The Nuclear Many-Body Problem

Quantum Monte Carlo

Second-Order Perturbation in Diffusion Monte Carlo

Current Work

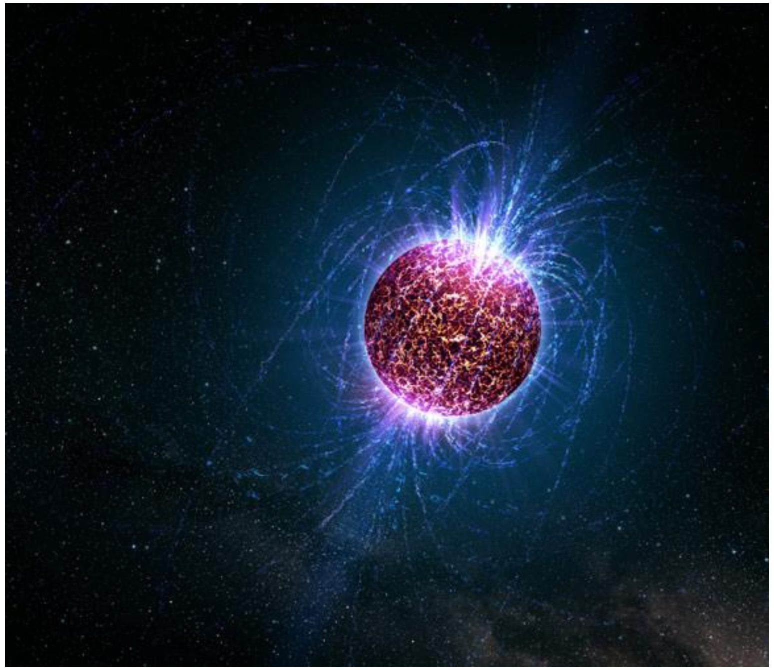
Probing the nuclear many-body problem with quantum Monte Carlo

Ryan Curry

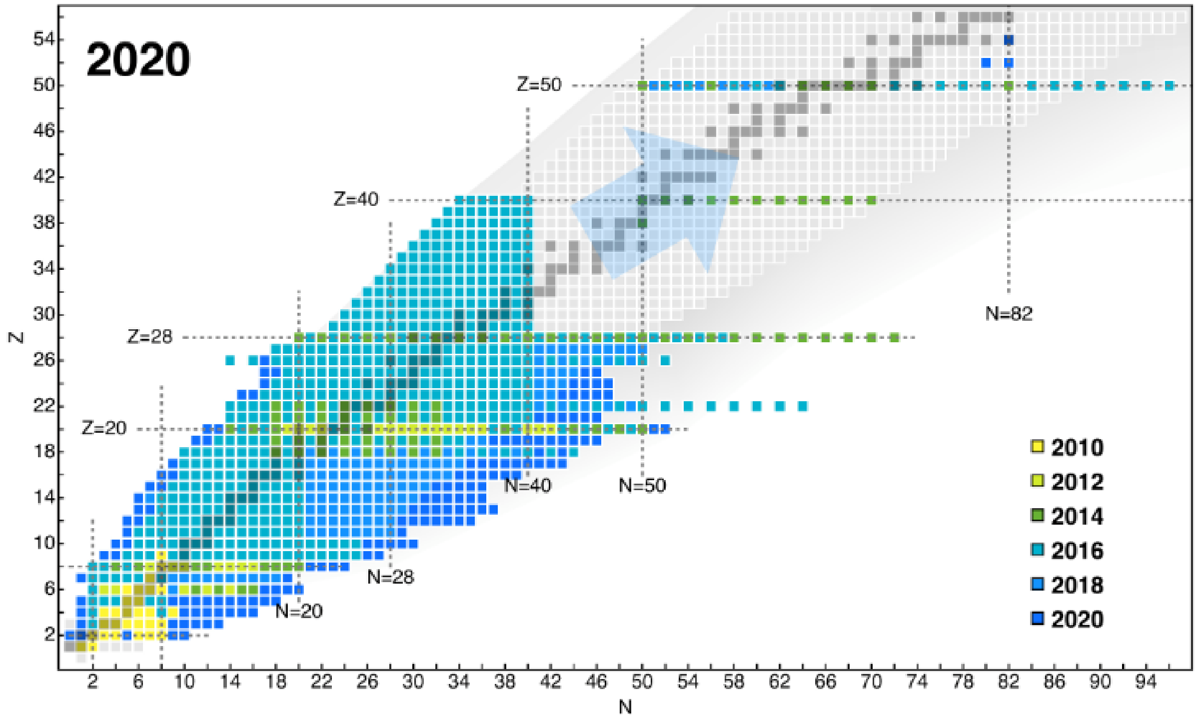
2024 CAP Congress
@ Western University
London, ON
2024-05-28

Nuclear Systems

Neutron stars



Nuclei



Nuclear Systems

Perturbing the Envelope

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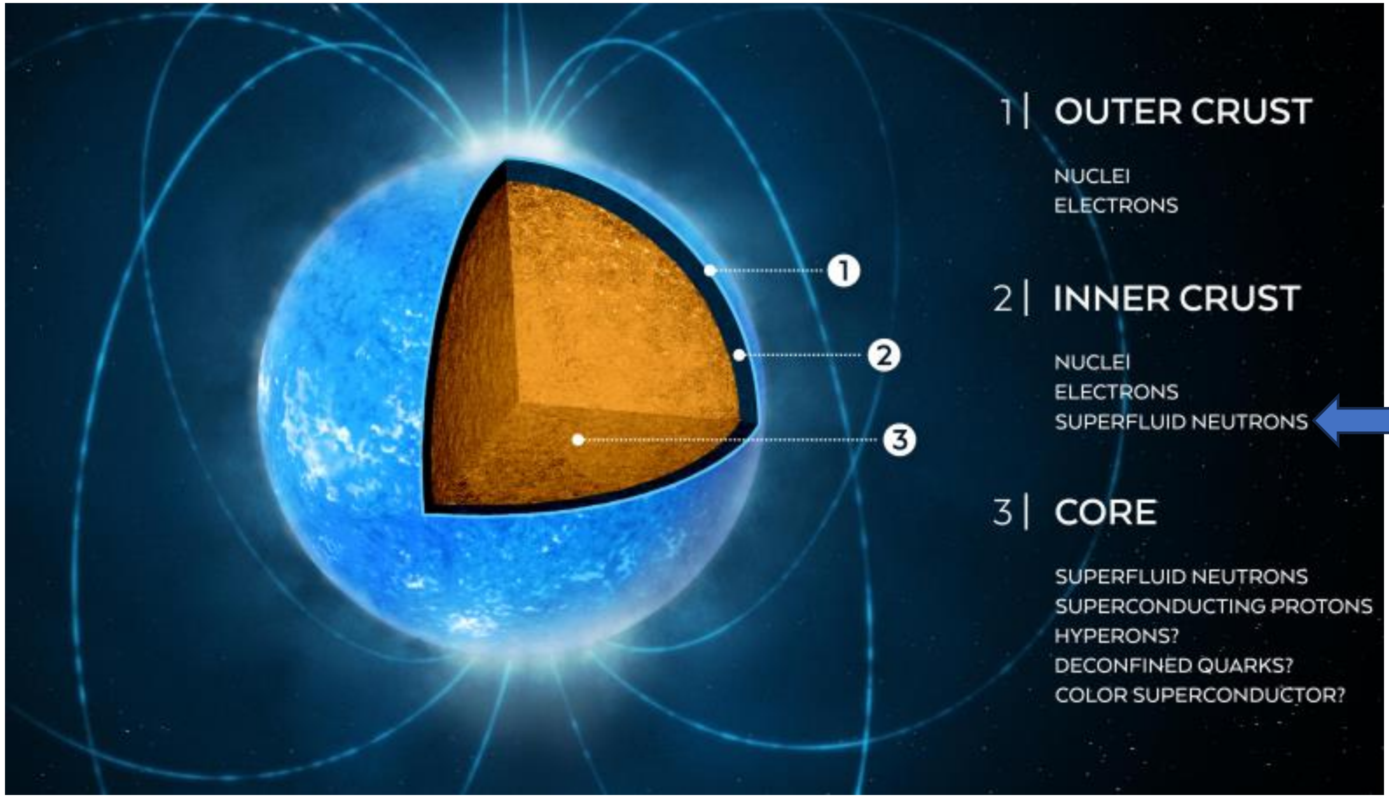


