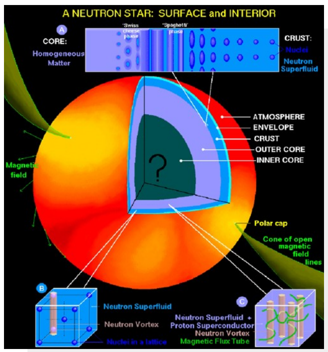
Perturbation theory in continuum quantum Monte Carlo
(arXiv:2302.07285)

Alex Gezerlis

UNIVERSITY of GUELPH

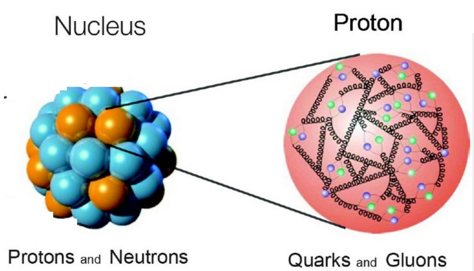
Workshop on Progress in Ab Initio Nuclear Theory
TRIUMF, Vancouver, BC
February 28, 2023

Outline

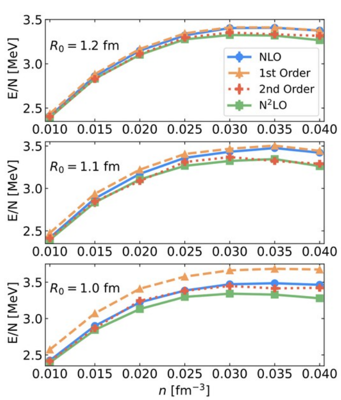


Credit: Dany Page

Motivation



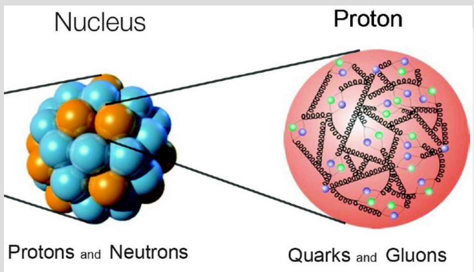
Nuclear methods



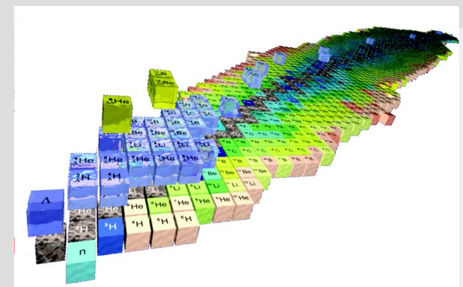
Recent results

Physical systems studied

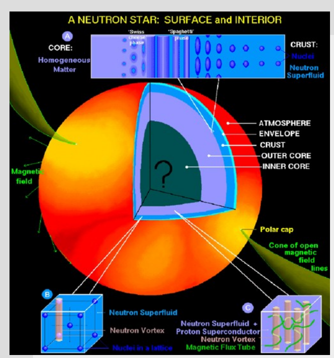
Nuclear forces

