How to consistently use modern nuclear forces in an *ab initio* technique

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- Submitted to PRL

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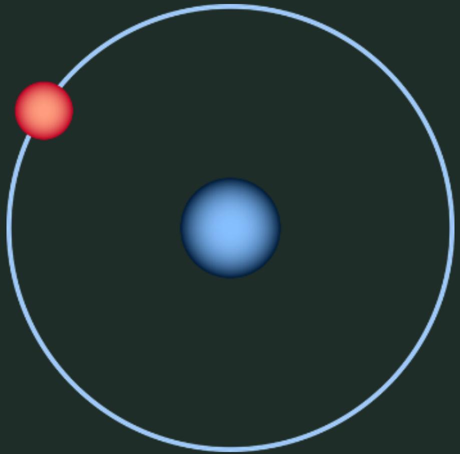
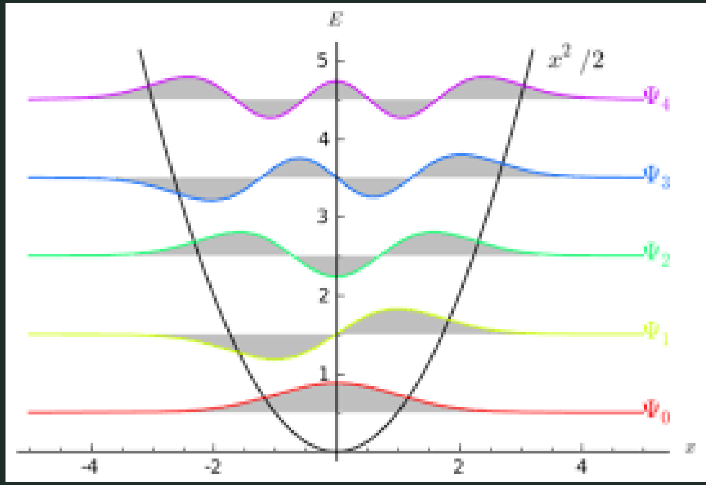
Nuclear Many-Body Problem

- Schrodinger Equation

$$H\Psi = E\Psi$$

- Analytically solvable for few idealized systems





- Realistic systems cannot be solved analytically

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

Neutron Stars

Second-Order Correction in QMC Calculations

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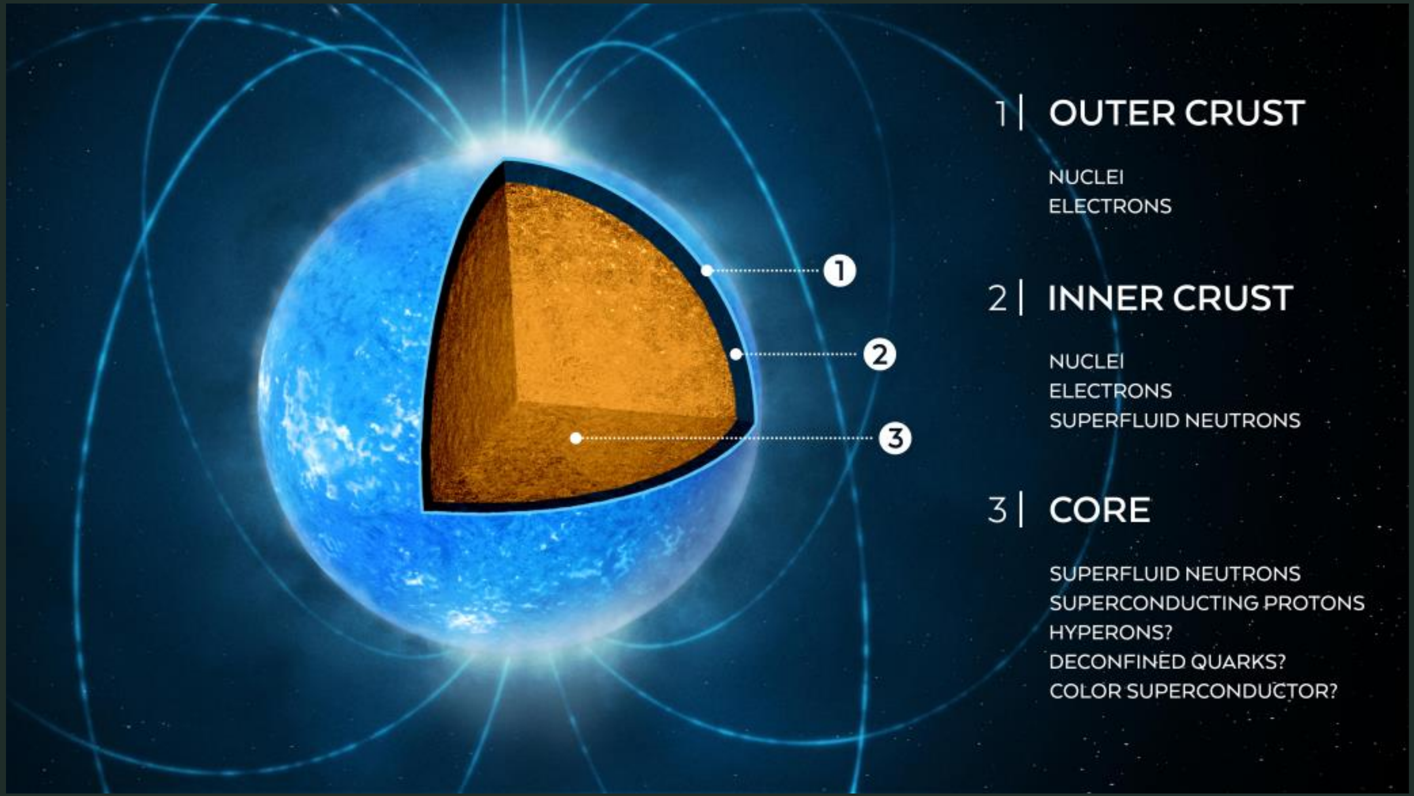
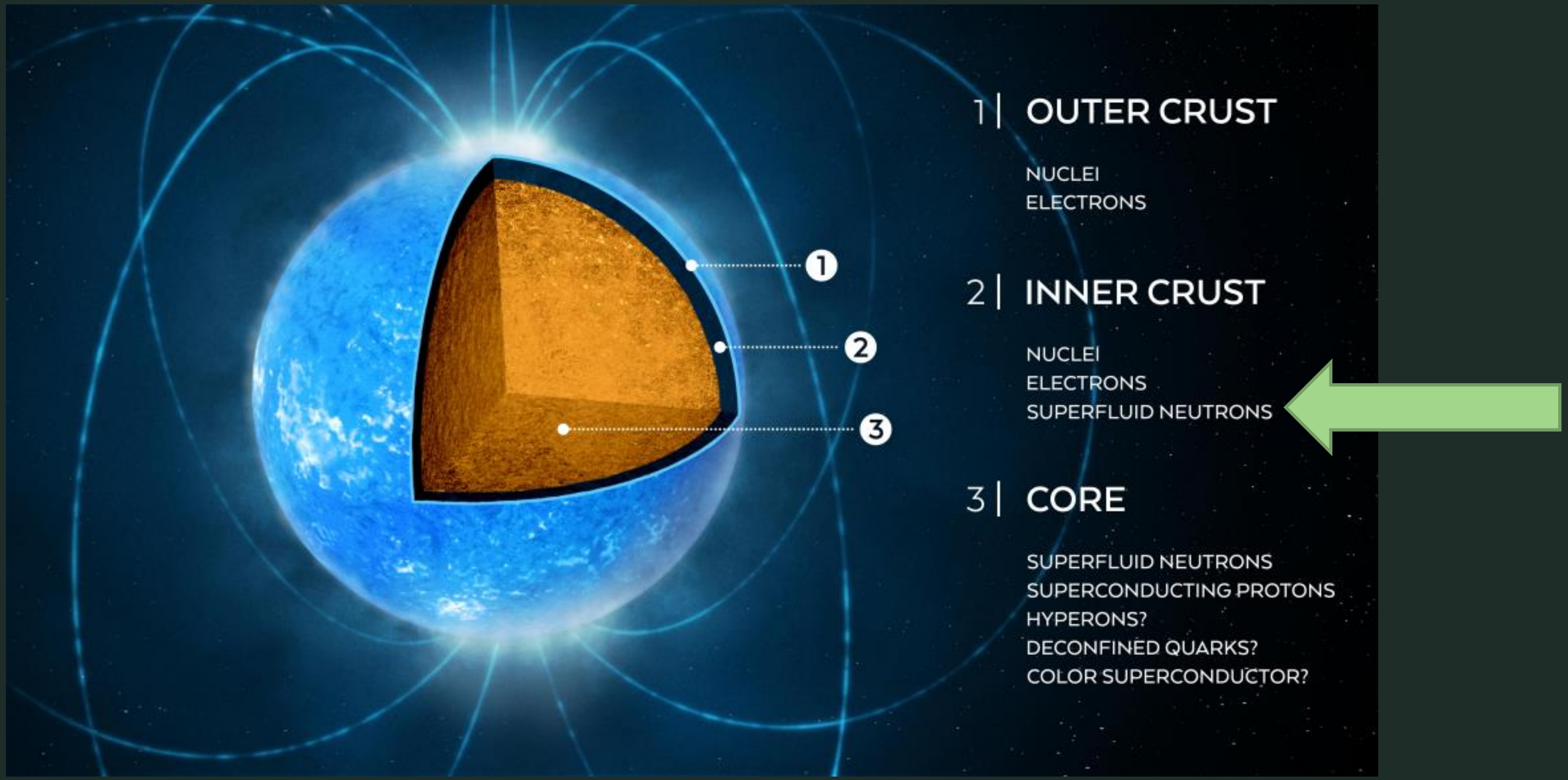


