Second-Order Perturbation Theory In Continuum Quantum Monte Carlo

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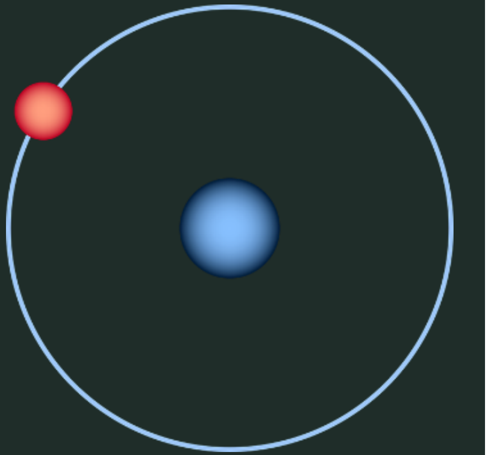
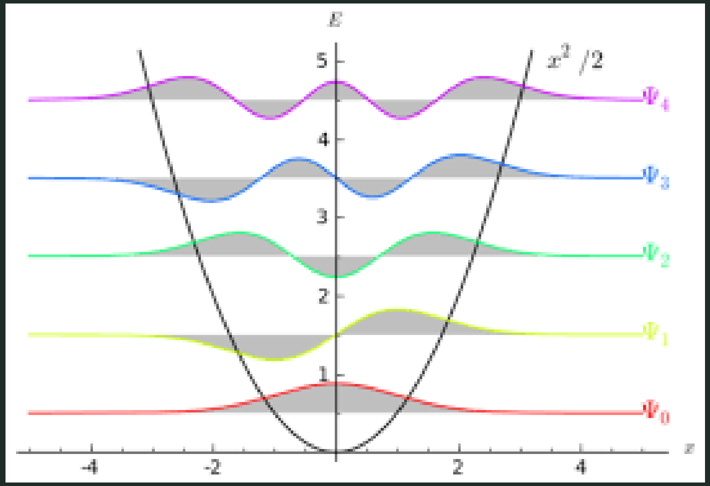
Nuclear-Many Body Problem

- Schrodinger Equation

$$H\Psi = E\Psi$$

- Analytically solvable for few idealized systems

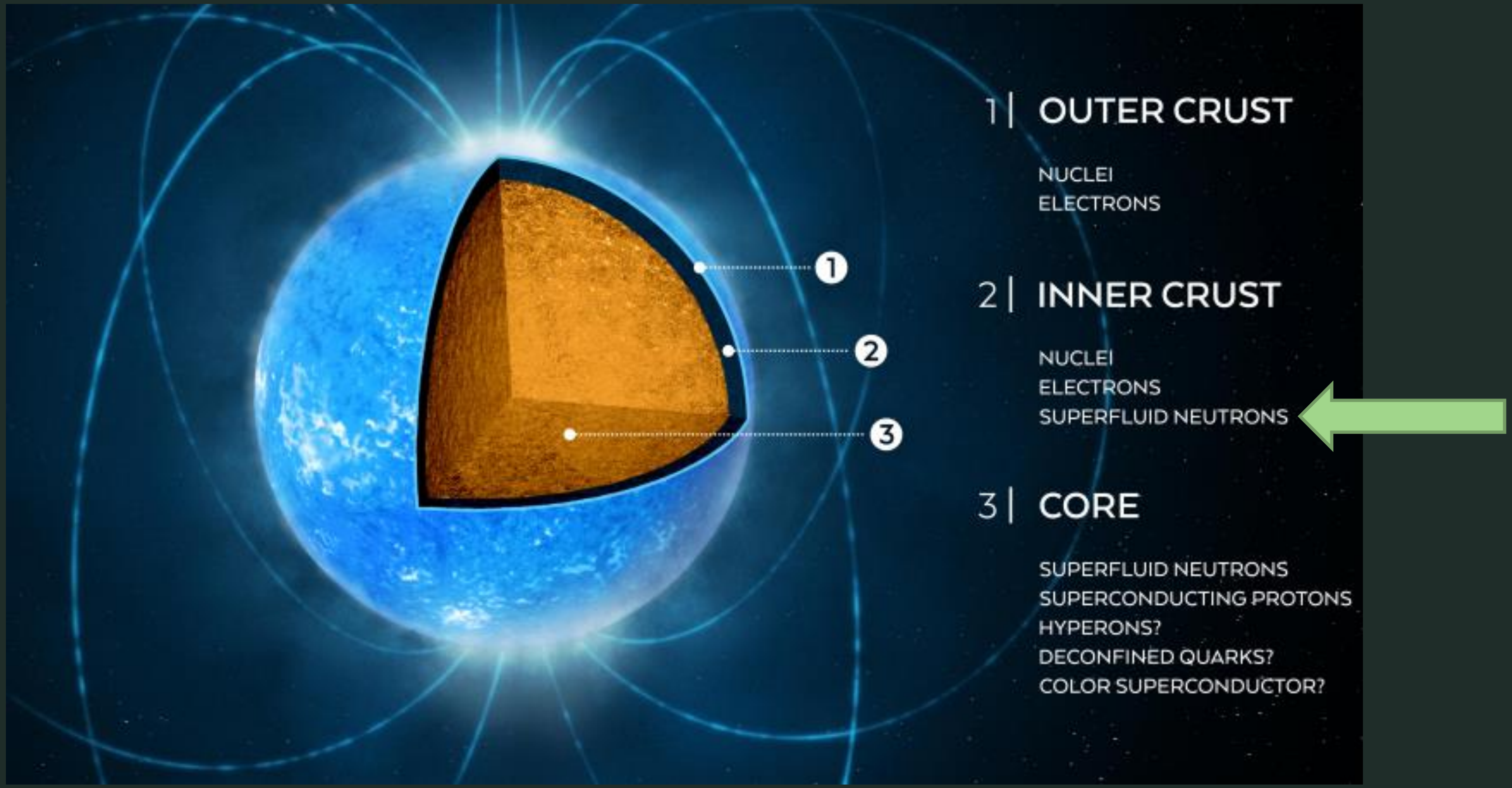




- Realistic systems cannot be solved analytically

$$H = \sum_{k=1}^{N}\left(-\frac{\hbar^2}{2m}\nabla_k^2\right) + \sum_{i<j\prime} V(\vec{r}_{ij\prime})$$

Neutron Stars



- From Anna L. Watts

- Pure infinite neutron matter
- S-wave interactions

Nucleon-Nucleon Interaction

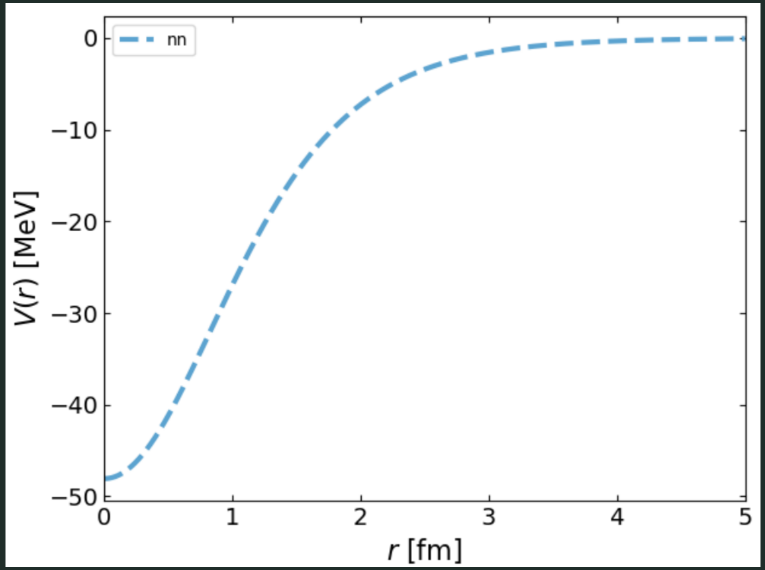
- Fully described by Quantum Chromodynamics (QCD)