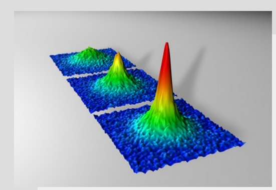


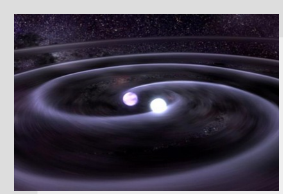
Nuclear structure



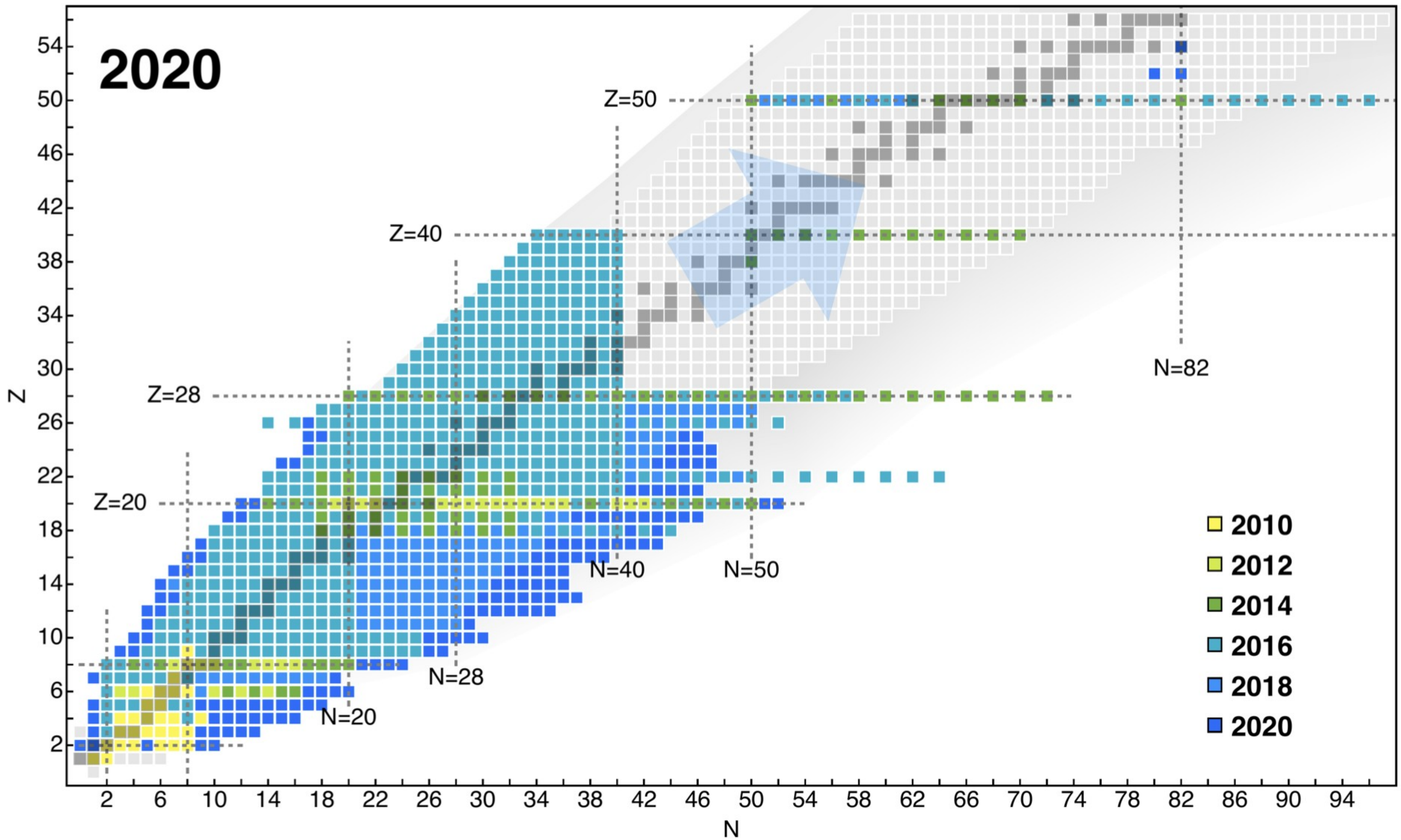
Nuclear astrophysics







Key system: nuclei

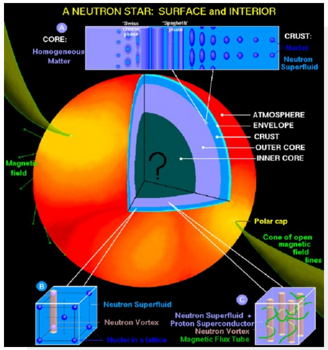


Credit:
Heiko Hergert
Front. Phys.
8:379 (2020)

- Lots of recent progress
- Open-shell nuclei are the current frontier

- Goal is to study nuclei *from first principles* (when possible)

Outline



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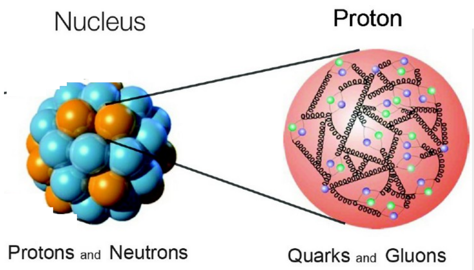
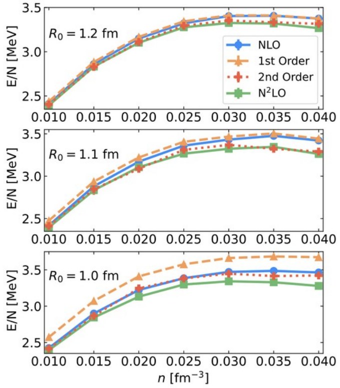
Motivation