- From Anna L. Watts

Neutron Stars



- From Anna L. Watts

- Pure infinite neutron matter
- S-wave interactions

Nucleon-Nucleon Interaction

Second-Order Correction in QMC Calculations

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The Nuclear Many-Body Problem

Perturbation Theory

Quantum Monte Carlo

Second-Order Correction

Perturbing between simple systems

Testing perturbativeness

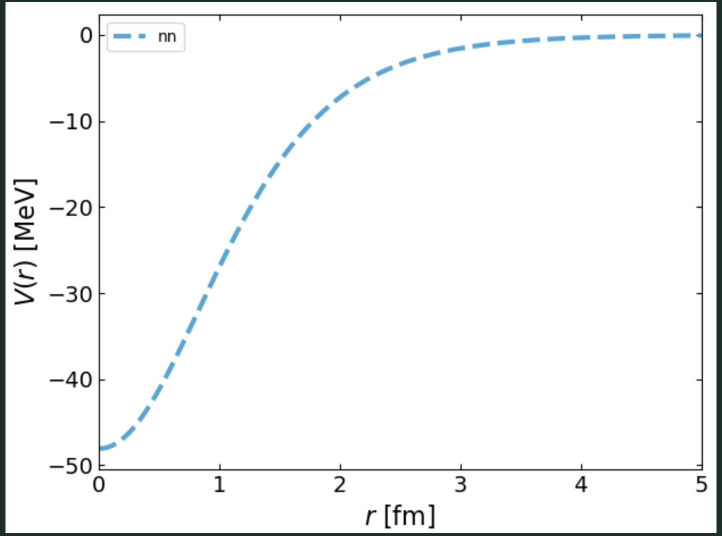
- Fully described by Quantum Chromodynamics (QCD)

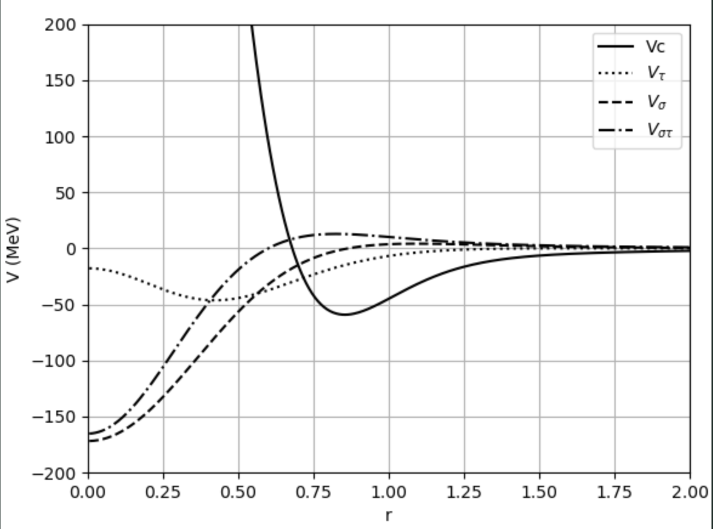
- Pöschl-Teller
  - Effective Range Expansion

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

- Argonne Group AV18
  - Operator Structure

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





[3]

[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 Correction in QMC Calculations