- From Anna L. Watts

- Radii $\approx 10 - 15$ km
- Masses $\approx 1.4\, M_{\odot} \leq 2.6 M_{\odot}$

- Pure infinite neutron matter
- S-wave interactions

- Many-body calculations of ground state inform EOS

Nuclear Many-Body Problem

Accurate description of the nuclear interaction + **Powerful computational approaches**

- Effective Range Expansion
- Argonne V18
  - Fit to Experimental Data
- Chiral EFT Interactions
  - Related to underlying theory (QCD)

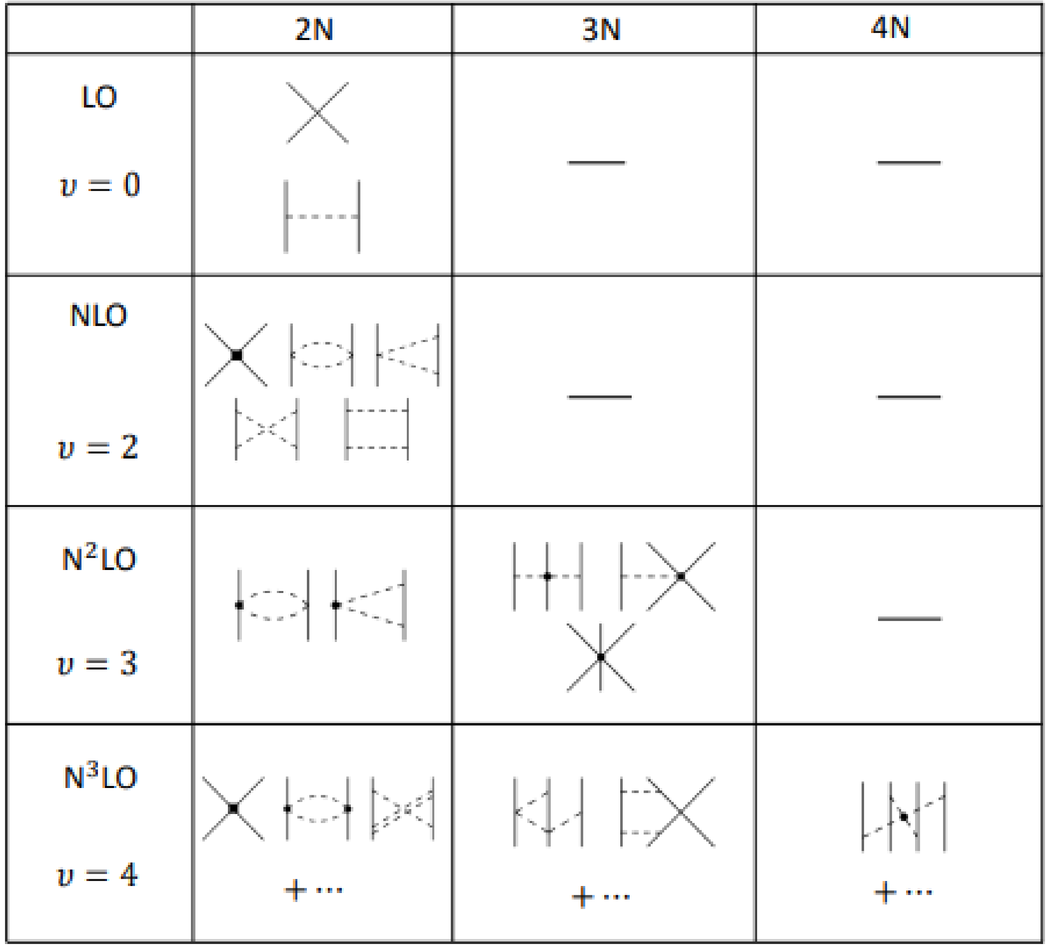
Phenomenology:

- Hartree-Fock (& extensions)
- BCS Theory
- Nuclear Shell Model
- Energy Density Functionals

Ab Initio:

- Exact Diagonalization
- Quantum Monte Carlo
- Many-Body Perturbation Theory
- Coupled Cluster
- In-Medium Similarity Renormalization Group
- Self-Consistent Green's Functions

Modern Nuclear Potentials



- Chiral Effective Field Theory
  - Expansion in powers in Q/Λ_b
  - Respects symmetries of QCD
  - Separation of scales quarks vs nucleons and pions
  - Power Counting
  - Many-body forces emerge naturally

S. Weinberg, Phys. Lett. B, **251**, 288 (1990).
U. van Kolck, Phys. Rev. C, **49**, 2932, (1994)
E. Epelbaum, H.-W. Hammer, Ulf-G. Meissner, Rev. Mod. Phys. **81**, 1773 (2009).

Local Chiral EFT

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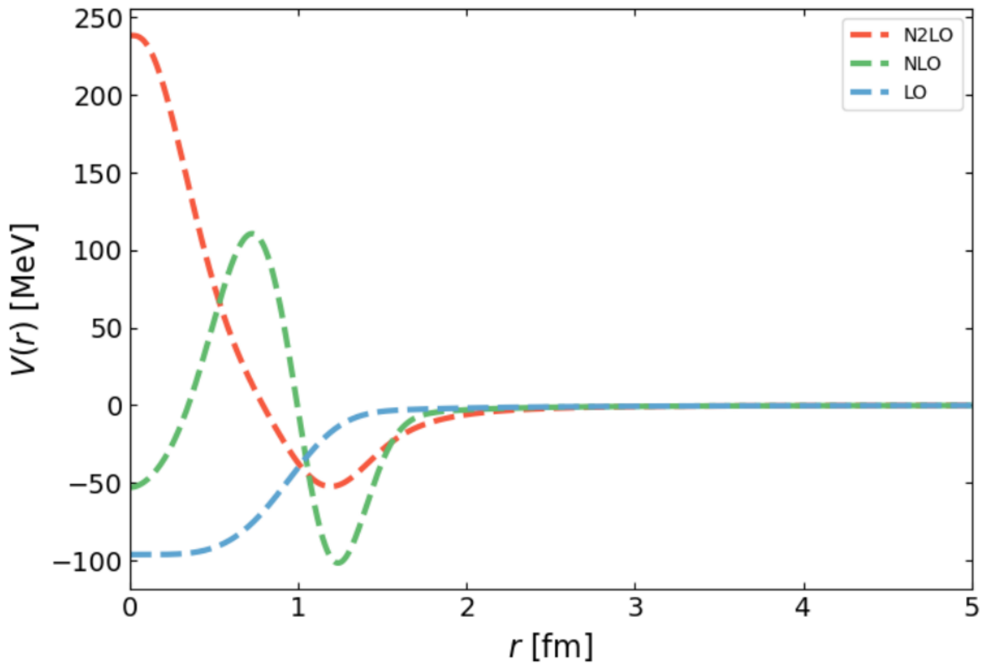
Current Work