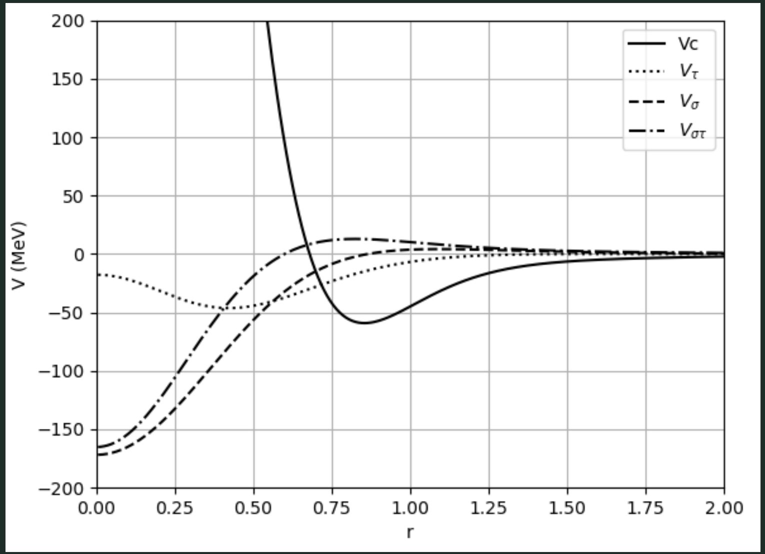
- Pöschl-Teller
  - Effective Range Expansion

$$k \cot \delta = -\frac{1}{a_0} + \frac{1}{2} r_e k^2 \cancel{- Pr^3 k^4 + \cdots}$$

- Argonne Group AV18
  - Operator structure
  - Fit to experimental data

$$1, \sigma_1 \cdot \sigma_2, \tau_1 \cdot \tau_2, \sigma_1 \cdot \sigma_2\ \tau_1 \cdot \tau_2, \ldots$$





[1] J. Carlson *et al,* Phys. Rev. Lett. **91**, 050401-1, (2003)
[2] H. Bethe, Phys. Rev. **76**, 38 (1949)
[3] R.B. Wiringa, V.G.J. Stoks and R. Schiavilla, Phys. Rev. C **76**, 38 (1995)

Chiral Effective Field Theory

Second-Order Perturbation Theory in QMC

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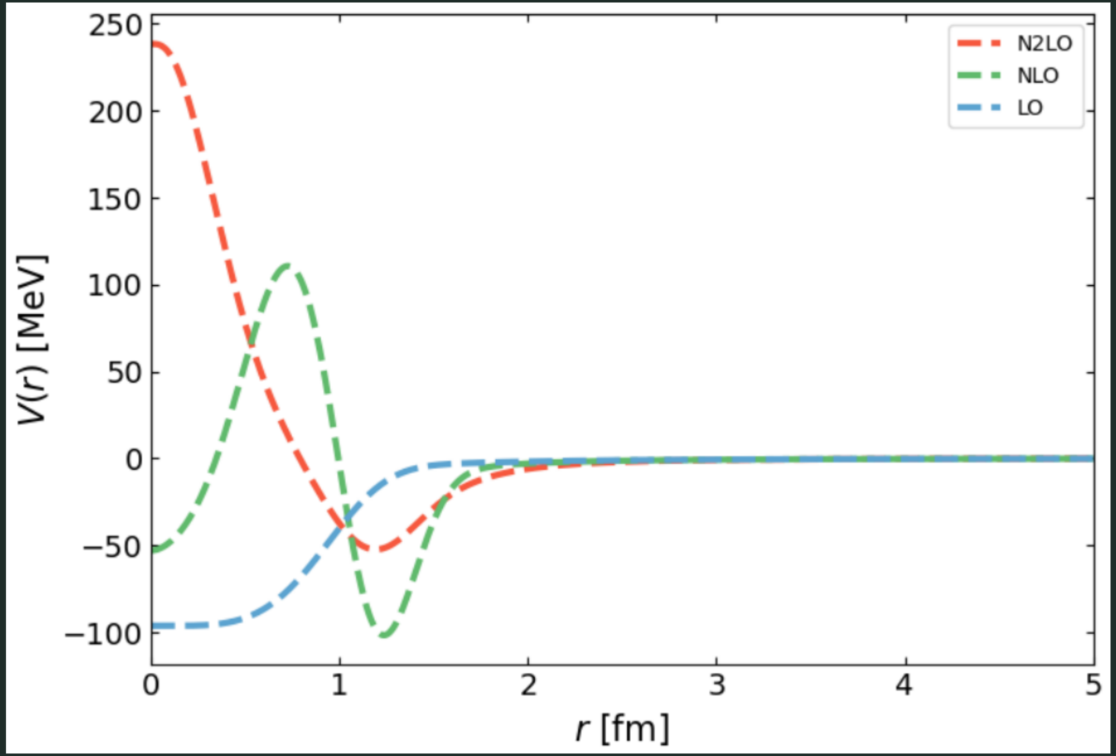
- Modern nuclear potentials

- Chiral Effective Field Theory
  - Power Counting
  - Respects symmetries of QCD
  - Expansion in powers in Q/Λ_b

$$V_{\text{chiral}} = V^{(0)} + V^{(2)} + V^{(3)} + \cdots$$

LO NLO N^{2}LO



[4] S. Weinberg, Phys. Lett. B, **251**, 288 (1990).
[5] E. Epelbaum *et al,* Rev. Mod. Phys. **81**, 1773 (2009).
[6]A. Gezerlis *et al,* Phys. Rev. Lett. **111**, 032501 (2013).

Second-Order Perturbation Theory in QMC

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Diffusion Monte Carlo

$$\psi(\tau) = e^{-(H-E_T)\tau}\psi_T$$

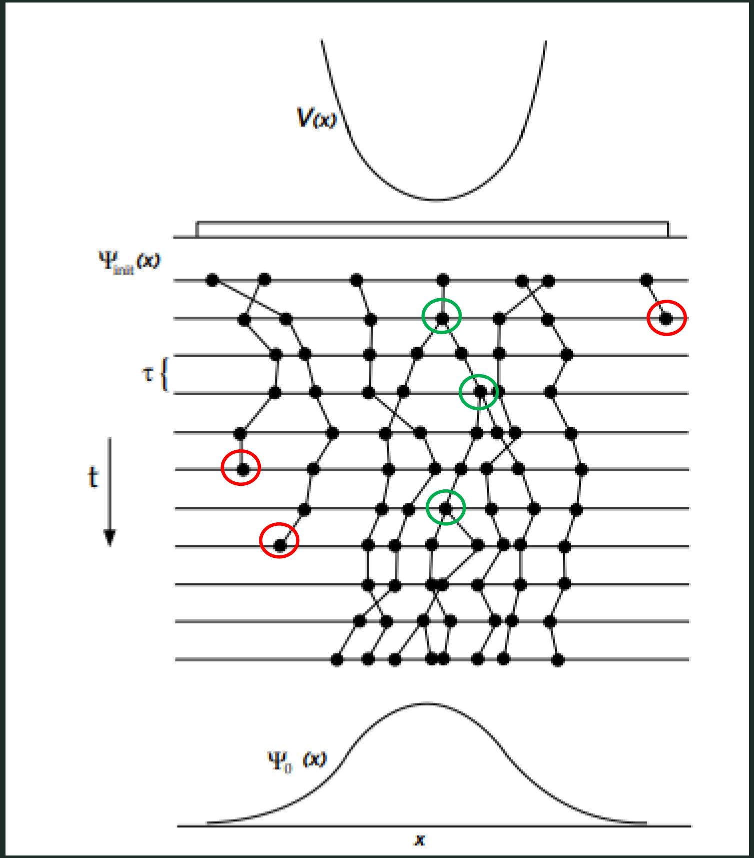
$$\psi(\tau) = \sum_{i=0}^{\infty} a_i e^{-(E_i-E_T)\tau}\psi_i$$

$$\psi(\tau) = a_0 e^{-(E_0-E_T)\tau}\psi_0 + a_0 e^{-(E_1-E_T)\tau}\psi_1 + a_0 e^{-(E_2-E_T)\tau}\psi_2 + \cdots$$

$$\psi(\tau) = a_0\psi_0 \qquad \lim \tau \to \infty$$

Diffusion Monte Carlo

$$\tau = it \longrightarrow -\frac{\partial}{\partial\tau}\psi = \left(-\frac{\hbar}{2m}\nabla^2 + V\right)\psi$$



$$-\frac{\partial}{\partial\tau}\psi = \left(-\frac{\hbar}{2m}\nabla^2 + \cancel{V}\right)\psi$$

Diffusion

$$-\frac{\partial}{\partial\tau}\psi = \left(\cancel{-\frac{\hbar}{2m}}\nabla^2 + V\right)\psi$$

Growth/Decay

[7] J.W.M.C. Foulkes *et al.* Rev. Mod. Phys., **73,** 33 (2001).