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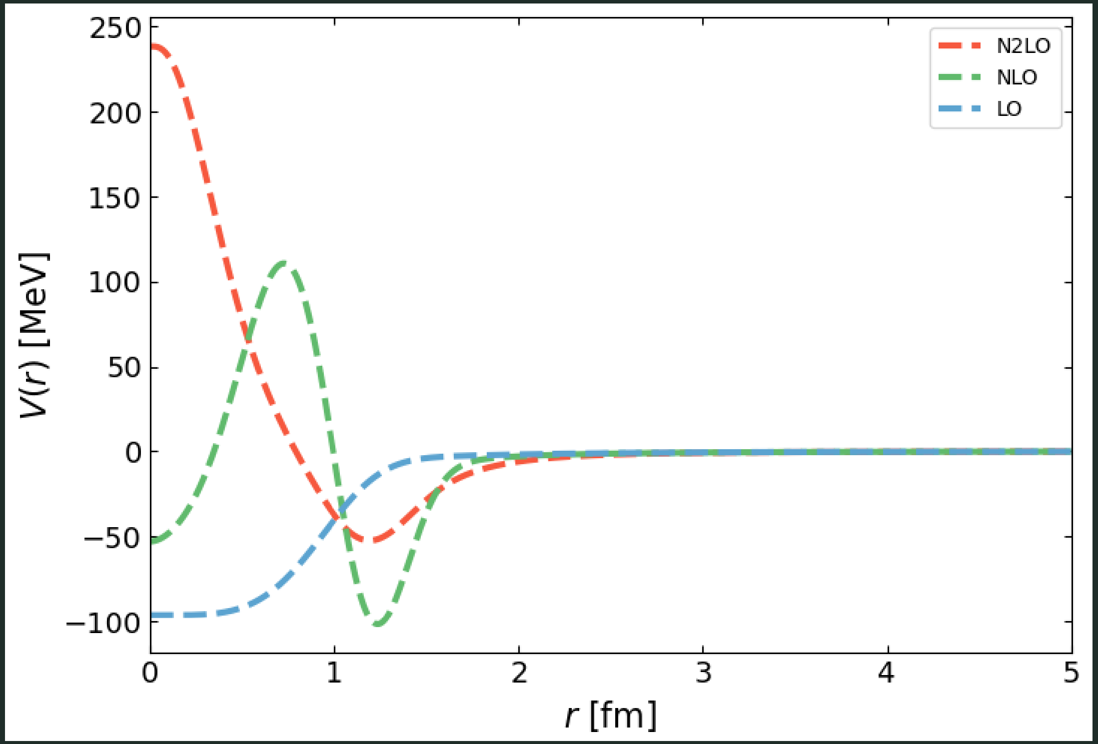
- Modern Nuclear Potentials

- Chiral Effective Field Theory
  - Power Counting
  - Respects Symmetries of QCD

- Expansion in powers of Q/Λ_b

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

LO NLO N^2LO



[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).

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

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

$$i \frac{\partial}{\partial t} \psi = \hat{H} \psi \xrightarrow{\tau = it} -\frac{\partial}{\partial \tau} \psi = \hat{H} \psi$$

[7] W.M.C. Foulkes, *et al.* Rev. Mod. Phys. **73**, 1 (2001).

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

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

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

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

Second-Order Correction

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

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

Second-Order Correction

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

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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

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

Second-Order Correction

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

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

Second-Order Correction

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

0 as $\tau \to \infty$

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

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

Second-Order Correction

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

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

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

Few Body Tests

Second-Order Correction in QMC Calculations

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The Nuclear Many-Body Problem