- Use only half, recover the rest through anti-symmetrization.

- Only S-wave interactions (for now)



$$V^{(0)} = \alpha_1 + \alpha_2 \boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2 + \alpha_3 \boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2 + \alpha_4 \boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2 \boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2$$

$$\begin{aligned} V^{(2)} = {} & \gamma_1 q^2 + \gamma_2 q^2 \boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2 + \gamma_3 q^2 \boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2 \\ & + \gamma_4 q^2 \boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2 \boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2 \\ & + \gamma_5 k^2 + \gamma_6 k^2 \boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2 + \gamma_7 k^2 \boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2 \\ & + \gamma_8 k^2 \boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2\, \boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2 + \gamma_9 k^2 (\boldsymbol{\sigma}_1 + \boldsymbol{\sigma}_2)(\boldsymbol{q} \times \boldsymbol{k}) \\ & + \gamma_{10} k^2 (\boldsymbol{\sigma}_1 + \boldsymbol{\sigma}_2)(\boldsymbol{q} \times \boldsymbol{k})\, \boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2 + \gamma_{11} (\boldsymbol{\sigma}_1 \cdot \boldsymbol{q})\, (\boldsymbol{\sigma}_2 \cdot \boldsymbol{q}) \\ & + \gamma_{12} (\boldsymbol{\sigma}_1 \cdot \boldsymbol{q})\, (\boldsymbol{\sigma}_2 \cdot \boldsymbol{q}) \boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2 + \gamma_{13} (\boldsymbol{\sigma}_1 \cdot \boldsymbol{k})\, (\boldsymbol{\sigma}_2 \cdot \boldsymbol{k}) \\ & + \gamma_{14} (\boldsymbol{\sigma}_1 \cdot \boldsymbol{k})\, (\boldsymbol{\sigma}_2 \cdot \boldsymbol{k}) \boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2 \end{aligned}$$

Fourier Transform
$q \rightarrow r$ local
$k \rightarrow \nabla$ non-local

Non-local terms must be treated perturbatively in QMC!

A. Gezerlis *et al,* Phys. Rev. C, **90**, 054323 (2014)

Continuum Quantum Monte Carlo

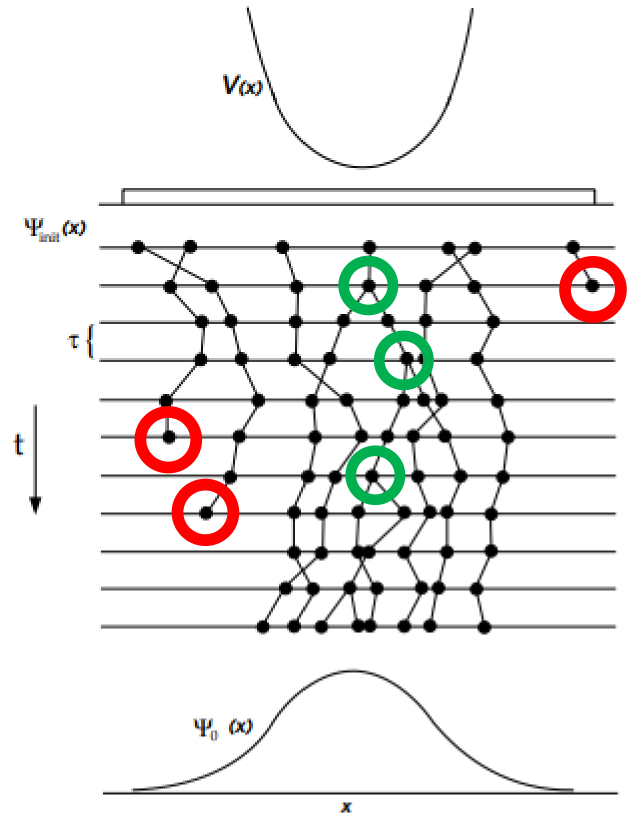
- Marry stochastic integration with quantum mechanics to probe the Quantum Many-Body problem

- Variational Monte Carlo
  Variational principle from QM
- Diffusion Monte Carlo
  Imaginary time evolution
- Green's Function Monte Carlo
  Imaginary time evolution with sums over spin states
- Auxiliary Field Diffusion Monte Carlo
  Imaginary time, Auxiliary fields to handle complicated interactions
- Path Integral Monte Carlo
  Path integral formalism, forward and backward walking
- …