Perturbation Theory

First- and Second-Order Corrections

$$E_0^{(1)} = \langle \psi_0 | V' | \psi_0 \rangle$$

$$E_0^{(2)} = -\sum_{k \neq 0}^{\infty} \frac{|\langle \psi_0 | V' | \psi_k \rangle|^2}{E_k - E_0}$$

Perturbation Theory

First- and Second-Order Corrections

$$E_0^{(1)} = \langle \psi_0 | V' | \psi_0 \rangle$$

The problem?

$$E_0^{(2)} = -\sum_{k\neq 0}^{\infty} \frac{|\langle \psi_0 | V' | \psi_k \rangle|^2}{E_k - E_0}$$

Diffusion Monte Carlo

$$\lim_{\tau\to\infty} \psi(\tau) = \lim_{\tau\to\infty} e^{-(H-E_0)\tau} \psi_T \propto \psi_0 \longrightarrow E_0$$

Second-Order Correction

$$I(\mathcal{T}) = \int_0^{\mathcal{T}} d\tau \left\langle \psi_0 \middle| V' e^{-[H_0 - E_0]\tau} V' \middle| \psi_0 \right\rangle$$

Second-Order Correction

$$I(\mathcal{T}) = \int_0^{\mathcal{T}} d\tau \left\langle \psi_0 \middle| V' e^{-[H_0 - E_0]\tau} V' \middle| \psi_0 \right\rangle$$

$$I(\mathcal{T}) = \sum_{k=0}^{\infty} \int_0^{\mathcal{T}} d\tau \, e^{-[E_k - E_0]\tau} \langle \psi_0 | V' | \psi_k \rangle \langle \psi_k | V' | \psi_0 \rangle$$

$$I(\mathcal{T}) = \int_0^{\mathcal{T}} d\tau \, |\langle \psi_0 | V' | \psi_0 \rangle|^2 + \sum_{k \neq 0}^{\infty} \int_0^{\mathcal{T}} e^{-[E_k - E_0]\tau} \, |\langle \psi_k | V' | \psi_0 \rangle|^2$$

Second-Order Perturbation Theory in QMC

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Second-Order Correction

$$I(\mathcal{T}) = \int_0^{\mathcal{T}} d\tau \left\langle \psi_0 \middle| V' e^{-[H_0 - E_0]\tau} V' \middle| \psi_0 \right\rangle$$

$$I(\mathcal{T}) = \sum_{k=0}^{\infty} \int_0^{\mathcal{T}} d\tau\, e^{-[E_k - E_0]\tau} \langle \psi_0 | V' | \psi_k \rangle \langle \psi_k | V' | \psi_0 \rangle$$

$$I(\mathcal{T}) = \int_0^{\mathcal{T}} d\tau\, |\langle \psi_0 | V' | \psi_0 \rangle|^2 + \sum_{k\neq 0}^{\infty} \int_0^{\mathcal{T}} e^{-[E_k - E_0]\tau} |\langle \psi_k | V' | \psi_0 \rangle|^2$$

$$E_0^{(1)} = \langle \psi_0 | V' | \psi_0 \rangle$$

Second-Order Correction

$$I(\mathcal{T}) = \int_0^{\mathcal{T}} d\tau \, \langle \psi_0 | V' e^{-[H_0 - E_0]\tau} V' | \psi_0 \rangle$$

$$I(\mathcal{T}) = \sum_{k=0}^{\infty} \int_0^{\mathcal{T}} d\tau \, e^{-[E_k - E_0]\tau} \langle \psi_0 | V' | \psi_k \rangle \langle \psi_k | V' | \psi_0 \rangle$$

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$$E_0^{(1)} = \langle \psi_0 | V' | \psi_0 \rangle$$

?

Second-Order Correction

$$I(\mathcal{T}) = \int_0^{\mathcal{T}} d\tau\, |\langle\psi_0|V'|\psi_0\rangle|^2 + \sum_{k\neq 0}^{\infty} \int_0^{\mathcal{T}} e^{-[E_k - E_0]\tau}\, |\langle\psi_k|V'|\psi_0\rangle|^2$$

Second-Order Correction

$$I(\mathcal{T}) = \int_0^{\mathcal{T}} d\tau \, |\langle\psi_0|V'|\psi_0\rangle|^2 + \sum_{k\neq 0}^{\infty} \int_0^{\mathcal{T}} e^{-[E_k - E_0]\tau} \, |\langle\psi_k|V'|\psi_0\rangle|^2$$

$$I(\mathcal{T}) = \left(E_0^{(1)}\right)^2 \mathcal{T} - \sum_{k\neq 0}^{\infty} \frac{|\langle\psi_k|V'|\psi_0\rangle|^2}{E_k - E_0} \left[e^{-[E_k - E_0]\mathcal{T}} - 1\right]$$

Second-Order Correction

$$I(\mathcal{T}) = \int_0^{\mathcal{T}} d\tau \, |\langle \psi_0 | V' | \psi_0 \rangle|^2 + \sum_{k \neq 0}^{\infty} \int_0^{\mathcal{T}} e^{-[E_k - E_0]\tau} \, |\langle \psi_k | V' | \psi_0 \rangle|^2$$

$$I(\mathcal{T}) = \left(E_0^{(1)}\right)^2 \mathcal{T} - \sum_{k \neq 0}^{\infty} \frac{|\langle \psi_k | V' | \psi_0 \rangle|^2}{E_k - E_0} \left[e^{-[E_k - E_0]\mathcal{T}} - 1\right]$$

$$E_0^{(2)} = -\sum_{k \neq 0}^{\infty} \frac{|\langle \psi_0 | V' | \psi_k \rangle|^2}{E_k - E_0}$$

Second-Order Correction

$$I(\mathcal{T}) = \int_0^{\mathcal{T}} d\tau \, |\langle\psi_0|V'|\psi_0\rangle|^2 + \sum_{k\neq0}^{\infty} \int_0^{\mathcal{T}} e^{-[E_k - E_0]\tau} \, |\langle\psi_k|V'|\psi_0\rangle|^2$$

0 as $\tau \rightarrow \infty$

$$I(\mathcal{T}) = \left(E_0^{(1)}\right)^2 \mathcal{T} - \sum_{k\neq0}^{\infty} \frac{|\langle\psi_k|V'|\psi_0\rangle|^2}{E_k - E_0} \left[\cancel{e^{-[E_k - E_0]\mathcal{T}}} - 1\right]$$

$$E_0^{(2)} = -\sum_{k\neq0}^{\infty} \frac{|\langle\psi_0|V'|\psi_k\rangle|^2}{E_k - E_0}$$

Second-Order Correction

$$I(\mathcal{T}) = \int_0^{\mathcal{T}} d\tau \, |\langle \psi_0 | V' | \psi_0 \rangle|^2 + \sum_{k \neq 0}^{\infty} \int_0^{\mathcal{T}} e^{-[E_k - E_0]\tau} \, |\langle \psi_k | V' | \psi_0 \rangle|^2$$

$$I(\mathcal{T}) = \left(E_0^{(1)}\right)^2 \mathcal{T} - \sum_{k \neq 0}^{\infty} \frac{|\langle \psi_k | V' | \psi_0 \rangle|^2}{E_k - E_0} \left[e^{-[E_k - E_0]\mathcal{T}} - 1\right]$$