Perturbation Theory

Quantum Monte Carlo

Second-Order Correction

Perturbing between simple systems

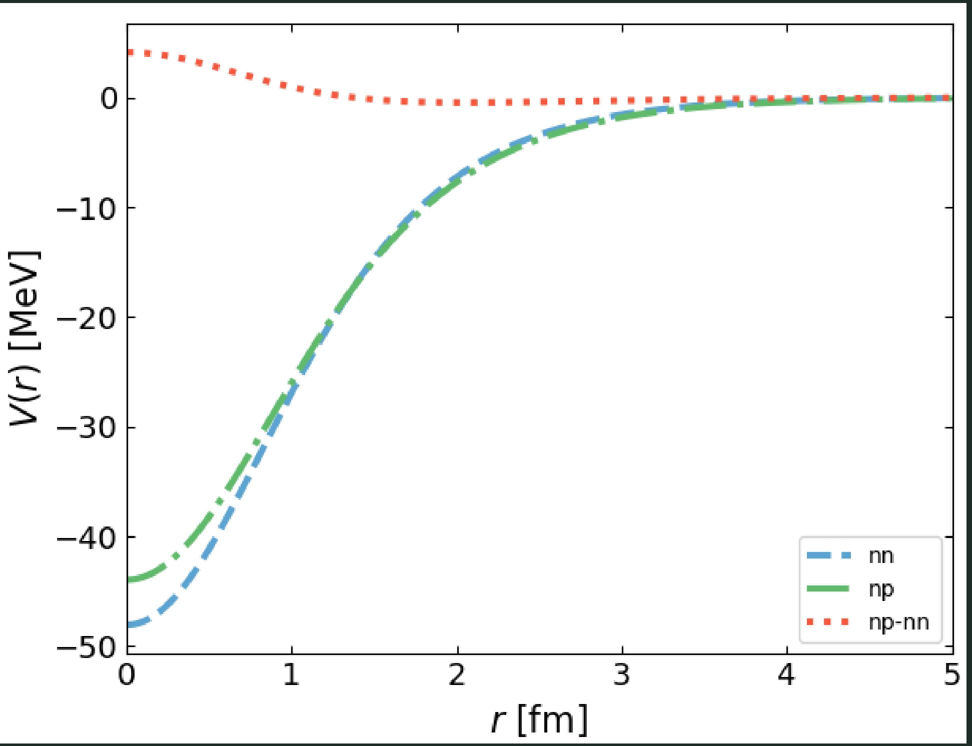
Testing perturbativeness

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

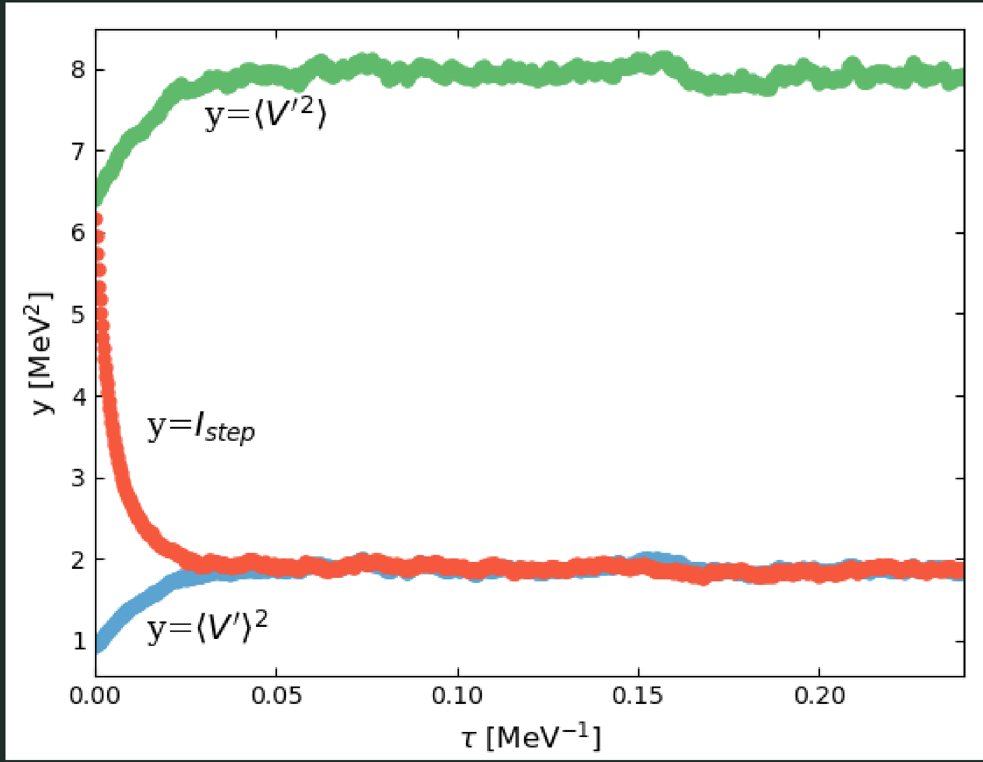
Neutron-Proton: $a_0 = -23.75$ fm, $r_e = 2.81$ fm



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

Few Body Tests

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



N	ω	$E^{[0]}$	$E^{[1]}$	$E^{[2]}$	Non-Pt.
2	1	2.57335(7)	2.58457(8)	2.58437(8)	2.58427(6)
4	1	6.5582(4)	6.5876(4)	6.5865(4)	6.5866(4)
6	1	10.0465(4)	10.0898(4)	10.0885(6)	10.0876(4)

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

Few Body Tests

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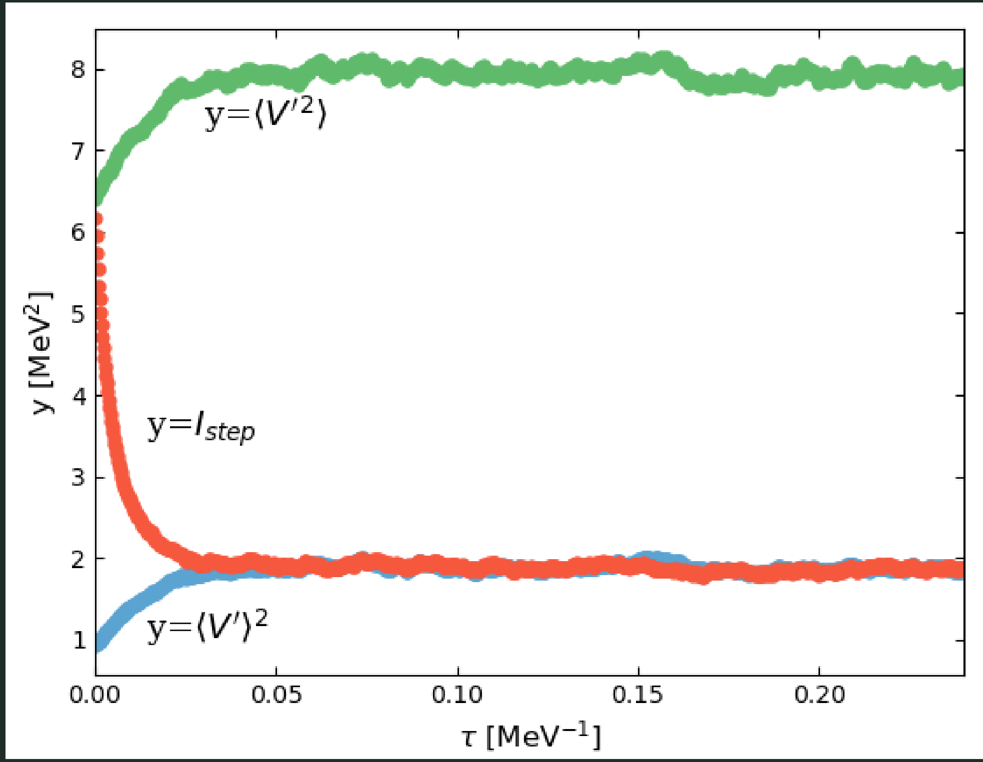
Fit → $$I(\mathcal{T}) = \int_0^{\mathcal{T}} d\tau \, |\langle\psi_0|V'|\psi_0\rangle|^2 + \sum_{k\neq 0}^{\infty} \int_0^{\mathcal{T}} e^{-[E_k - E_0]\tau} \, |\langle\psi_k|V'|\psi_0\rangle|^2$$



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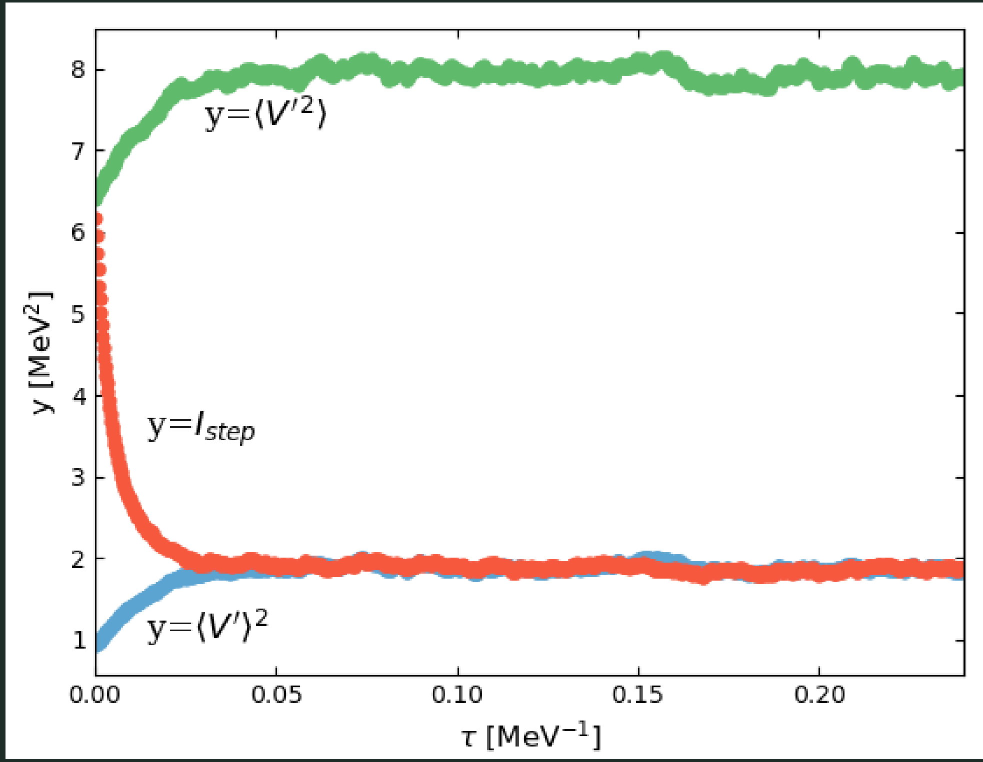
Few Body Tests



