i, S_i) \sim \pi_V} \frac{\langle R_i S_i | H | \Psi_V \rangle}{\langle R_i S_i | \Psi_V \rangle}$$

We need to compute the local energy, which is the sum of a kinetic and potential contribution

$$\begin{aligned} \frac{\langle RS | T | \Psi_V \rangle}{\langle RS | \Psi_V \rangle} &= -\frac{1}{2m} \sum_i \frac{\nabla_i^2 \Psi_V(R,S)}{\Psi_V(R,S)} \\ &= -\frac{1}{2m} \sum_i \left[\nabla_i^2 U(R) + (\nabla_i U(R))^2 \right] \end{aligned}$$

Automatic differentiation (and tailored variants) are employed to efficiently compute it.

LOCAL ENERGY

The potential energy is particularly complicated in Nuclear Physics!

$$\frac{\langle RS|V|\Psi_V\rangle}{\langle RS|\Psi_V\rangle} = \sum_{i<j}\sum_p v^p(r_{ij})\frac{\langle RS|O^p_{ij}|\Psi_V\rangle}{\langle RS|\Psi_V\rangle}$$

We pre-compute the local operators corresponding to exchanging the spin, the isospin, and both.

$$P^\sigma_{ij}(R,S) = \frac{\langle RS|\hat{P}^\sigma_{ij}|\Psi_V\rangle}{\langle RS|\Psi_V\rangle} \quad ; \quad P^\tau_{ij}(R,S) = \frac{\langle RS|\hat{P}^\tau_{ij}|\Psi_V\rangle}{\langle RS|\Psi_V\rangle} \quad ; \quad P^{\sigma\tau}_{ij}(R,S) = \frac{\langle RS|\hat{P}^\sigma_{ij}\hat{P}^\tau_{ij}|\Psi_V\rangle}{\langle RS|\Psi_V\rangle}$$

LOCAL ENERGY

$$\frac{\langle RS|V|\Psi_V\rangle}{\langle RS|\Psi_V\rangle} = \sum_{i<j}\Big\{4v^{\sigma\tau}(r_{ij})P_{ij}^{\sigma\tau}(R,S) + 2[v^{\sigma}(r_{ij}) - v^{\sigma\tau}(r_{ij})]P_{ij}^{\sigma}(R,S)$$

$$+ 2[v^{\tau}(r_{ij}) - v^{\sigma\tau}(r_{ij})]P_{ij}^{\tau}(R,S)$$

$$+ [v^{c}(r_{ij}) - v^{\sigma}(r_{ij}) - v^{\tau}(r_{ij}) + v^{\sigma\tau}(r_{ij})\Big\}$$

LOCAL ENERGY FOR THE DEUTERON

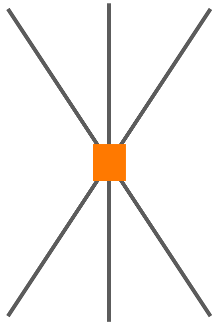
$$|\Phi\rangle = |\uparrow\uparrow\rangle \otimes \frac{1}{\sqrt{2}}\left(|pn\rangle - |np\rangle\right) \quad \rightarrow \quad \begin{cases} \sigma_{12}|\Phi\rangle = |\Phi\rangle \\ \tau_{12}|\Phi\rangle = -3|\Phi\rangle \\ \sigma_{12}\tau_{12}|\Phi\rangle = -3|\Phi\rangle \end{cases}$$