Diffusion Monte Carlo

- Schrödinger equation in imaginary time

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



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

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

W. Foulkes, L. Mitas, R. Needs, G. Rajagopal, Rev. Mod. Phys., **73,** 33 (2001).

Diffusion Monte Carlo

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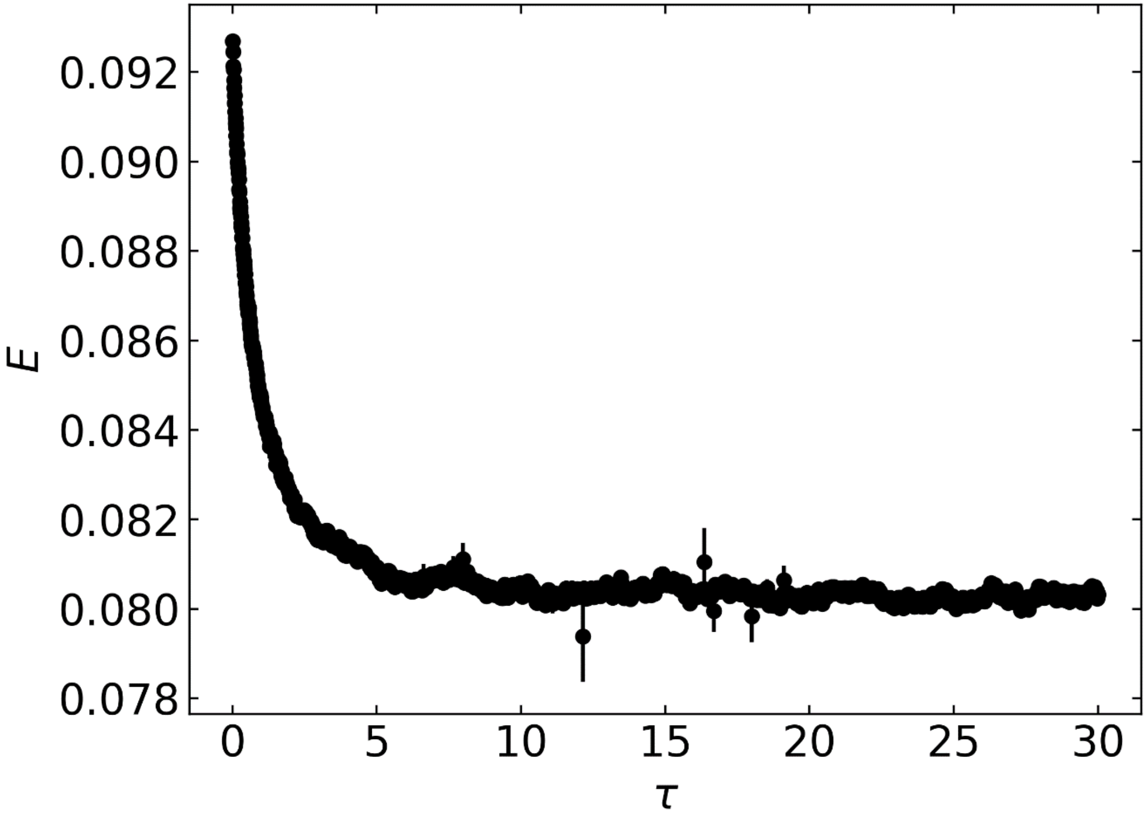
Current Work

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

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

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



The Goal?

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Current Work

What do we have?

- A perturbative nuclear interaction (Chiral EFT)
- A non-perturbative many-body method (QMC)

What would we like to have?

A technique to fuse a non-perturbative many-body technique to treat interactions perturbatively

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

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Current Work

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

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

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Current Work

Formalism

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

R. Curry, J.E. Lynn, K.E. Schmidt, and A. Gezerlis, Phys. Rev. Res., **5**, L042021, (2023)

Formalism

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

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

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

R. Curry, J.E. Lynn, K.E. Schmidt, and A. Gezerlis, Phys. Rev. Res., **5**, L042021, (2023)

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

?

R. Curry, J.E. Lynn, K.E. Schmidt, and A. Gezerlis, Phys. Rev. Res., **5**, L042021, (2023)

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

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Formalism

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Current Work

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

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

R. Curry, J.E. Lynn, K.E. Schmidt, and A. Gezerlis, Phys. Rev. Res., **5**, L042021, (2023)

Formalism

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0 as $\tau \to \infty$

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

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0 as $\tau \to \infty$

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

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

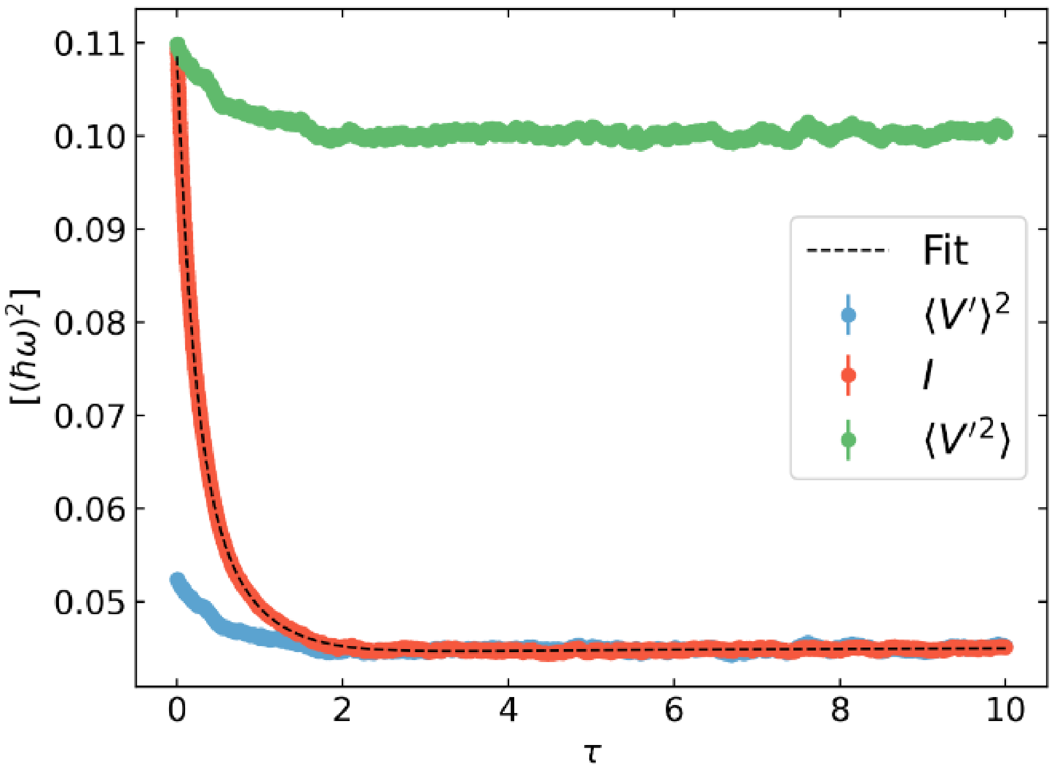
1st and 2nd order corrections from imaginary time propagation

R. Curry, J.E. Lynn, K.E. Schmidt, and A. Gezerlis, Phys. Rev. Res., **5**, L042021, (2023)

Practically

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

$$I_{step} \approx \frac{\sum_i^{\mathcal{N}} w_i V'(\boldsymbol{R}_i) V'(\boldsymbol{R}'_i)}{\sum_i^{\mathcal{N}} w_i}$$