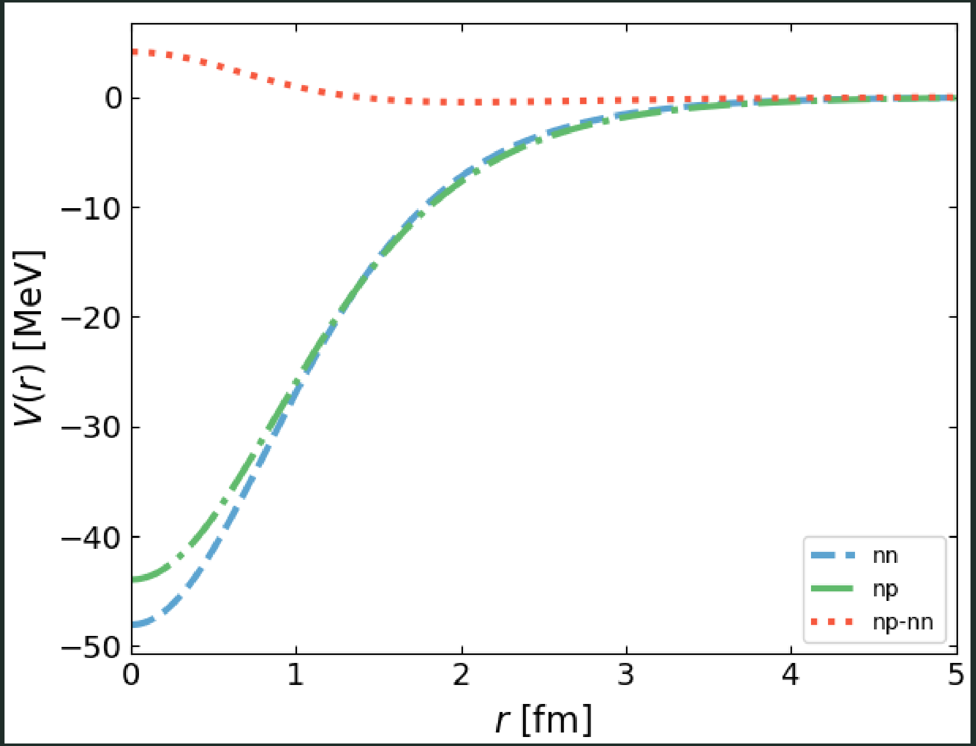
$$I(\mathcal{T} \to \infty) = \left(E_0^{(1)}\right)^2 \mathcal{T} - E_0^{(2)}$$

Few Body Tests

Neutron-Neutron → Neutron-Proton

$$V(r) = -2v_0 \frac{\mu^2}{\cosh\,^2(\mu r)}$$

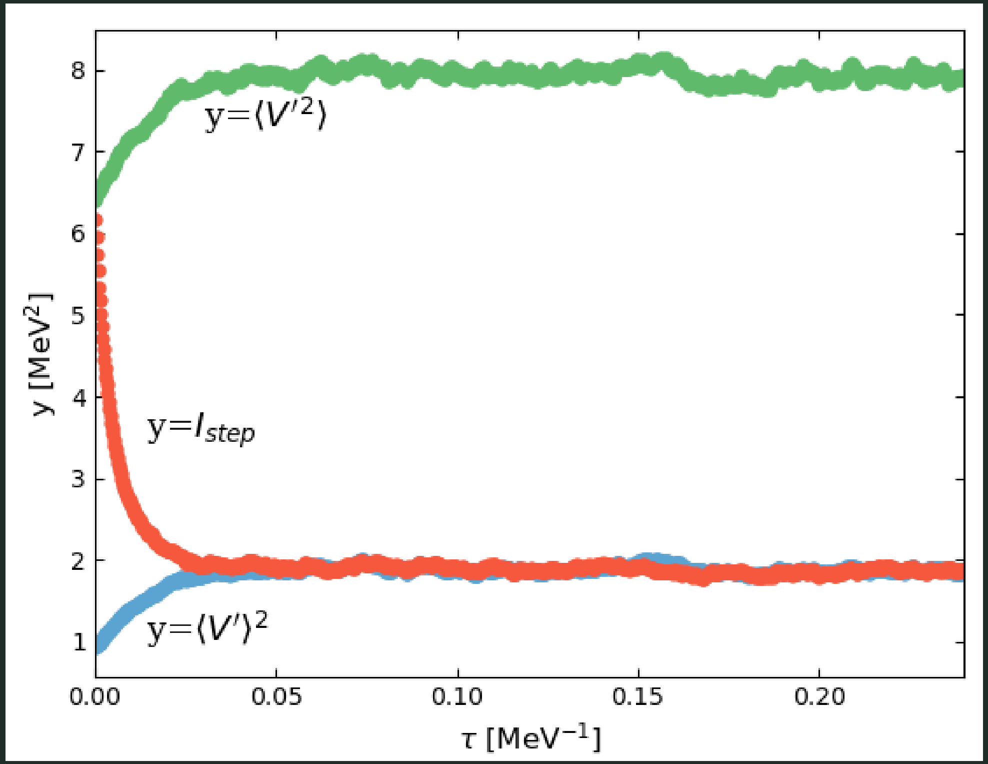
Neutron-Neutron	$a_0 = -18.5$ fm $r_e = 2.7$ fm
Neutron-Proton	$a_0 = -23.75$ fm $r_e = 2.81$ fm

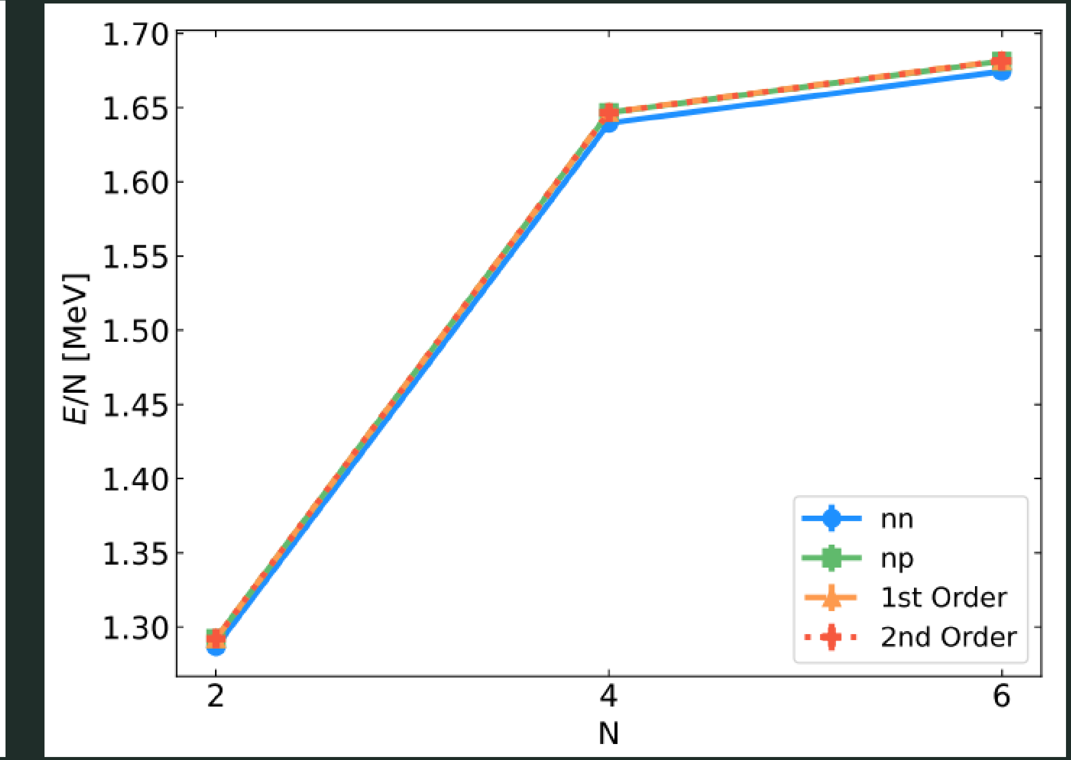


[8] R. Curry, J.E. Lynn, K.E. Schmidt, and A. Gezerlis, arxiv: 2302.07285 Nucl. Th.