Therefore, the potential becomes effectively spin-isospin independent

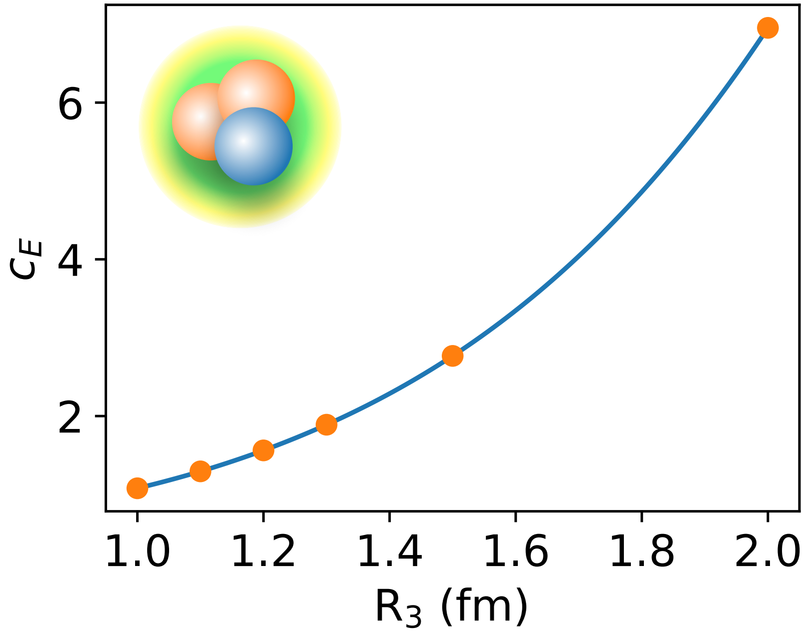
$$\frac{\langle RS|V|\Psi_V\rangle}{\langle RS|\Psi_V\rangle} = \sum_{i<j}\left[v^c(r_{ij}) - 3v^\tau(r_{ij}) + v^\sigma(r_{ij}) - 3v^{\sigma\tau}(r_{ij})\right]$$

SOLVING THE DEUTERON

- Three-nucleons potential adjusted to reproduce the energy of ^{3}H.