R. Curry, J.E. Lynn, K.E. Schmidt, and A. Gezerlis, Phys. Rev. Res., **5**, L042021, (2023)

Testing Perturbativeness

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Current Work

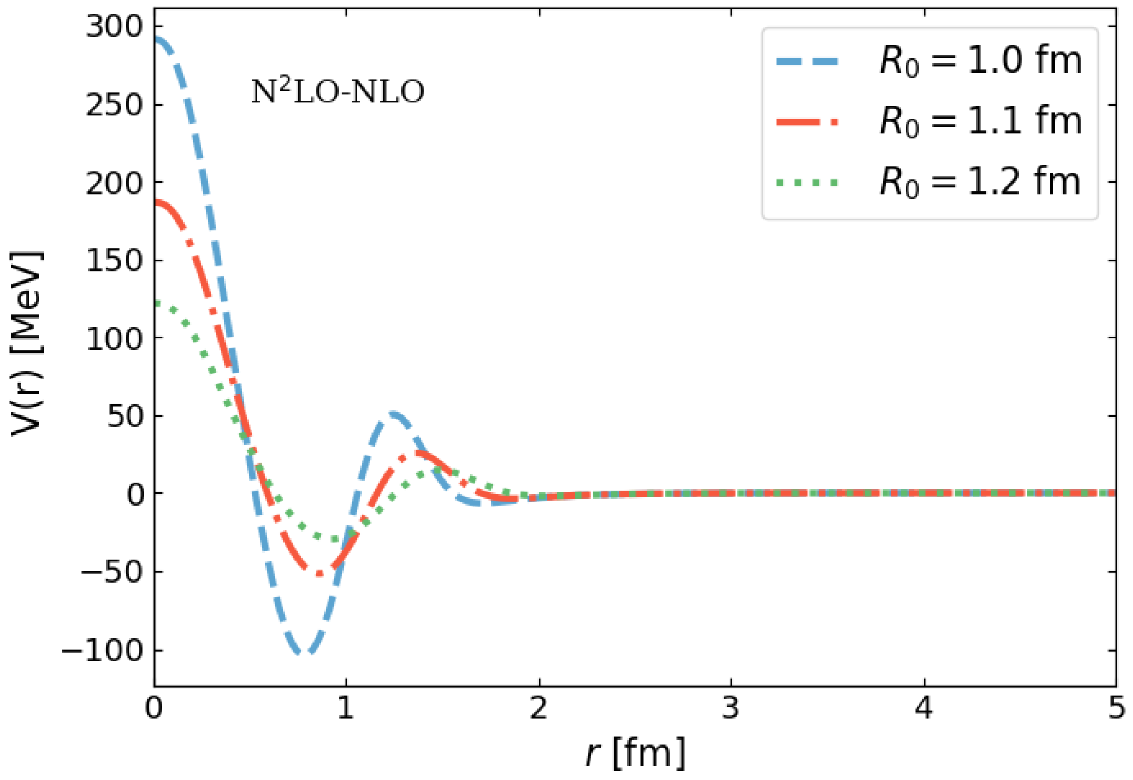
$$V_{\text{chiral}} = V^{(0)} + V^{(2)} + V^{(3)} + \cdots$$

LO NLO $\mathrm{N^2LO}$

66 Neutrons

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

Coordinate Space Cutoff R_0
~ Potential Softness



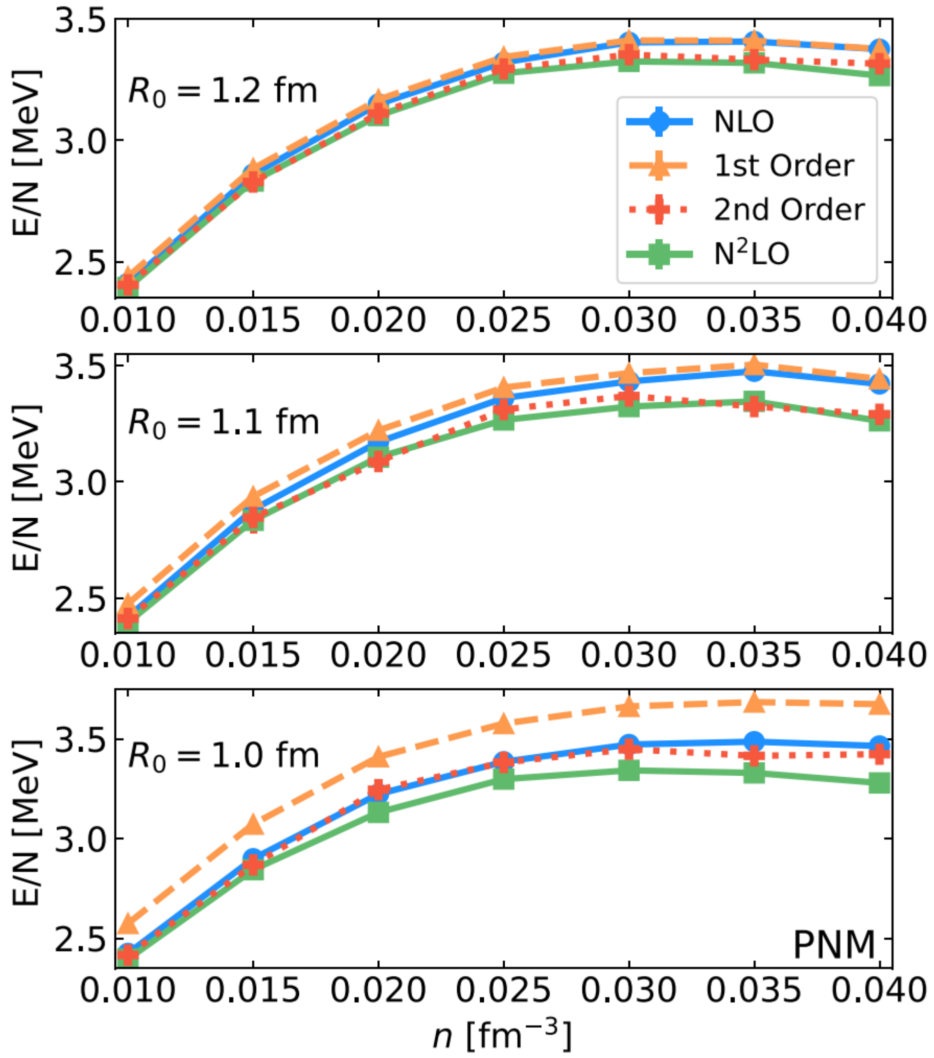
R. Curry, J.E. Lynn, K.E. Schmidt, and A. Gezerlis, Phys. Rev. Res., **5**, L042021, (2023)
G. Palkanoglou, F. K. Diakonos, A. Gezerlis, Phys. Rev. C 102, 064324 (2020)

Testing Perturbativeness

- Softest potential ($R_0 = 1.2$ fm) has excellent agreement

- At ($R_0 = 1.0$ fm) there is no agreement between second-order and non-perturbative results

- Cast doubt on perturbativeness of chiral EFT interactions.



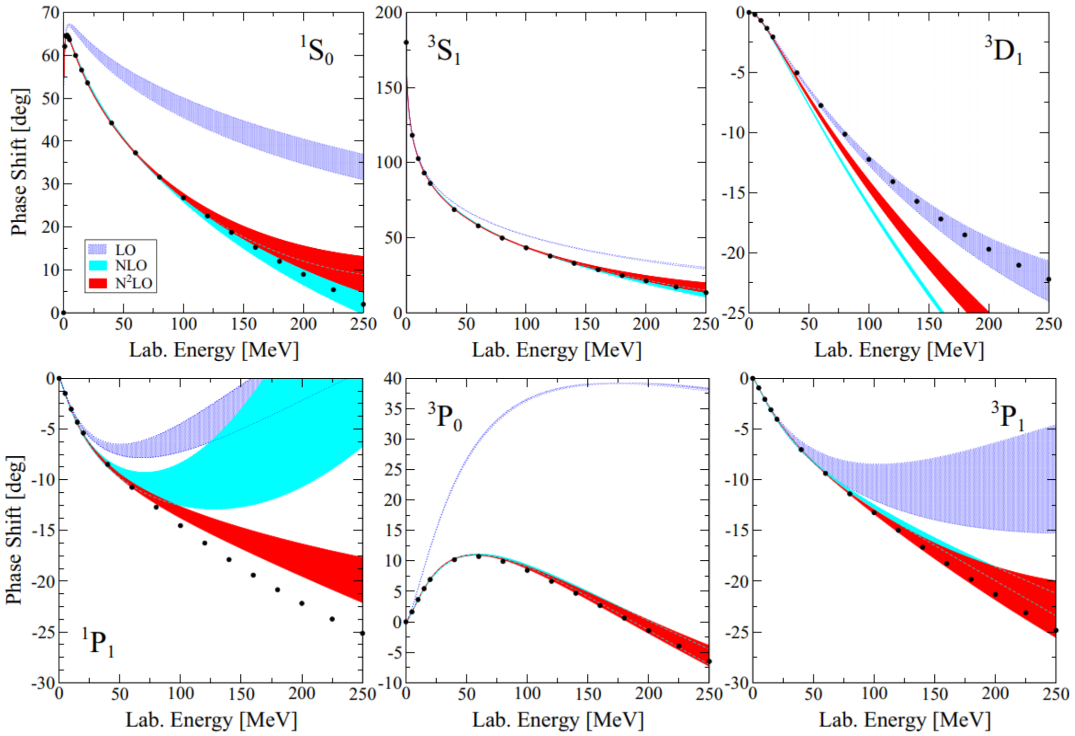
R. Curry, J.E. Lynn, K.E. Schmidt, and A. Gezerlis, Phys. Rev. Res., **5**, L042021, (2023)