Few Body Tests

$$I(\mathcal{T}) = \int_0^{\mathcal{T}} d\tau \, \underbrace{\langle \psi_0 | V' e^{-[H_0-E_0]\tau} V' | \psi_0 \rangle}_{}$$

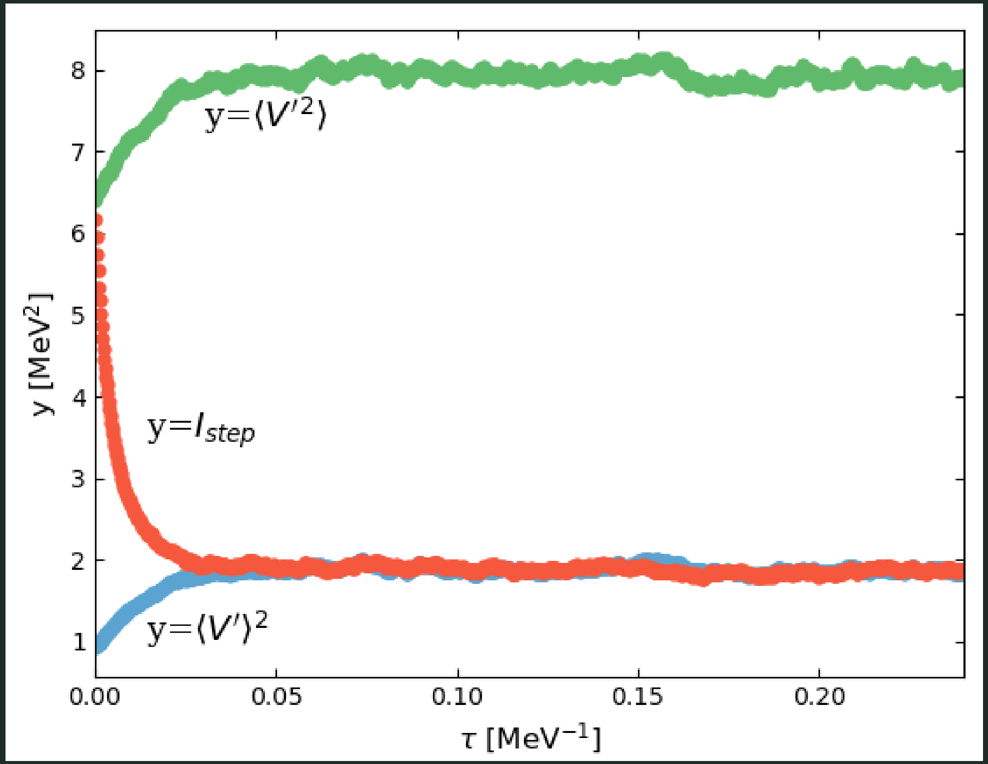


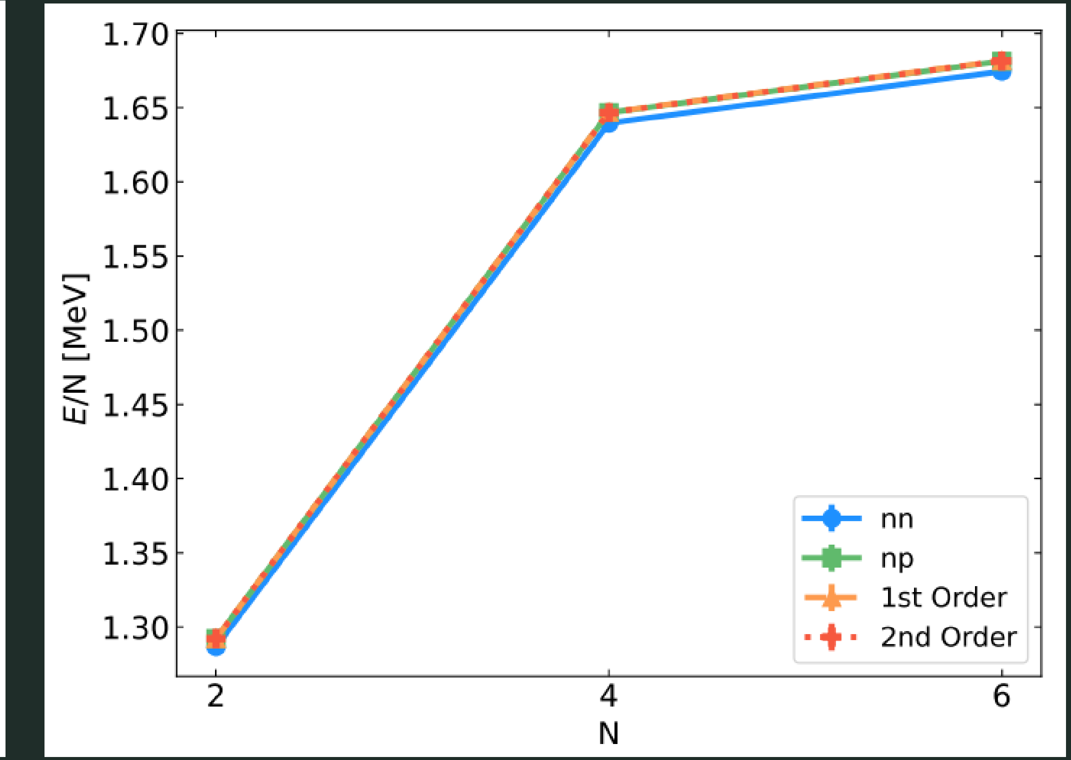


[8] R. Curry, J.E. Lynn, K.E. Schmidt, and A. Gezerlis, arxiv: 2302.07285 Nucl. Th.

Few Body Tests

$$\text{Fit} \longrightarrow \quad I(\mathcal{T}) = \int_0^{\mathcal{T}} d\tau \, |\langle\psi_0|V'|\psi_0\rangle|^2 + \sum_{k\neq 0}^{\infty} \int_0^{\mathcal{T}} e^{-[E_k-E_0]\tau} \, |\langle\psi_k|V'|\psi_0\rangle|^2$$





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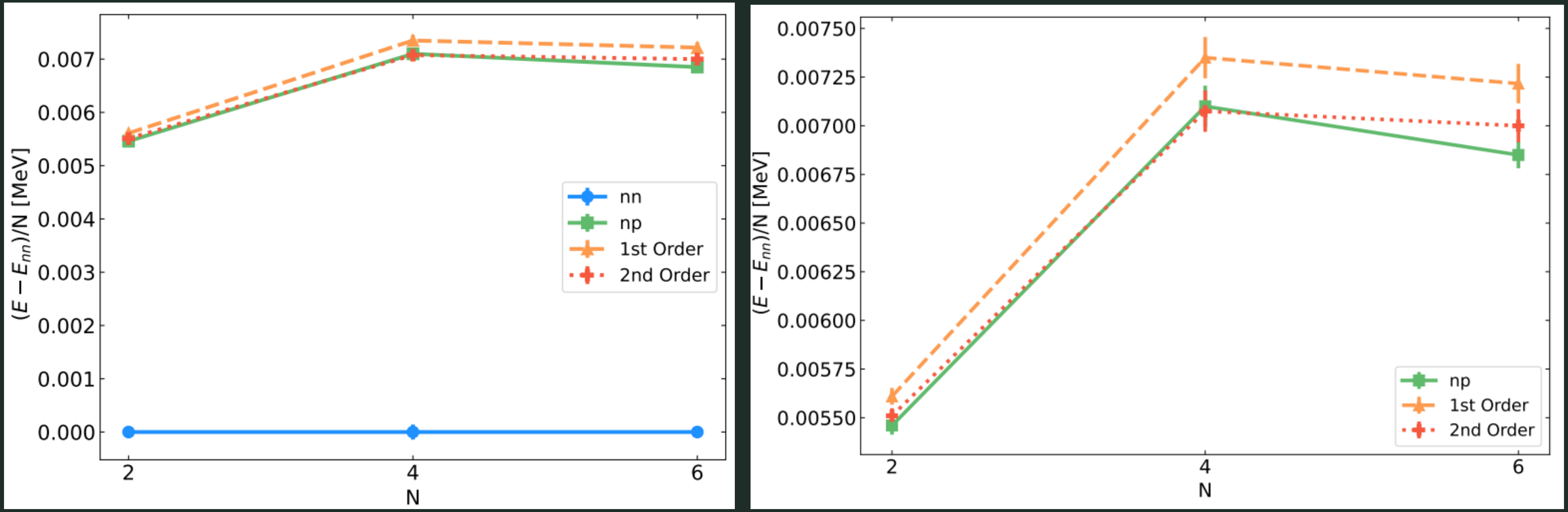
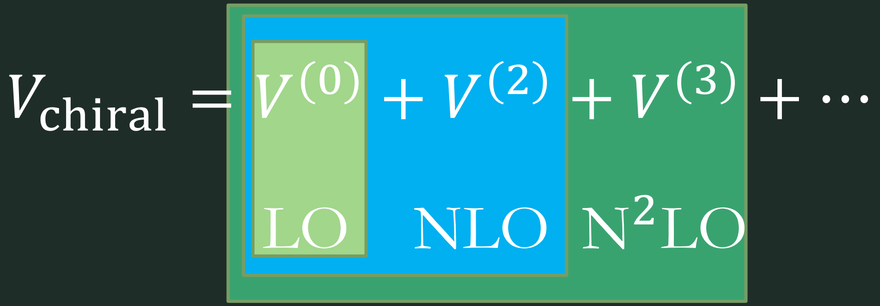
Few Body Tests



- First-Order correction insufficient!