Neutron-Neutron

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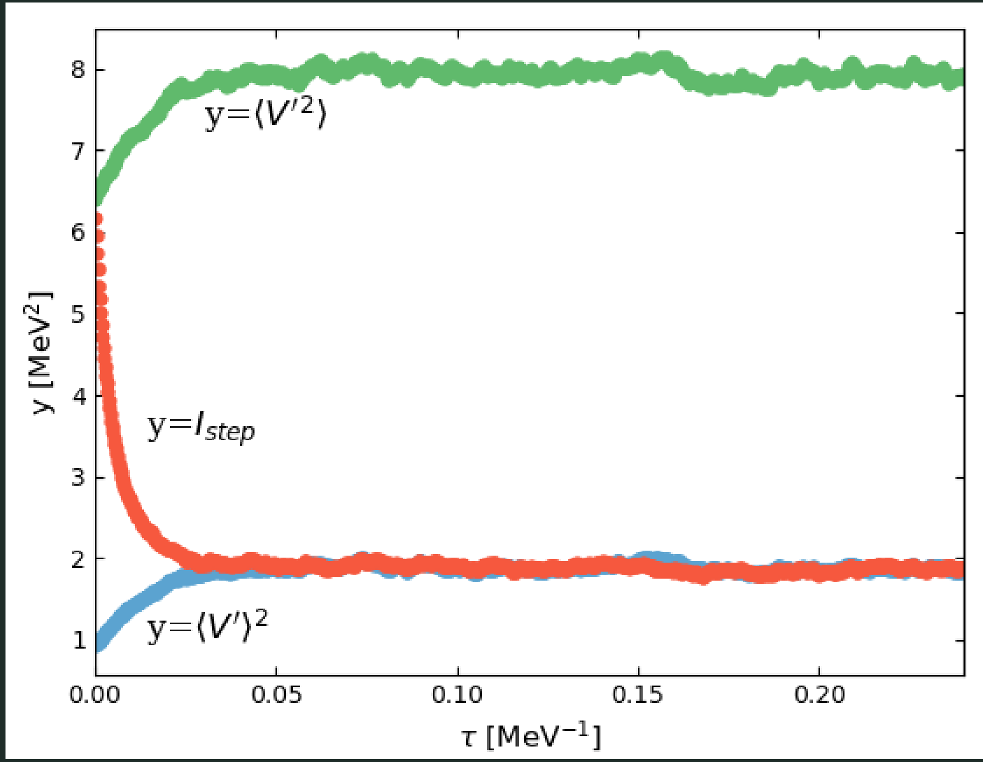
Neutron-Proton

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

Few Body Tests



First Order

N	ω	$E^{[0]}$	$E^{[1]}$	$E^{[2]}$	Non-Pt.
2	1	2.57335(7)	2.58457(8)	2.58437(8)	2.58427(6)
4	1	6.5582(4)	6.5876(4)	6.5865(4)	6.5866(4)
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Neutron-Proton

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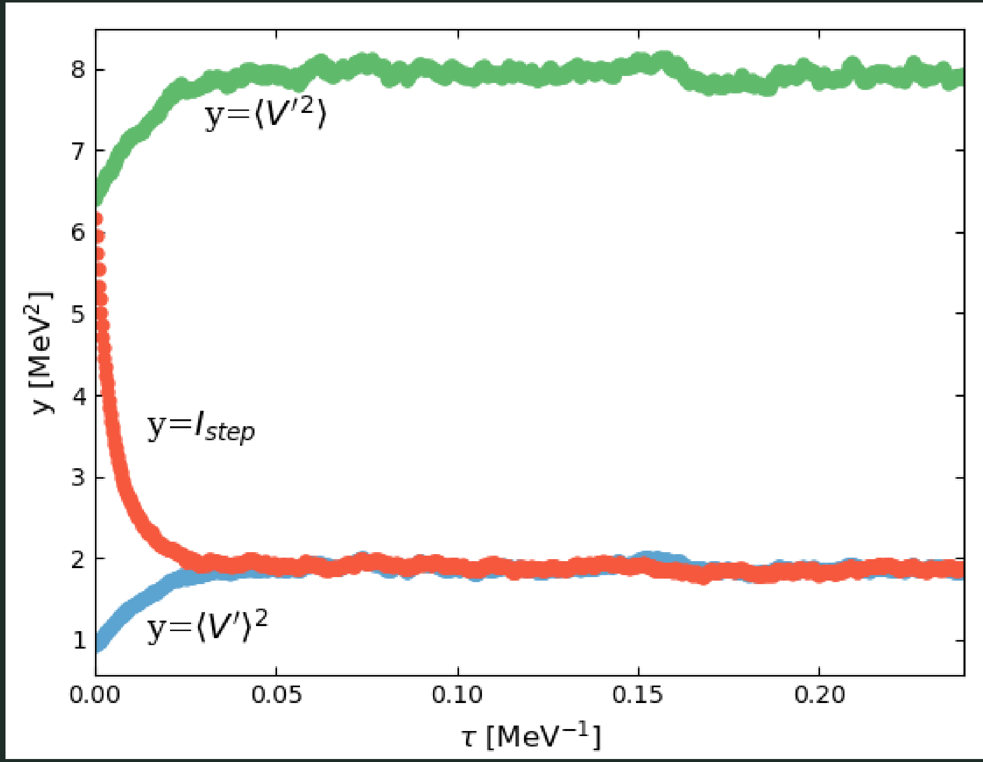

Second Order

N	ω	$E^{[0]}$	$E^{[1]}$	$E^{[2]}$	Non-Pt.
2	1	2.57335(7)	2.58457(8)	2.58437(8)	2.58427(6)
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Neutron-Proton