Next steps

- Nuclear interaction goes well beyond s-wave

- Higher chiral orders cannot avoid non-local operators

- Need to test our method for realistic nuclear interactions and non-local operators

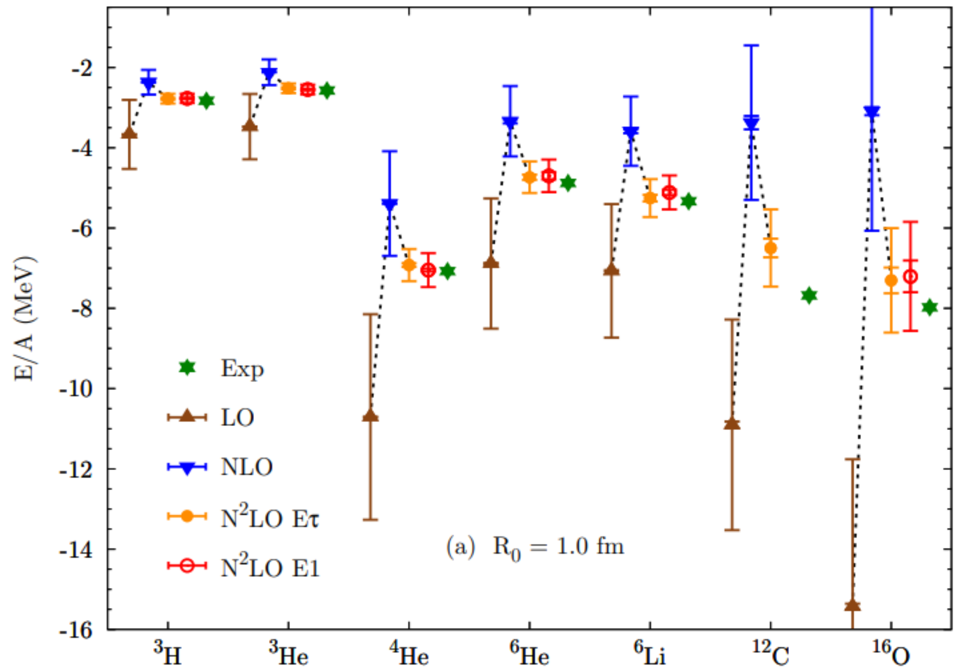


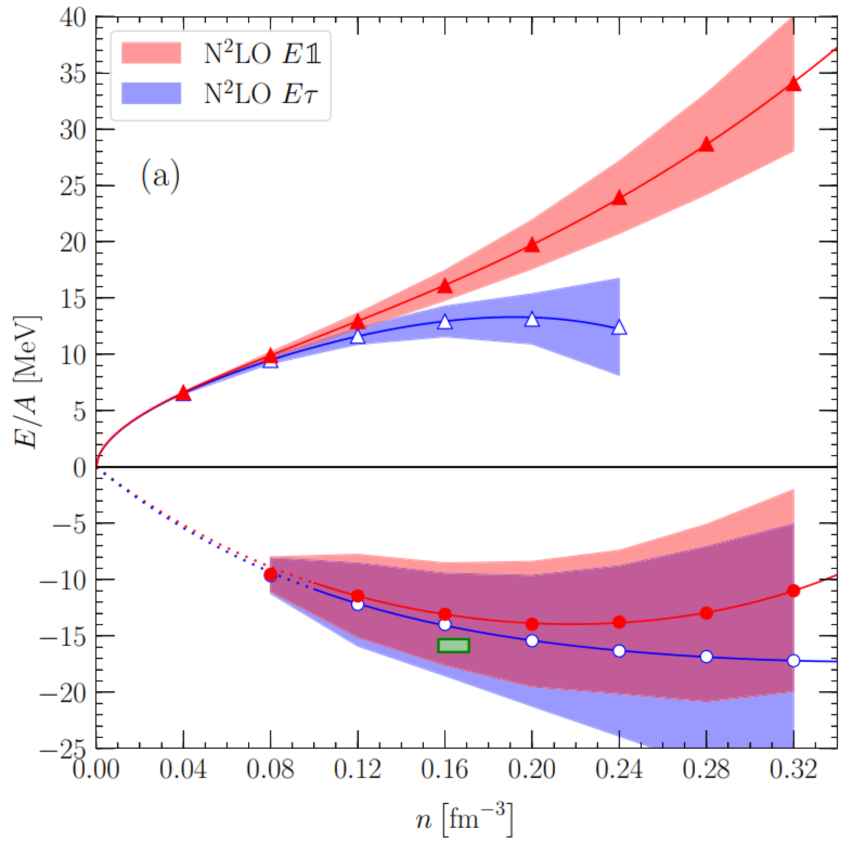
A. Gezerlis *et al,* Phys. Rev. C, **90**, 054323 (2014)
R. Somasundaram, J.E. Lynn, L. Huth, A. Schwenk and I. Tews, Phys. Rev. C, **109**, 034005, (2024)

Auxiliary Field Diffusion Monte Carlo

- All imaginary time propagation carries over

- Spin/isospin operators treated with auxiliary fields through HS transformation





K.E. Schmidt and S. Fantoni, Phys. Lett. B, **446**, 99 (1999)
D. Lonardoni, S. Gandolfi, J.E. Lynn, C. Petrie, J. Carlson, K.E. Schmidt, A. Schwenk, Phys. Rev. C, **97**, 044318 (2018)
D. Lonardoni, I. Tews, S. Gandolfi, J. Carlson, Phys. Rev. Res., **2**, 022033 (2020)

Non-local operators

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Current Work

- Non-local operators cannot be included in imaginary time propagator (must be treated perturbatively)