Nuclear methods



Recent results

Nuclear physics is difficult

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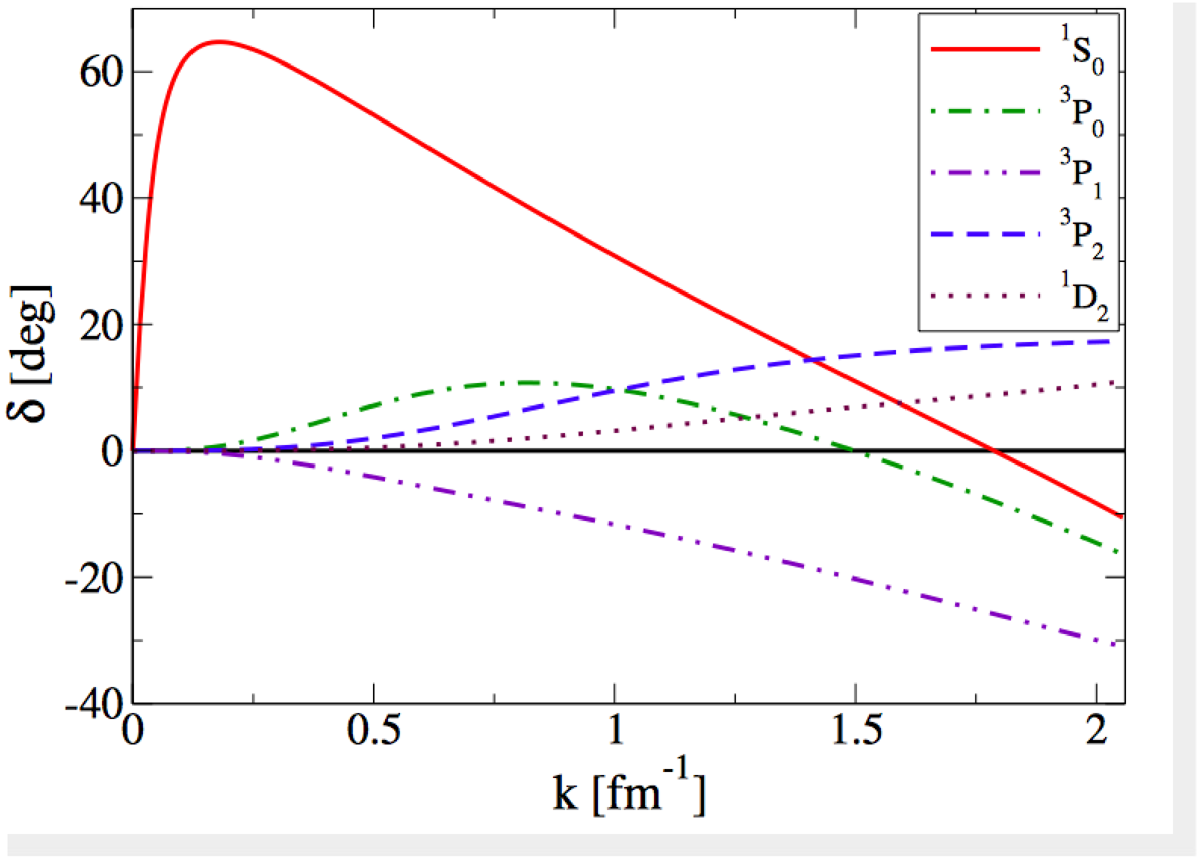
Scattering phase shifts: different "channels" have different behavior.



Any potential that reproduces them must be spin (and isospin) dependent

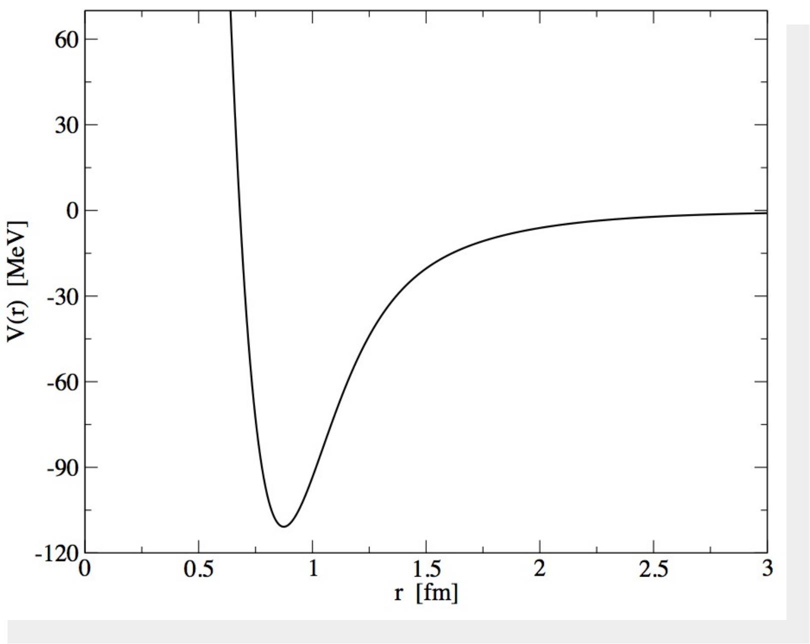
Nuclear interactions

Meson exchanges: phenomenology treats NN scattering without connecting with the underlying level

$$V_2 = \sum_{j<k} v_{jk} = \sum_{j<k} \sum_{p=1}^{8} v_p(r_{jk}) O^{(p)}(j,k)$$

$$O^{p=1,8}(j,k) = (1, \sigma_j \cdot \sigma_k, S_{jk}, \mathbf{L}_{jk} \cdot \mathbf{S}_{jk}) \otimes (1, \tau_j \cdot \tau_k)$$