$< 1\sigma$ difference

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

Testing Perturbativeness

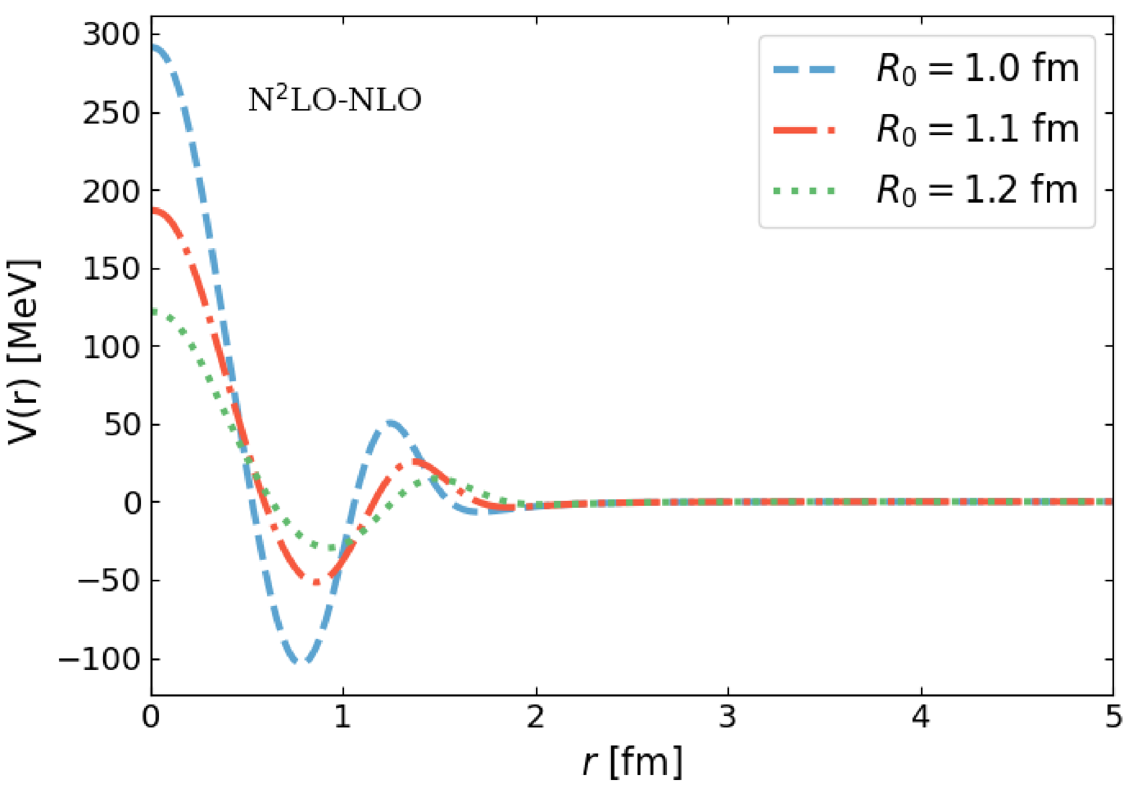
$$V_{\text{chiral}} = V^{(0)} + V^{(2)} + V^{(3)} + \cdots$$

LO NLO N^{2}LO

66 Neutrons

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

Coordinate Space Cutoff R_0
~ Potential Softness



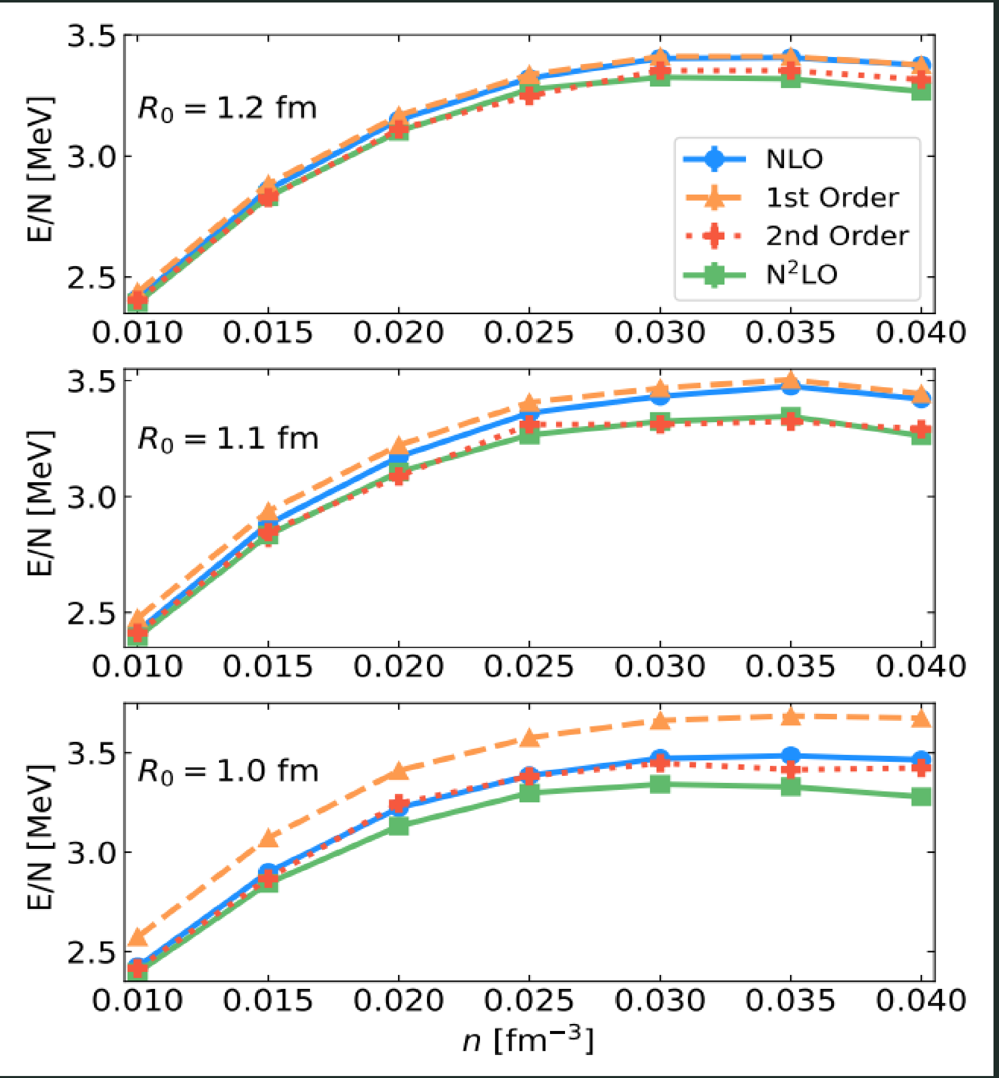
[9] G. Palkanoglou, F. K. Diakonos, A. Gezerlis, Phys. Rev. C 102, 064324 (2020)

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.