- Replace a single local operator with its non-local equivalent and treat perturbatively

$$V^{(2)} = \gamma_1 q^2 + \gamma_2 q^2 \boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2 + \gamma_3 q^2 \boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2$$
$$+ \gamma_4 q^2 \boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2 \boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2$$
$$+ \gamma_5 k^2 + \gamma_6 k^2 \boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2 + \gamma_7 k^2 \boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2$$
$$+ \gamma_8 k^2 \boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2\, \boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2 + \gamma_9 k^2 (\boldsymbol{\sigma}_1 + \boldsymbol{\sigma}_2)(\boldsymbol{q} \times \boldsymbol{k})$$
$$+ \gamma_{10} k^2 (\boldsymbol{\sigma}_1 + \boldsymbol{\sigma}_2)(\boldsymbol{q} \times \boldsymbol{k})\, \boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2 + \gamma_{11} (\boldsymbol{\sigma}_1 \cdot \boldsymbol{q})\, (\boldsymbol{\sigma}_2 \cdot \boldsymbol{q})$$
$$+ \gamma_{12} (\boldsymbol{\sigma}_1 \cdot \boldsymbol{q})\, (\boldsymbol{\sigma}_2 \cdot \boldsymbol{q}) \boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2 + \gamma_{13} (\boldsymbol{\sigma}_1 \cdot \boldsymbol{k})\, (\boldsymbol{\sigma}_2 \cdot \boldsymbol{k})$$
$$+ \gamma_{14} (\boldsymbol{\sigma}_1 \cdot \boldsymbol{k})\, (\boldsymbol{\sigma}_2 \cdot \boldsymbol{k}) \boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2$$

Fourier Transform

$q \rightarrow r$		local
$k \rightarrow \nabla$		non-local

Non-local operators

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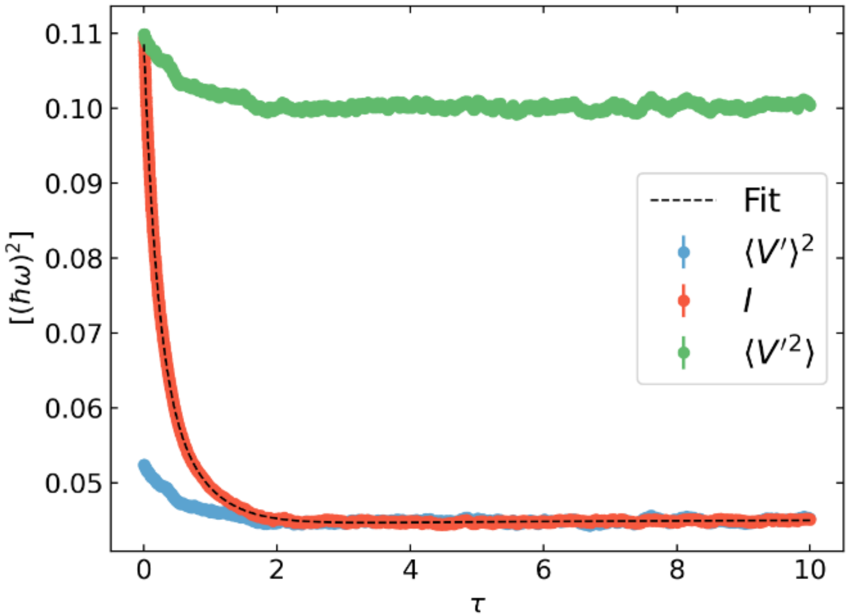
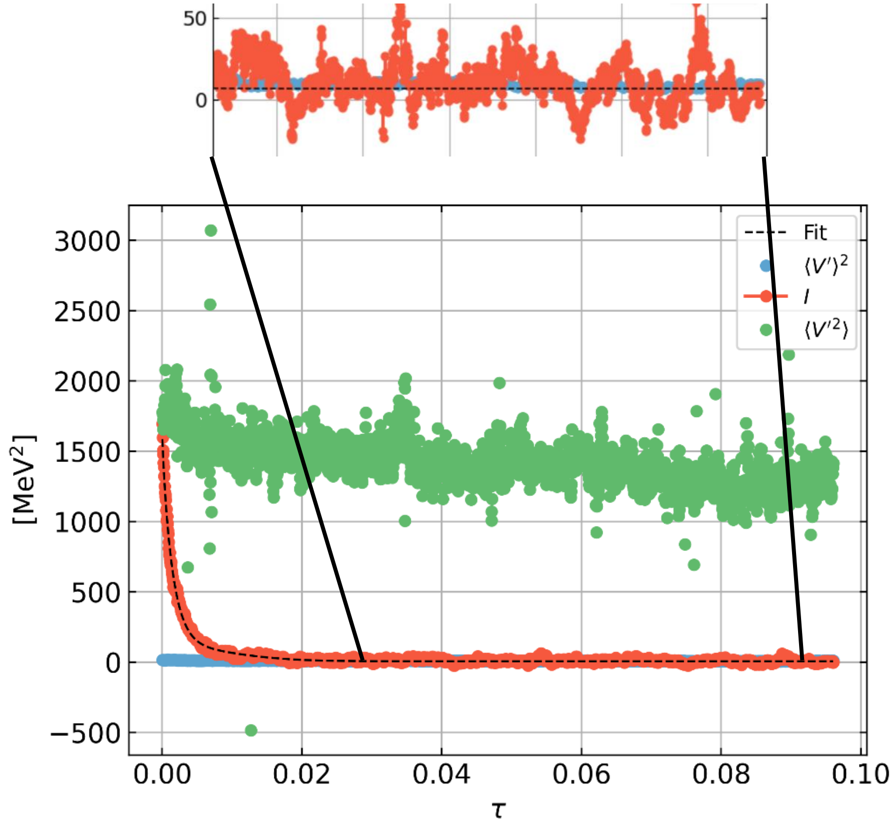
Current Work

$$k^2 \xrightarrow{\text{FT}} \left[-\frac{1}{4}(\nabla^2\delta_{R_0})\psi(\boldsymbol{r}) - \frac{1}{r}\frac{\partial\delta_{R_0}}{\partial r}\left(\boldsymbol{r}\cdot\nabla\psi(\boldsymbol{r})\right) - \delta_{R_0}\nabla^2\psi(\boldsymbol{r})\right]$$