Such potentials are hard, making them non-perturbative at the many-body level



Nuclear interactions

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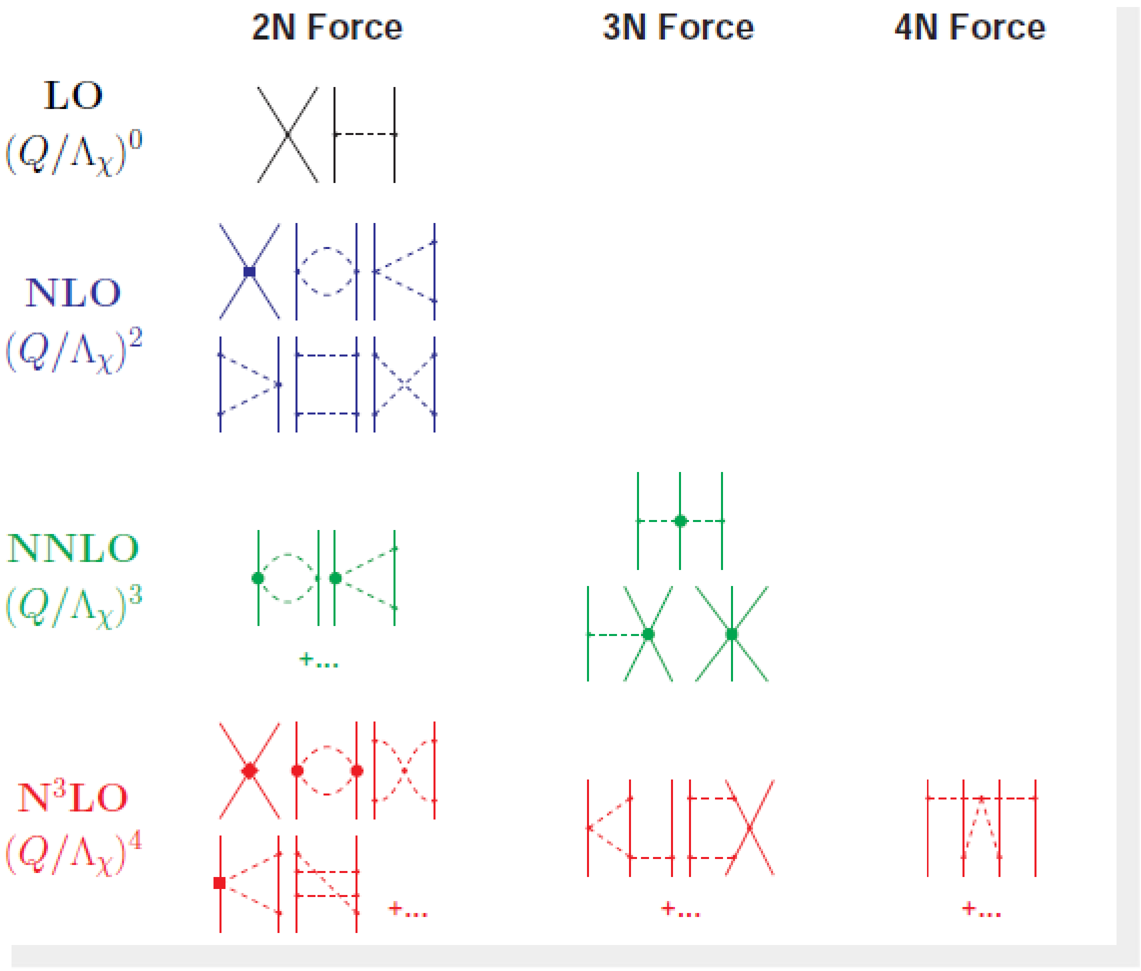
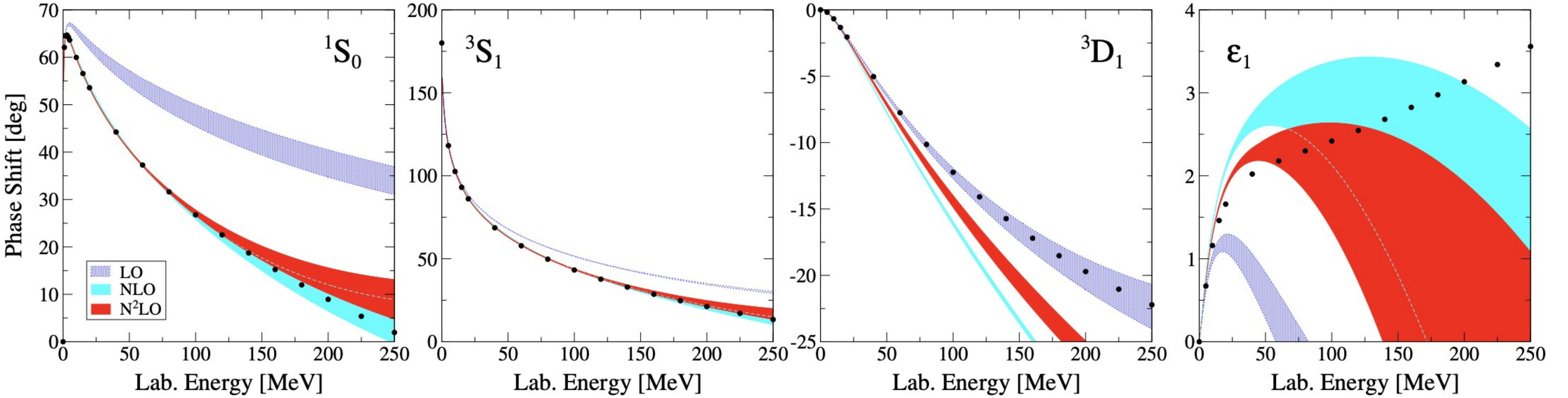


- Attempts to connect with underlying theory (QCD)
- Low-momentum expansion
- Naturally emerging many-body forces
- Low-energy constants from experiment or lattice QCD
- Now available in non-local, local, or semi-local varieties
- Power counting's relation to renormalization actively investigated