Summary & Outlook

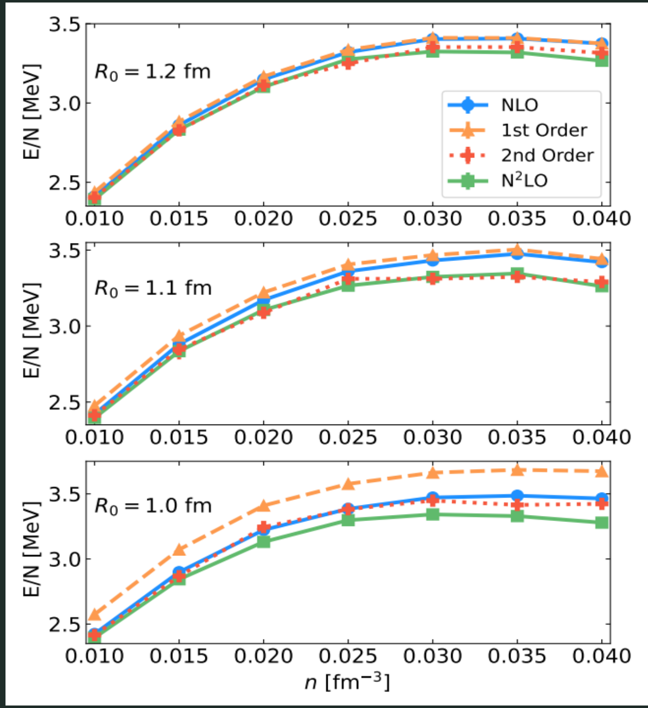
- Developed a new method for calculating Second-Order correction in *ab initio* many body context.

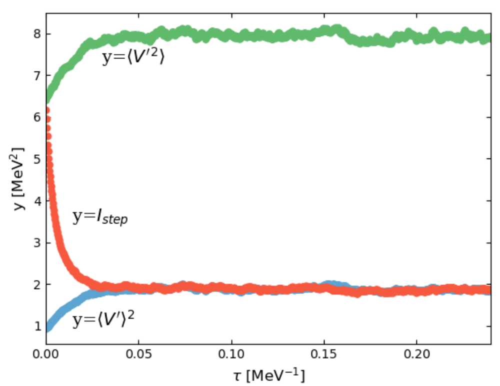
- First continuum Nuclear many-body calculations with Second-Order corrections

- First many-body tests of perturbativeness for modern chiral EFT potentials

- Hard core potentials need third-order corrections or higher. Cast doubt on perturbativeness of chiral EFT potentials.

- Widely applicable to anyone using DMC or extensions (e.g. AFDMC, GFMC, etc)





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

Second-Order Correction

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

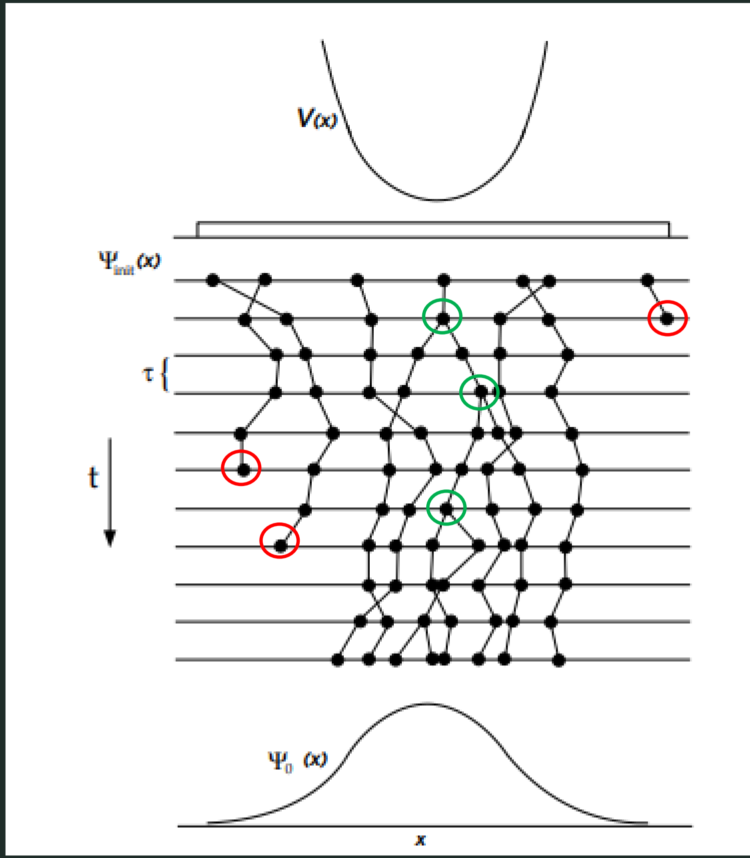
$$I(\mathcal{T}) = \int_o^{\mathcal{T}} \langle \psi_0 \, | V' e^{-[H_0 - E_0]} \sum_{k=0}^{\infty} |\psi_k\rangle \langle \psi_k | V' | \psi_0 \rangle$$

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

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

Diffusion Monte Carlo

$$i\frac{\partial}{\partial t}\psi = \left(-\frac{1}{2}\nabla^2 + V\right)\psi \longrightarrow -\frac{\partial}{\partial \tau}\psi = \left(-\frac{\hbar}{2m}\nabla^2 + V\right)\psi$$



[7]

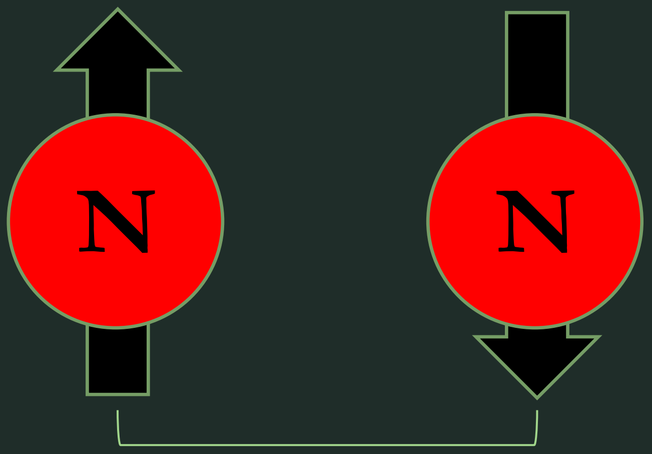
$$-\frac{\partial}{\partial \tau}\psi = \left(-\frac{\hbar}{2m}\nabla^2 + V\right)\psi$$ Diffusion