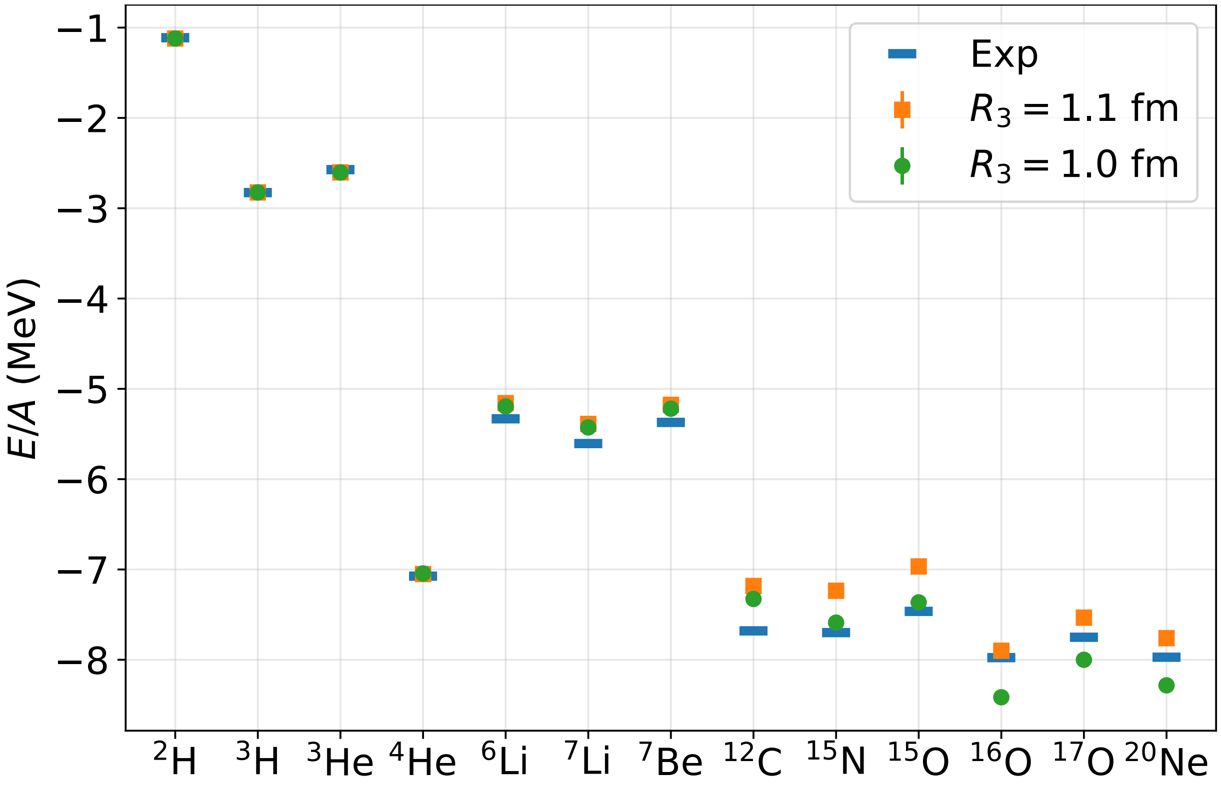


$$V_{ijk} \propto c_E \sum_{\text{cyc}} e^{-(r_{ij}^2 + r_{jk}^2)/R_3^2}$$



R. Schiavilla, AL, PRC **103**, 054003 (2021)

VMC+NQS: UNDERSTAND NUCLEAR FORCES



A. Gnech, et al., Phys. Rev. Lett. 133 (2024) **14**, 142501

NEUTRON STARS

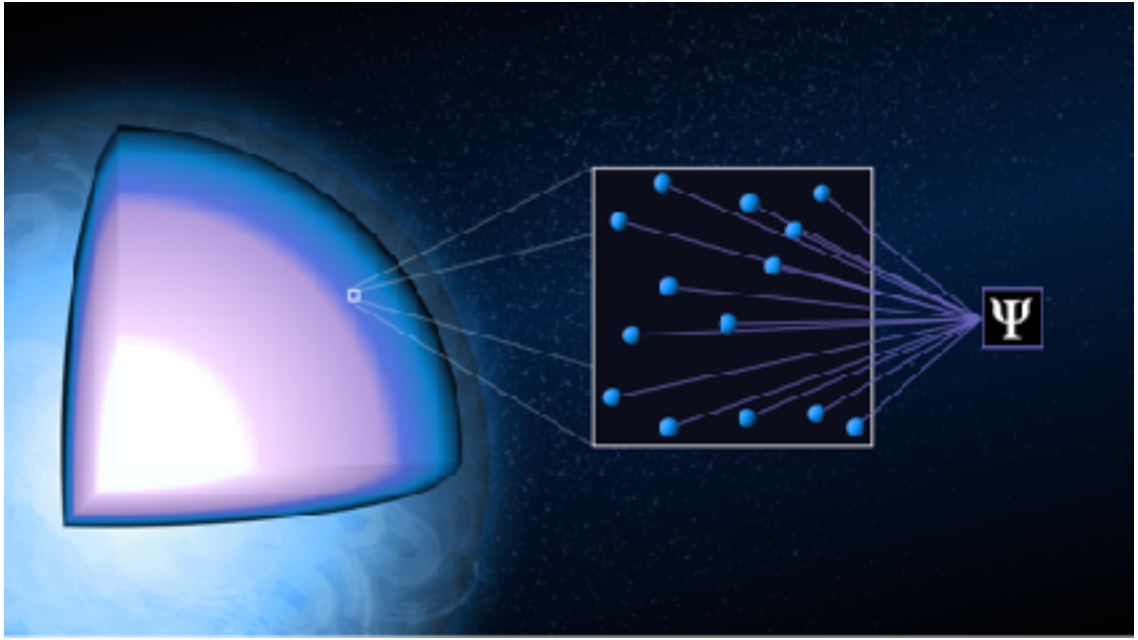
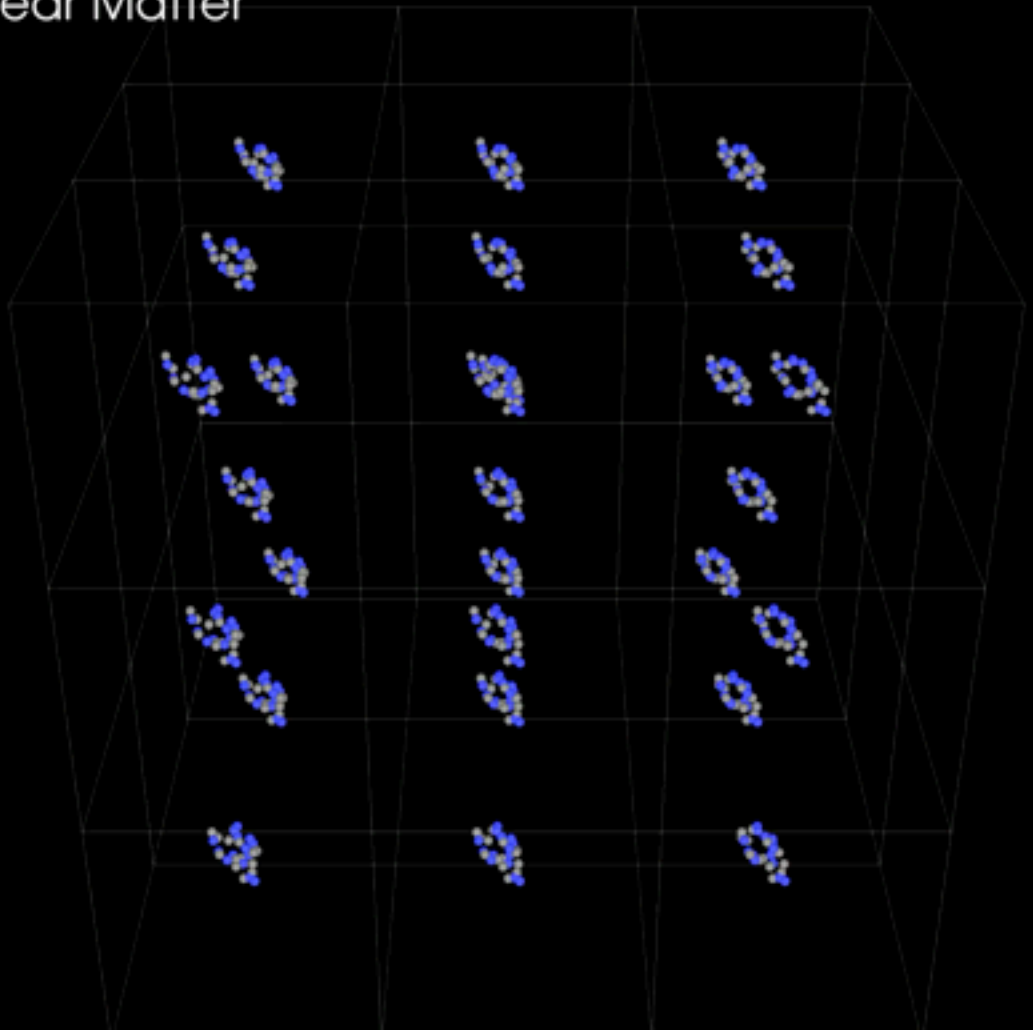


Image Credit: Jane Kim

Symmetric Nuclear Matter

$n_B = 0.001\ fm^{-3}$



BACKUP

GITHUB REPOSITORY

https://github.com/alelovato/EIC_School/

QUANTUM HARMONIC OSCILLATOR

Let us consider the prototypal problem of a collection of A independent (decoupled) quantum Harmonic oscillators, in N dimensions with unit mass

$$H = -\frac{1}{2}\sum_{i=1}^{A}\nabla_i^2 + \sum_{i=1}^{A}\frac{\mathbf{r}_i^2}{2}$$