Local

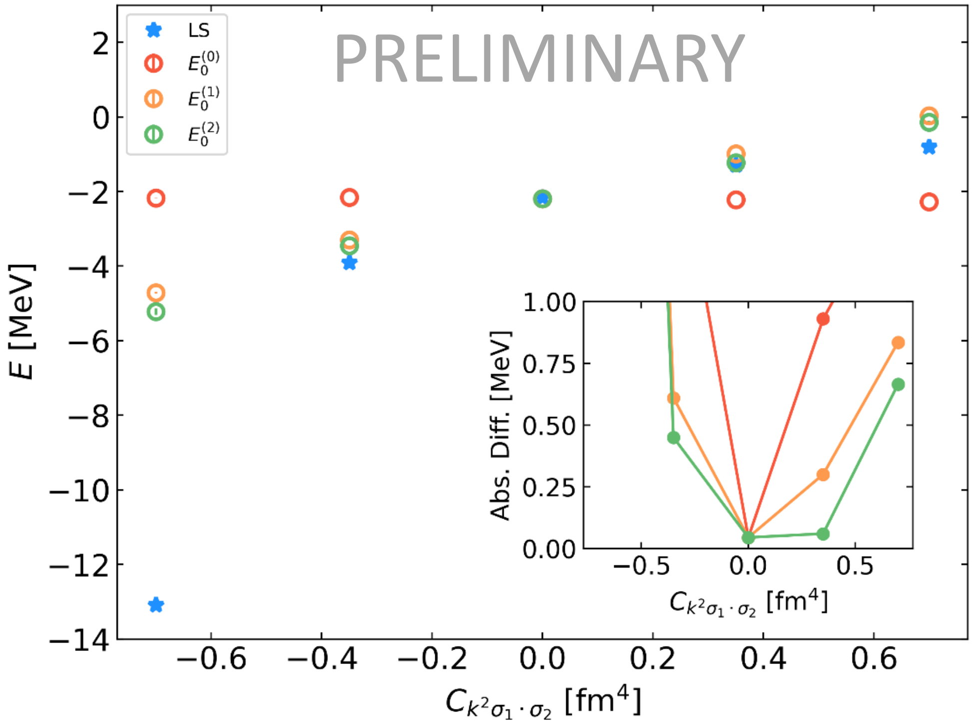


Non-Local

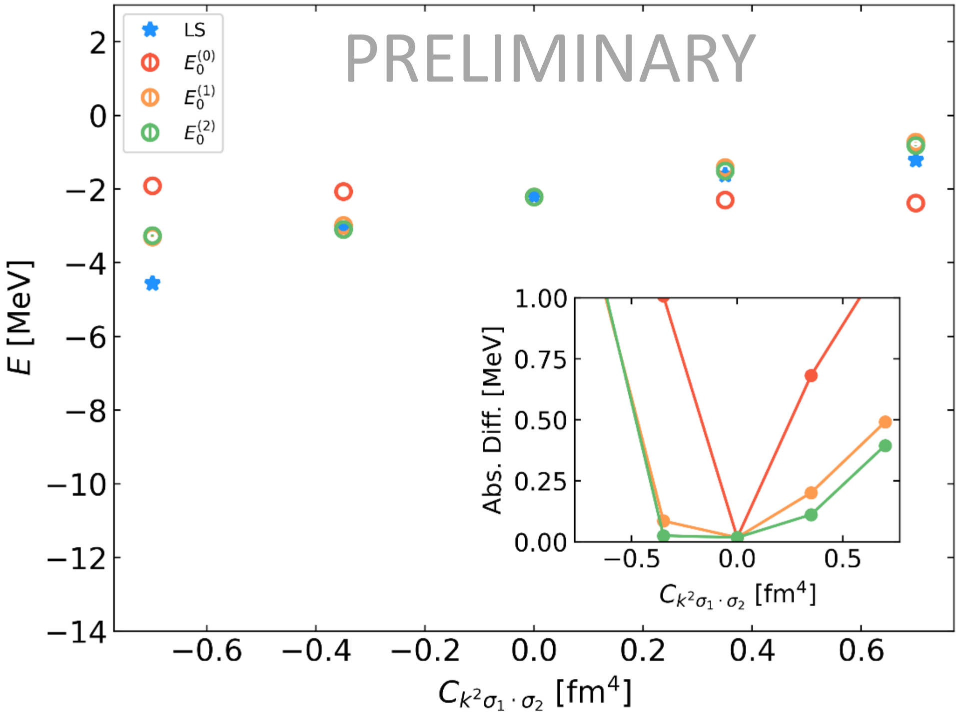
Deuteron with non-local operator

- $k^2\sigma_1 \cdot \sigma_2$ included perturbatively, for two cutoffs

- Compare against exact Lippmann-Schwinger solution



$R_0 = 0.6$ fm



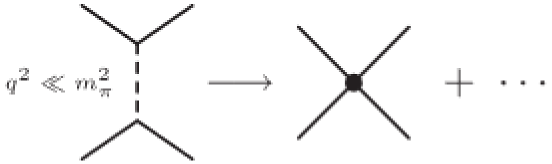
$R_0 = 0.9$ fm

Outlook

- Study neutron matter using AFDMC, treating non-local terms perturbatively

- Extend our treatment to N^3LO potentials, terms that <u>must</u> be treated perturbatively.

- Pionful Chiral EFT vs Pionless EFT ?

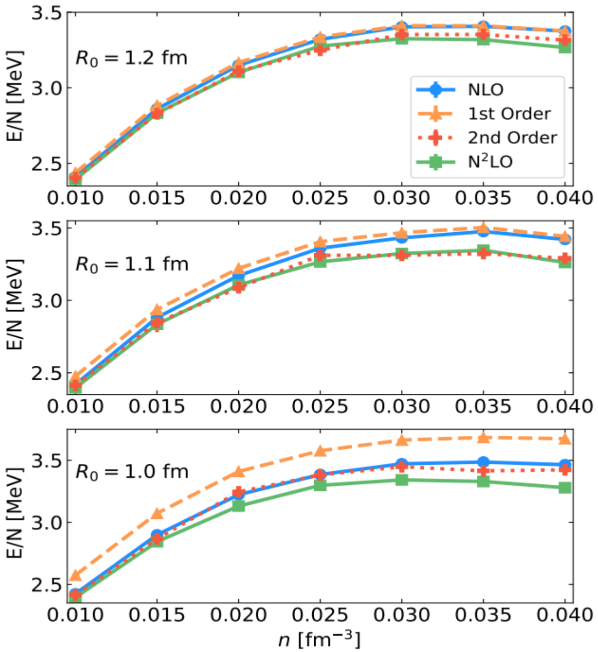


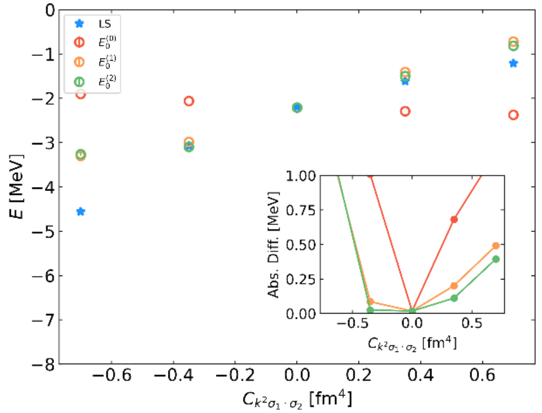
- Third-Order Corrections?

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

Summary

- Developed a new method for calculating Second-Order correction in *ab initio* many body context.
- Tested perturbativeness of modern chiral EFT potentials
- Hard core potentials need third-order corrections or higher. Cast doubt on perturbativeness of chiral EFT interactions.
- Deuteron calculations with non-local term treated perturbatively





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Current Work

Thank You for listening!

Alexandros Gezerlis………….... University of Guelph

Joel E. Lynn…………………… Institut für Kernphysik Technische Universität Darmstadt

Kevin E. Schmidt……………… Arizona State University

Ingo Tews………………………
Stefano Gandolfi………………..Los Alamos National Laboratory
Rahul Somasundaram…………..

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NSERC CRSNG
SHARCNET™