Testing Perturbativeness



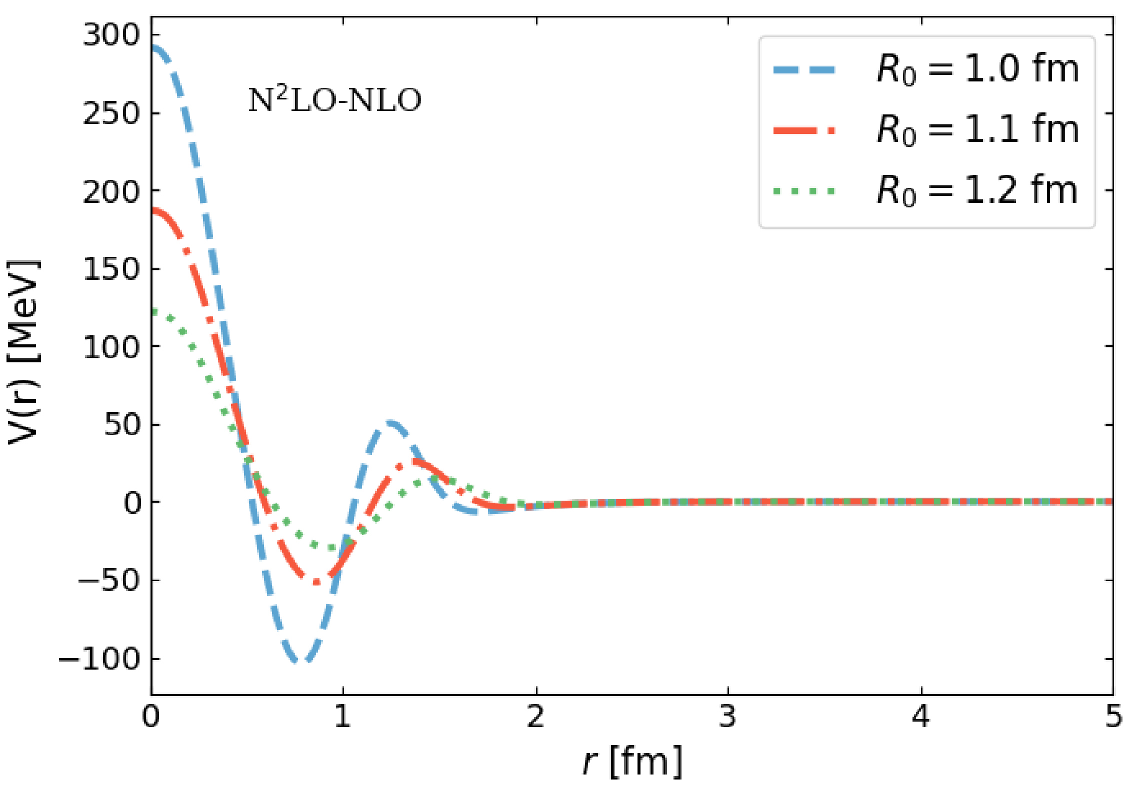
$$V_{\text{chiral}} = V^{(0)} + V^{(2)} + V^{(3)} + \cdots$$

66 Neutrons

$$V' = \text{N}^2\text{LO} - \text{NLO}$$

Coordinate Space Cutoff R_0

~ Potential Softness



[9] G. Palkanoglou, F. K. Diakonos, A. Gezerlis, Phys. Rev. C 102, 064324 (2020)

Second-Order Perturbation Theory in QMC

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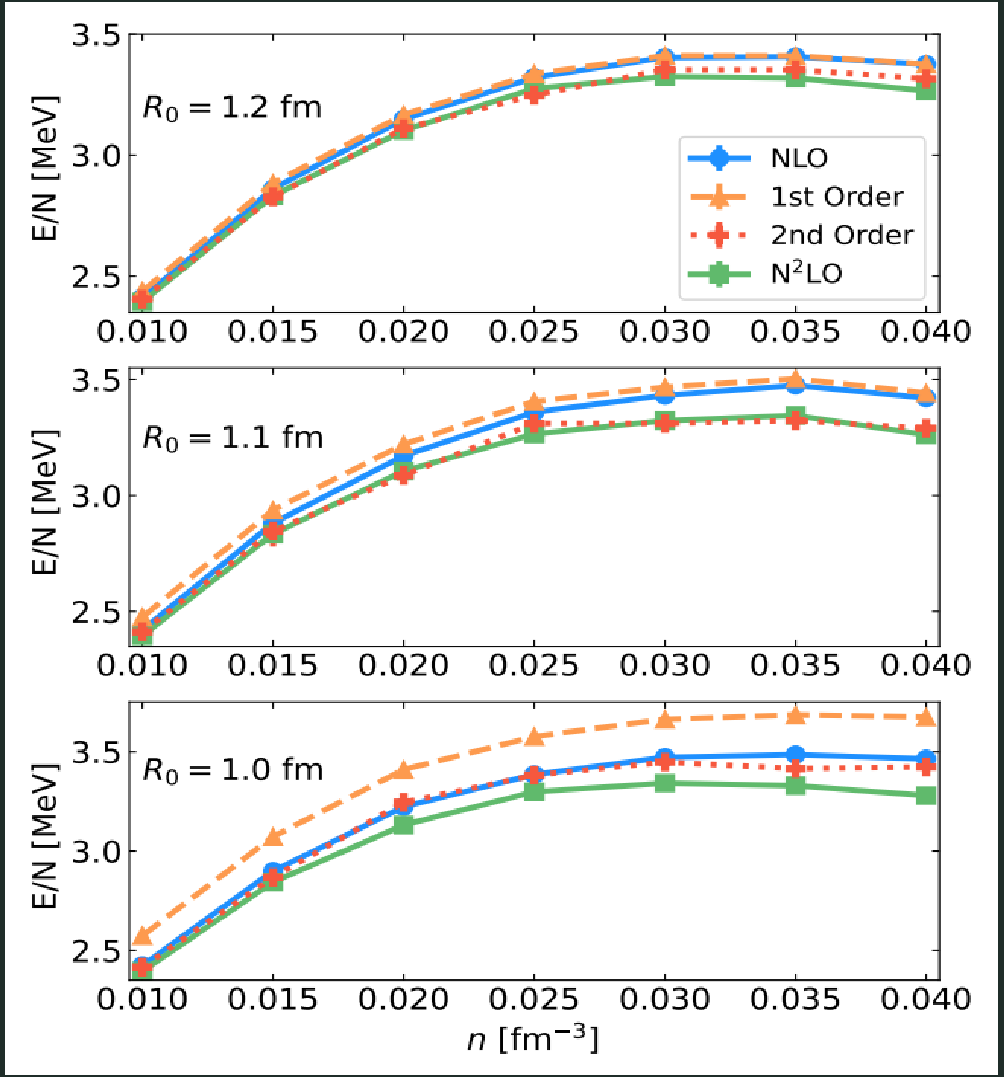
Testing Perturbativeness

- Easier to perturb from NLO to N^2LO with softer potentials.

- $R_0 = 1.1$ fm and 1.2 fm: $\leq 1\%$ difference between non-perturbative results and new results.

- Second-Order correction insufficient for hard core potentials.



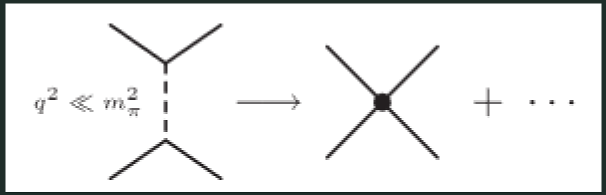
[8] R. Curry, J.E. Lynn, K.E. Schmidt, and A. Gezerlis, arxiv: 2302.07285 Nucl. Th.

Outlook & Summary

- Non-local operators (Spin, Isospin, etc) only treatable perturbatively in Diffusion Monte Carlo

- N^3LO potentials have terms that must be treated perturbatively.