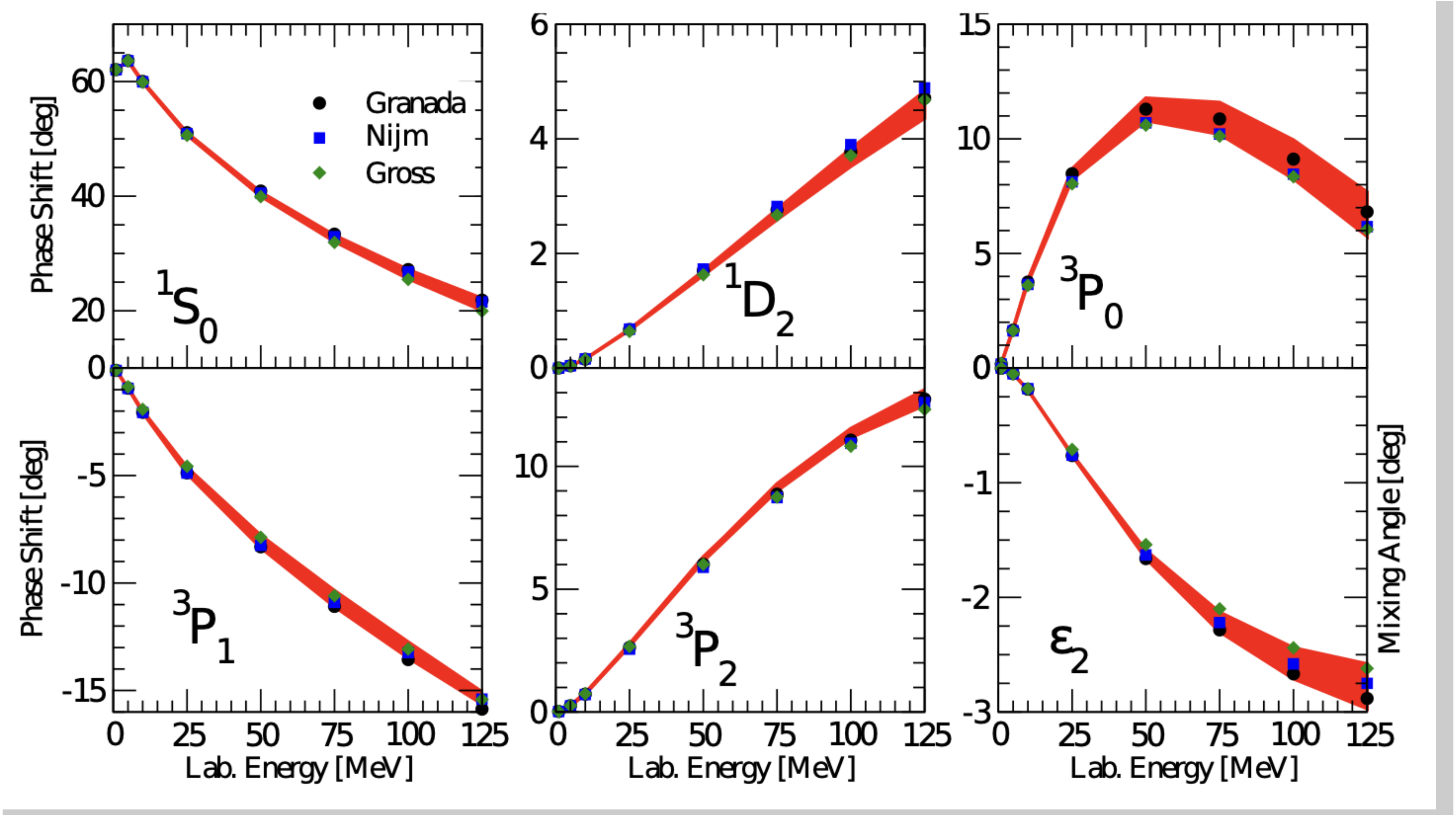
S. Weinberg, U. van Kolck, E. Epelbaum, N. Kaiser ...

Local chiral EFT



A. Gezerlis, I. Tews, E. Epelbaum, M. Freunek, S. Gandolfi, K. Hebeler, A. Nogga, and A. Schwenk, Phys. Rev. C **90**, 054323 (2014)

Local chiral EFT



M. Piarulli, L. Girlanda, R. Schiavilla, A. Kievsky, A. Lovato, L. E. Marcucci, S. C. Pieper, M. Viviani, and R. B. Wiringa, Phys. Rev. C **94**, 054007 (2016)

But even with the interaction in place,
how do you solve the many-body problem?