We assume a variational wave function of the exponential form

$$\Psi_V(R) \equiv \langle R|\Psi_V\rangle = \exp\left(-b\sum_{i=1}^{A}\mathbf{r}_i^2\right)$$

Note that the exact ground state is recovered by taking b = 1/2

$$\Psi_0(R) = \exp\left(-\frac{1}{2}\sum_{i=1}^{A}\mathbf{r}_i^2\right) \longrightarrow E_0 = A \times N \times \frac{1}{2}$$

QUANTUM HARMONIC OSCILLATOR

The local energy is the sum of the kinetic and potential contributions

$$E_L(R) \equiv \frac{\langle R|H|\Psi_V\rangle}{\langle R|\Psi_V\rangle} = \frac{\langle R|T|\Psi_V\rangle}{\langle R|\Psi_V\rangle} + \frac{\langle R|V|\Psi_V\rangle}{\langle R|\Psi_V\rangle}$$

The kinetic energy involves the second derivative of the variational wave function

$$T_L(R) = -\frac{1}{2}\sum_{i=1}^{A} \frac{\nabla_i^2 \Psi_V(R)}{\Psi_V(R)}$$

Let us first compute the first derivative analytically

$$\nabla_i \Psi_V(R) = -2b\mathbf{r}_i \Psi_V(R)$$

So that:

$$\nabla_i^2 \Psi_V(R) = (-2Nb + 4b^2\mathbf{r}_i^2)\Psi_V(R) \longrightarrow \quad T_L(R) = \sum_{i=1}^{A}(bN - 2b^2\mathbf{r}_i^2)$$

QUANTUM HARMONIC OSCILLATOR

The potential energy is more immediate to evaluate, as it is diagonal in coordinate space

$$V_L(R) = \sum_{i=1}^{A} \frac{\mathbf{r}_i^2}{2}$$

The total energy then reads

$$E_L(R) = \sum_{i=1}^{A} \left[bN + \left(\frac{1}{2} - 2b^2 \right) \mathbf{r}_i^2 \right]$$

Question: what happens when b = 1/2?

Question 2: do you notice anything “strange”?

QUANTUM HARMONIC OSCILLATOR

The potential energy is more immediate to evaluate, as it is diagonal in coordinate space

$$V_L(R) = \sum_{i=1}^{A} \frac{\mathbf{r}_i^2}{2}$$

The total energy then reads

$$E_L(R) = \sum_{i=1}^{A} \left[bN + \left(\frac{1}{2} - 2b^2 \right) \mathbf{r}_i^2 \right]$$

Question: what happens when b = 1/2?

$$E_L(R) = A \times N \times \frac{1}{2} = E_0$$

Question 2: do you notice anything “strange”?

ZERO-VARIANCE PRINCIPLE

The Monte Carlo variance vanishes for exact variational wave functions

$$\sigma_{E_V} = \sqrt{\frac{\langle E_L^2 \rangle - \langle E_L \rangle^2}{N_s - 1}} \quad ; \quad \langle E_L \rangle \simeq \frac{1}{N_s} \sum_{R_n} E_L(R_n) \quad ; \quad \langle E_L^2 \rangle \simeq \frac{1}{N_s} \sum_{R_n} E_L^2(R_n)$$

For an exact variational wave function, the local energy is independent of the sample

$$E_L(R) \equiv \frac{\langle R|H|\Psi_V \rangle}{\langle R|\Psi_V \rangle} = E_0 \frac{\langle R|\Psi_V \rangle}{\langle R|\Psi_V \rangle} = E_0$$

As a consequence:

$$\begin{cases} \langle E_L \rangle = E_0 \\ \langle E_L^2 \rangle = E_0^2 \end{cases} \longrightarrow \quad \sigma_{E_V} = 0$$

REFERENCES

*Hermann et al., Nature Chemistry, **12**, 891 (2020)*

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

*J. Stokes et al., PRB, **102**, 205122 (2020)*

*J. R. Moreno, et al., PRL **125**, 076402 (2022)*