- Pionful Chiral EFT vs Pionless EFT

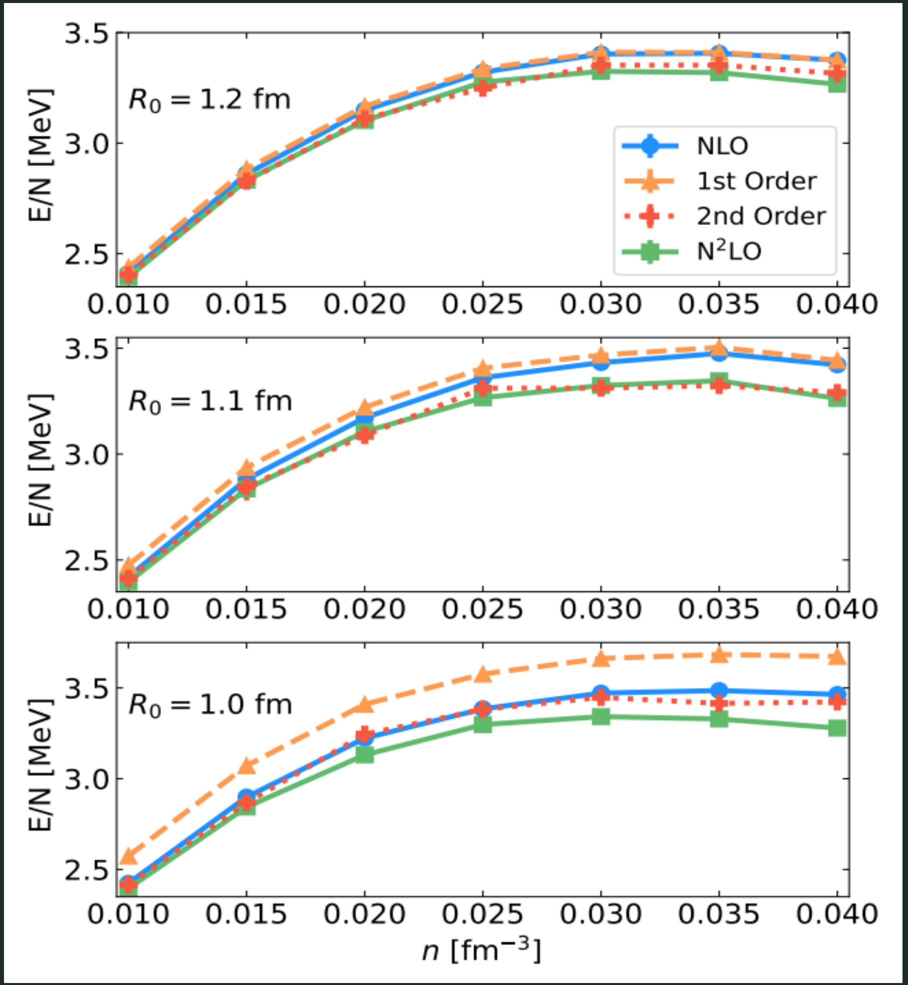


- Third-Order Corrections?

$$E_0^{(3)} = \sum_{k\neq 0}\sum_{m\neq 0} \frac{\langle\psi_0|V'|\psi_m\rangle\langle\psi_m|V'|\psi_k\rangle\langle\psi_k|V'|\psi_0\rangle}{(E_0 - E_m)(E_0 - E_k)} - \langle\psi_0|V'|\psi_0\rangle \sum_{m\neq 0} \frac{|\langle\psi_0|V'|\psi_m\rangle|^2}{(E_0 - E_m)^2}$$

Outlook & Summary

- Developed a new method for calculating Second-Order correction in *ab initio* many body context.
- First continuum Nuclear many-body calculations with Second-Order corrections
- Tested perturbativeness of modern chiral EFT potentials
- Hard core potentials need third-order corrections or higher. Cast doubt on perturbativeness of chiral EFT potentials.
- Exciting opportunities to probe nuclear many-body systems!



Thank you

Collaborators

Dr. Alexandros Gezerlis	**University of Guelph**
Dr. Joel E. Lynn	**Intitut für Kernphysik, Technische Universität Darmstadt**
Dr. Kevin Schmidt	**Arizona State University**

Funding / Computational Resources

NSERC CRSNG

SHARCNET™

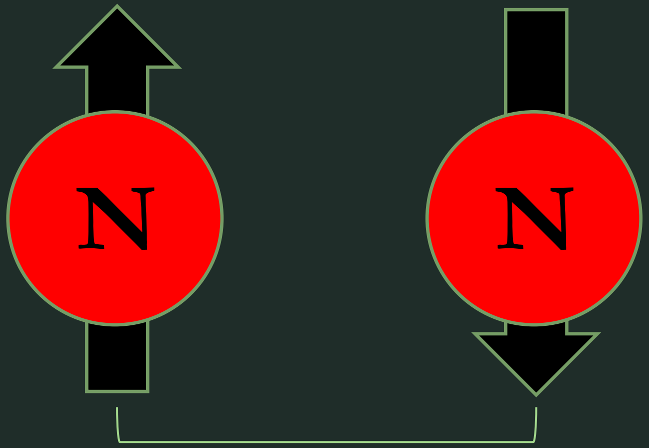
INNOVATION
Canada Foundation for Innovation
Fondation canadienne pour l'innovation

NERSC

Trial Wavefunction

$$\psi_T(R) = \left[\prod_{i<j} f(r_{ij})\right]\Phi(R)$$

- Symmetric correlation function $f(r)$
- Antisymmetric determinant Φ(R)