Nuclear many-body problem

$$H\Psi = E\Psi$$

where $$H = \sum_i K_i + \sum_{i<j} V_{ij} + \sum_{i<j<k} V_{ijk}$$

Wave function depends on coordinates, spin projections, and isospin projections, so we are faced with a large number of complex coupled second-order differential equations

Nuclear many-body methods

- Phenomenological
- Ab initio

Two complementary approaches

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Phenomenological

- *Shell model*
  mainstay of nuclear physics, still very important
- *Hartree-Fock/Hartree-Fock-Bogoliubov (HF/HFB)*
  mean-field theory, a priori inapplicable, unreasonably effective
- *Energy-density functionals (EDF)*
  like mean-field but with wider applicability

Two complementary approaches

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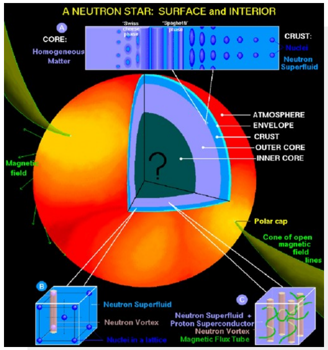
Ab initio

- *Exact diagonalization techniques (e.g., HH or NCSM)*
  fully ab initio, in contradistinction to traditional SM
- *Quantum Monte Carlo (QMC), continuum or lattice*
  stochastically propagate in imaginary time
- *Perturbative Theories (PT)*
  first few orders only
- *Resummation schemes (e.g. SCGF)*
  selected class of diagrams up to infinite order
- *Coupled cluster (CC) and In-Medium Similarity Renormalization Group (IMSRG)*
  decoupling transformation of Hamiltonian/generate *n*p-*n*h excitations of a reference state

Outline



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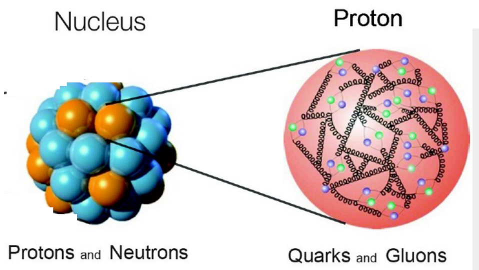
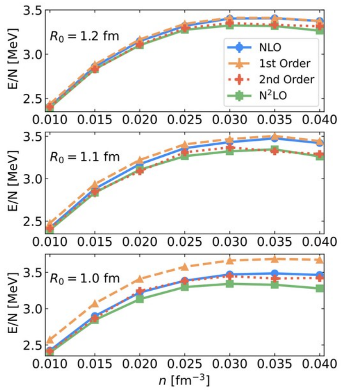


Nuclear methods



Recent results

Perturbative or non-perturbative?

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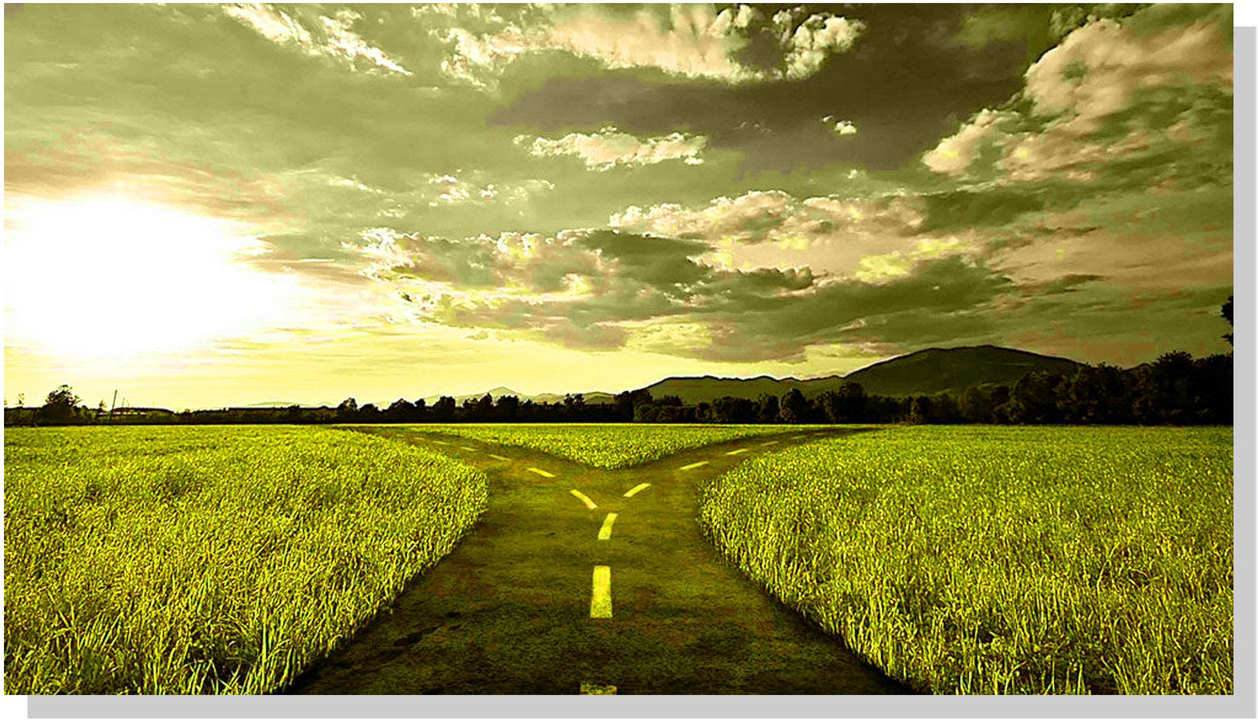
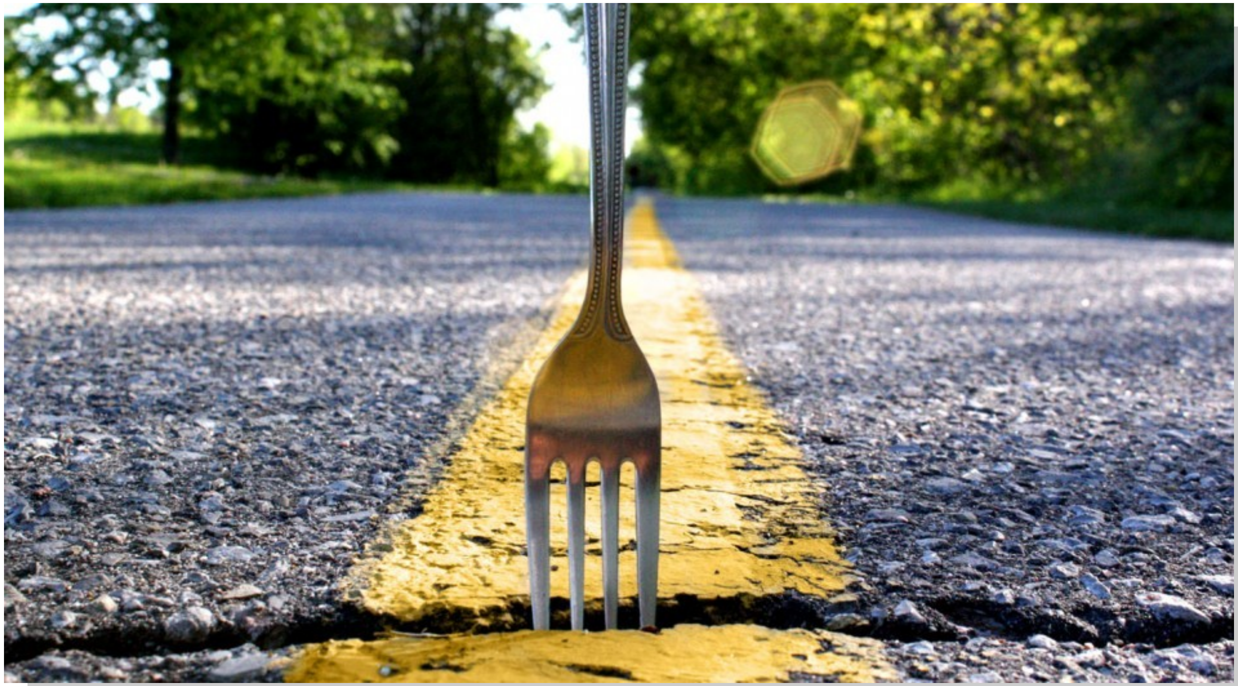