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

Trial Wavefunction

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

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

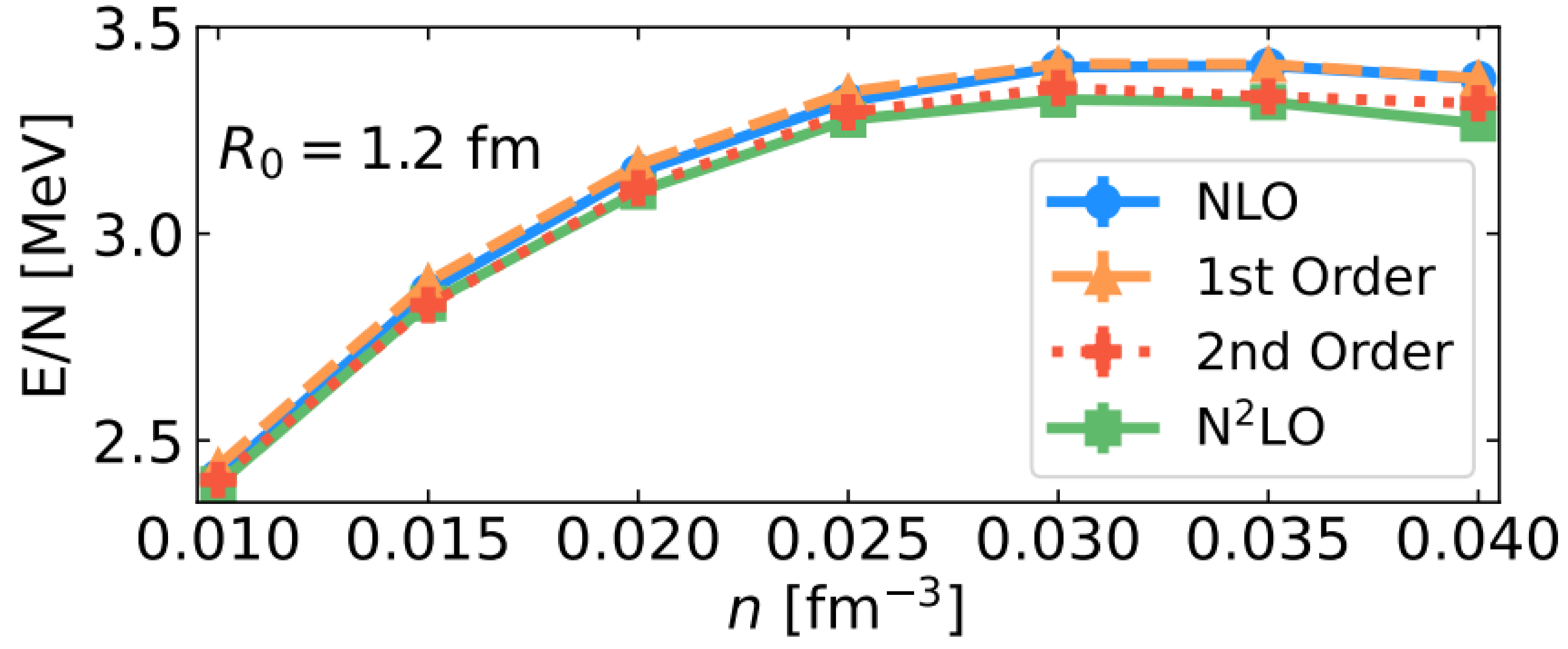


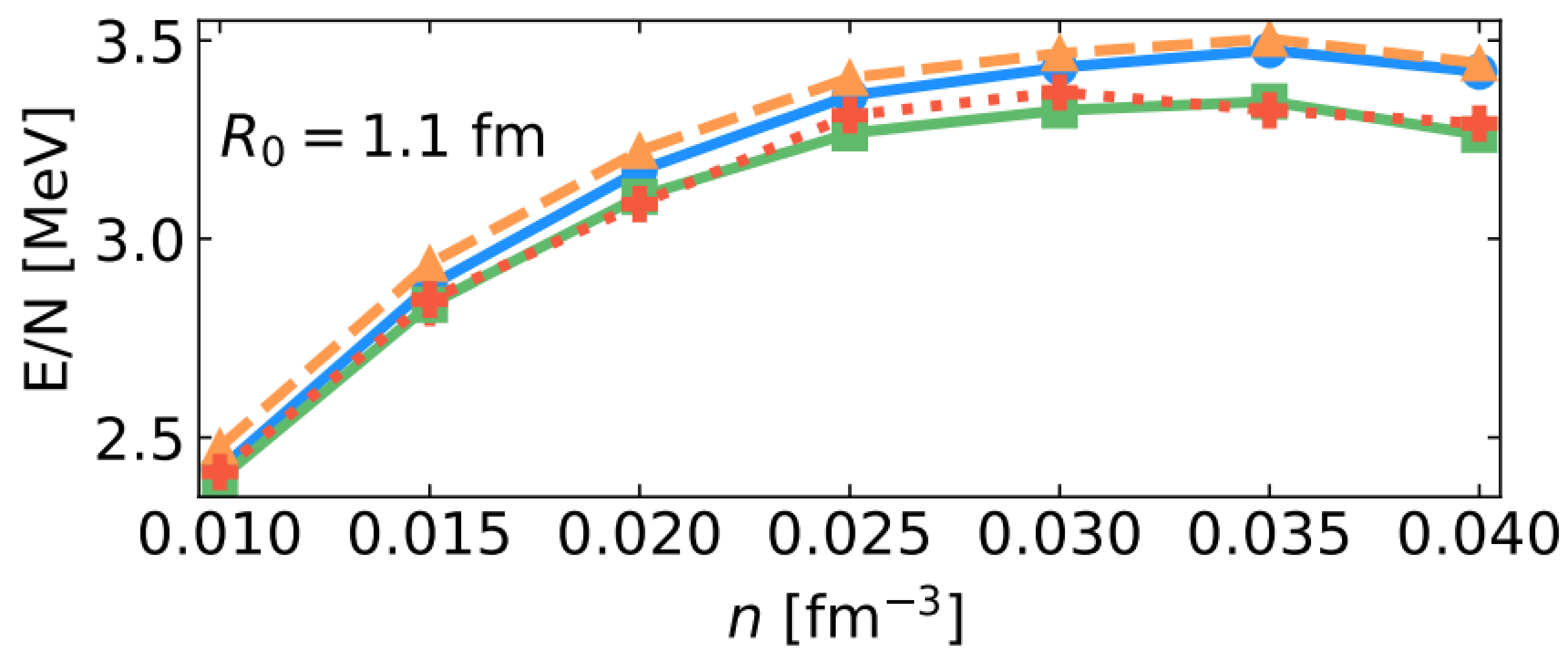
BCS Wavefunction

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

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

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


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


3.5
3.0
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E/N [MeV]
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0.010
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Second-Order Correction in QMC Calculations

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