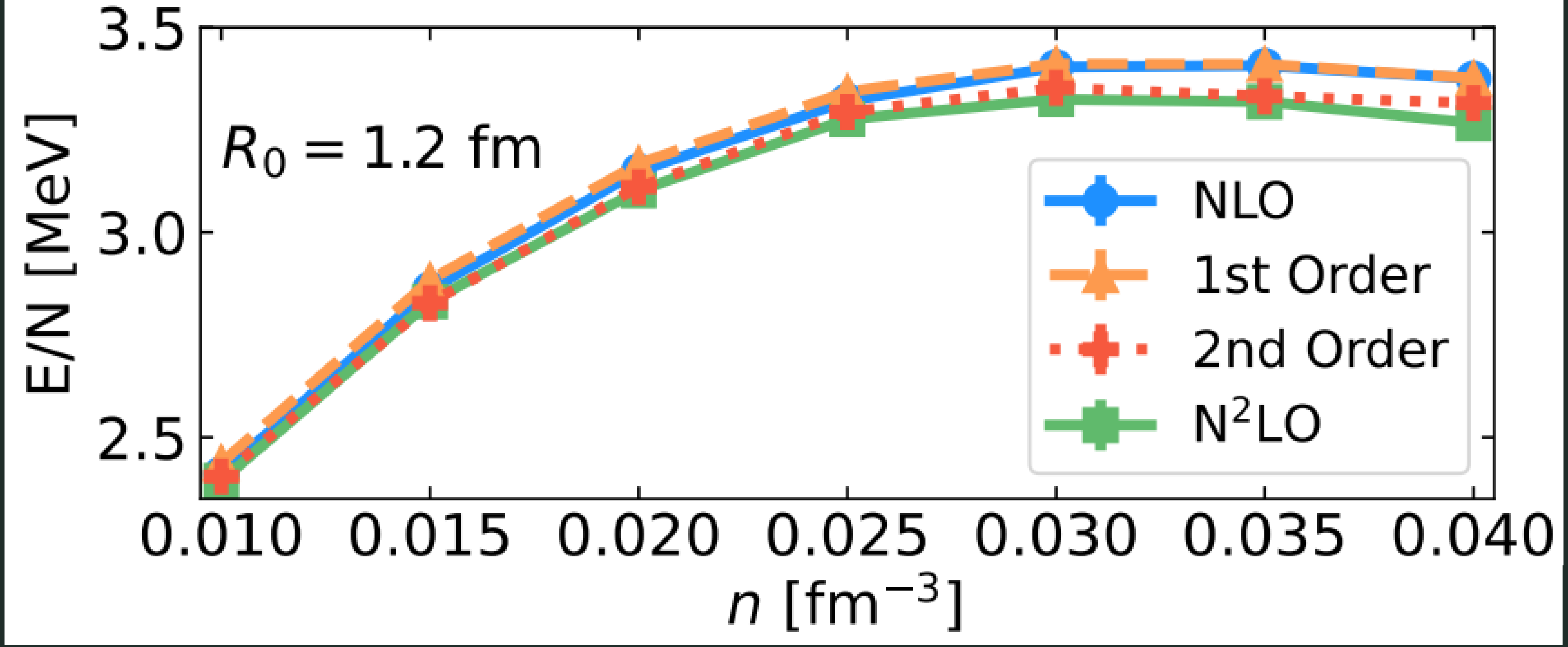


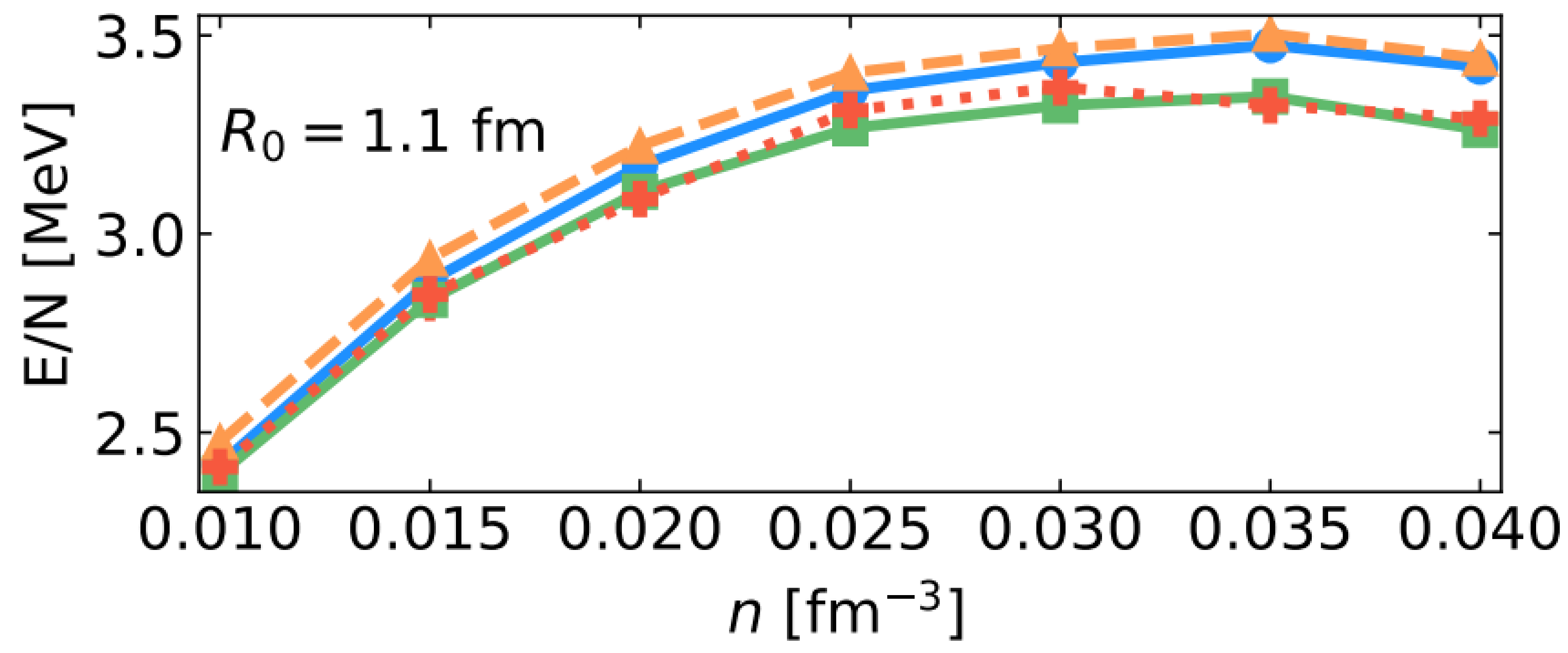
BCS Wavefunction

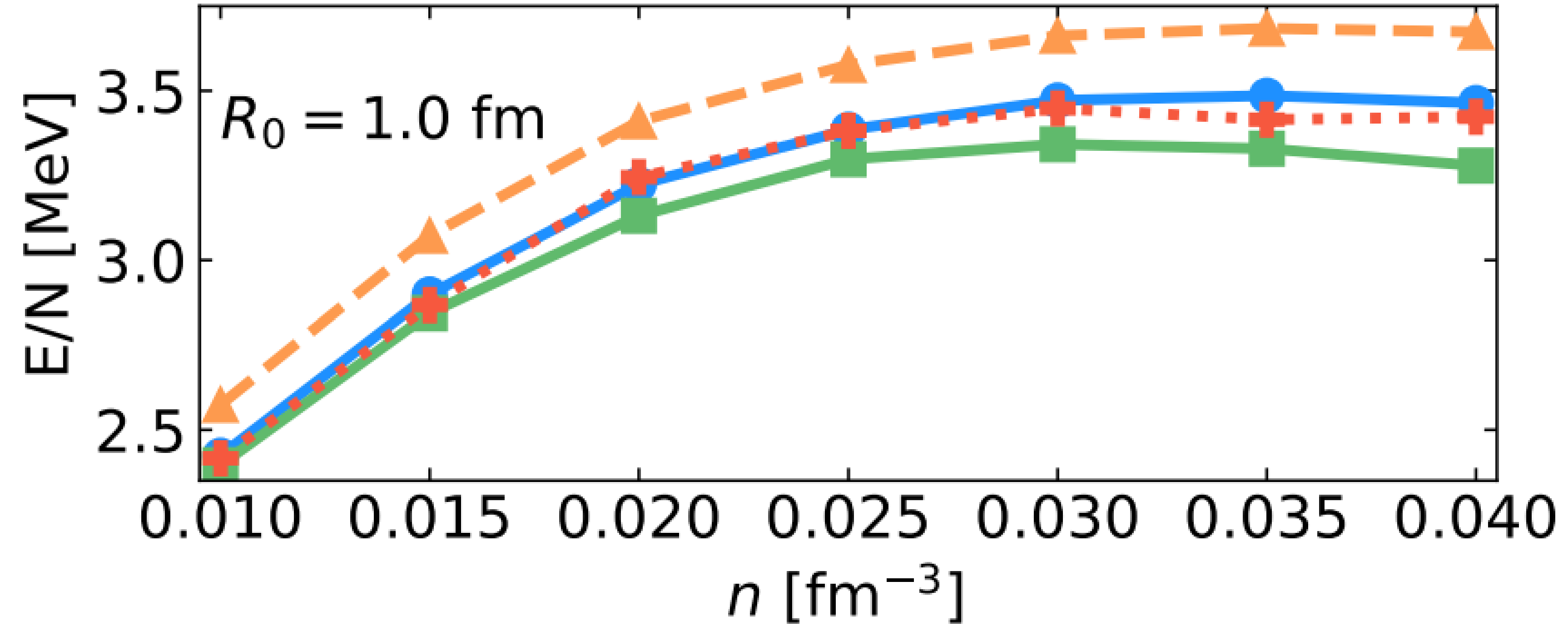
$$\Phi_{BCS} = \begin{vmatrix} \phi(r_{11'}) & \phi(r_{12'}) & \cdots & \phi\left(r_{1N'_\downarrow}\right) \\ \phi(r_{21'}) & \phi(r_{22'}) & \cdots & \phi\left(r_{2N'_\downarrow}\right) \\ \vdots & \vdots & \ddots & \vdots \\ \phi(r_{N_\uparrow 1'}) & \phi(r_{N_\uparrow 2'}) & \cdots & \phi\left(r_{N_\uparrow N'_\downarrow}\right) \end{vmatrix}$$

$$\phi(\vec{r}_{ij'}) = \sum_n \alpha_n e^{i\vec{k}_n\cdot\vec{r}_{ij'}} + \tilde{\beta}(r_{ij'})$$

[10] A. Gezerlis and J. Carlson, Phys. Rev. C. **81**, 025803 (2010)


$R_0 = 1.2$ fm
NLO
1st Order
2nd Order
N^{2}LO
E/N [MeV]
3.5
3.0
2.5
0.010
0.015
0.020
0.025
0.030
0.035
0.040
n [fm^{-3}]


$R_0 = 1.1$ fm
E/N [MeV]
3.5
3.0
2.5
0.010
0.015
0.020
0.025
0.030
0.035
0.040
n [fm^{-3}]


$R_0 = 1.0$ fm
E/N [MeV]
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n [fm^{-3}]