"When you come to a fork in the road, take it"

Perturbative or non-perturbative?



“When you come to a fork in the road, take it”

Setting the stage

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Split your Hamiltonian:

$$\hat{H} = \hat{H}_0 + V'$$

Nearly everyone can do a first-order perturbation:

$$E_0^{(1)} = \frac{\left\langle \psi_0^{(0)} \middle| V' \middle| \psi_0^{(0)} \right\rangle}{\left\langle \psi_0^{(0)} \middle| \psi_0^{(0)} \right\rangle}$$

Things not so easy when it comes to the second order:

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

Deuteron

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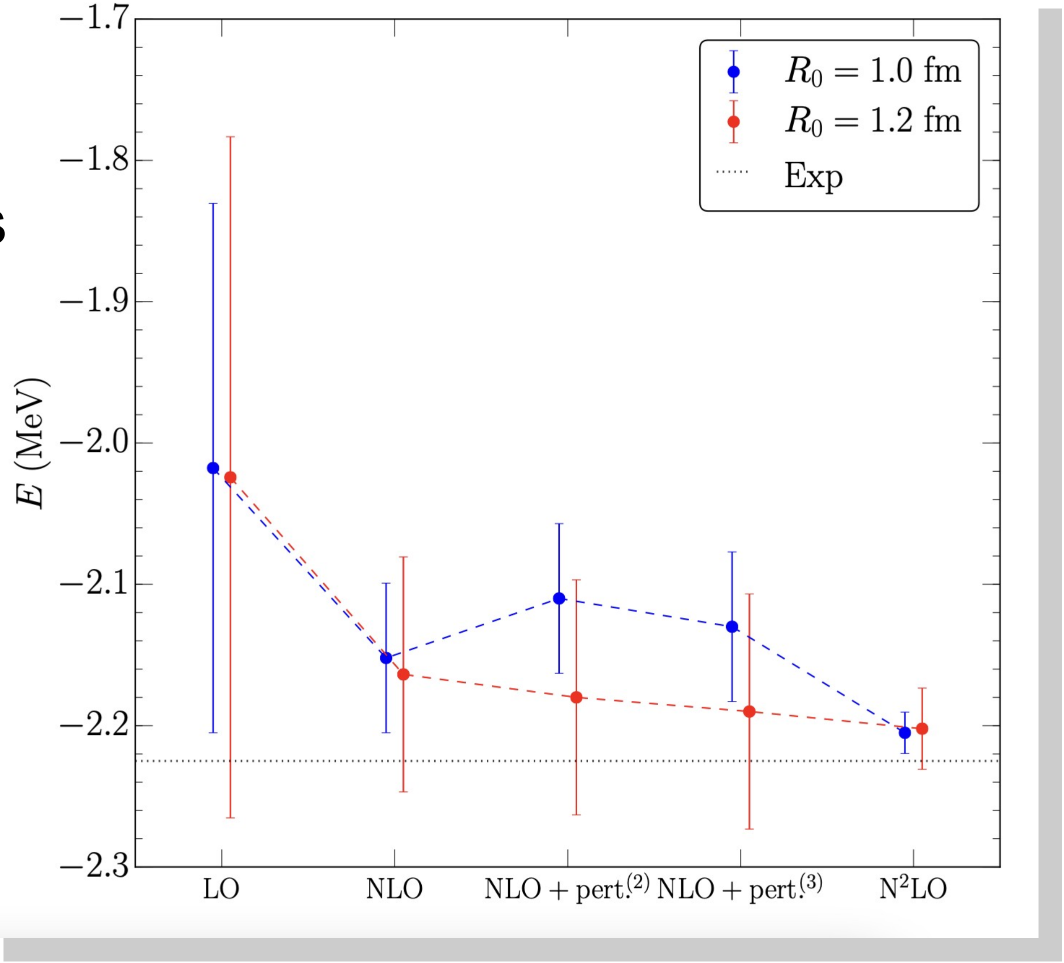
Up to 3rd order

Two zeroth-order Hamiltonians (and two cutoffs).

Speed of convergence appears to depend on softness of interaction.



J. E. Lynn, I. Tews, J. Carlson, S. Gandolfi, A. Gezerlis, K. E. Schmidt, A. Schwenk, Phys. Rev. C **96**, 054007 (2017)

Deuteron

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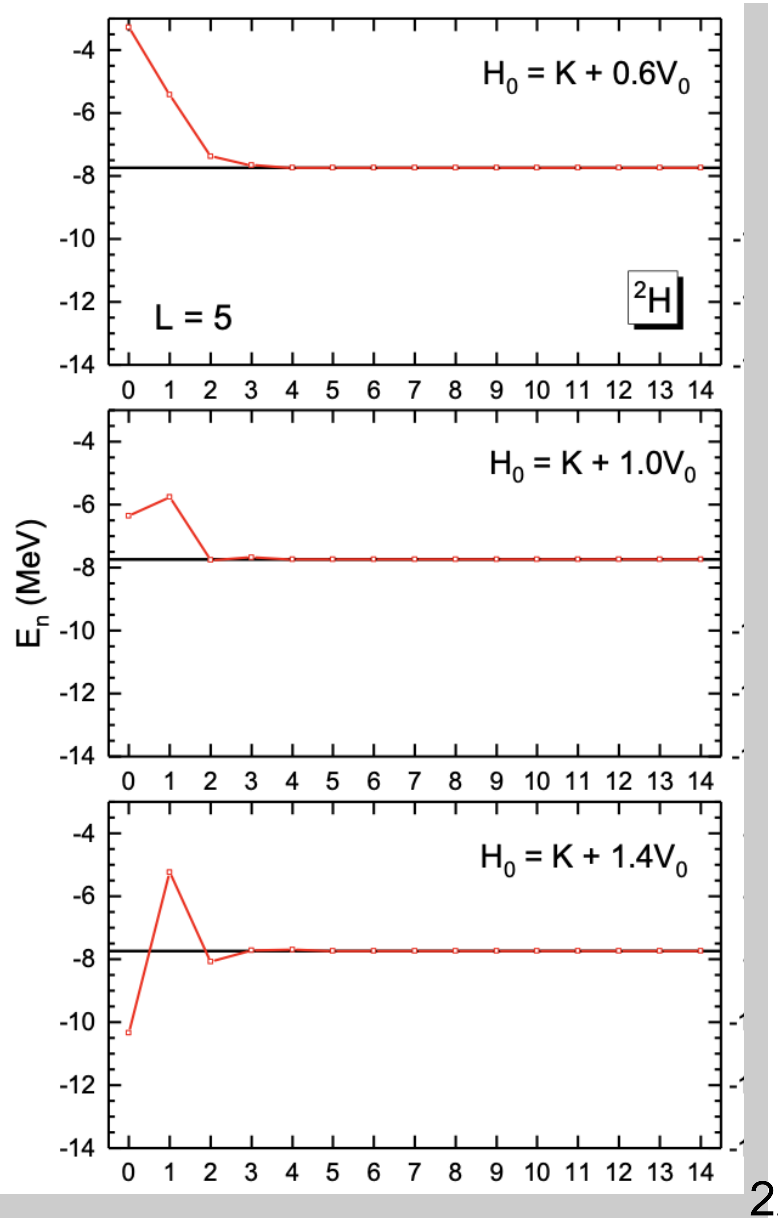
Up to 14th order

Many zeroth-order Hamiltonians (but single momentum cutoff).

Beyond second-order effects small.



B.-N. Lu, N. Li, S. Elhatisari, Y.-Z. Ma, D. Lee, U.-G. Meissner, Phys. Rev. Lett. **128**, 242501 (2022)

Beyond the deuteron

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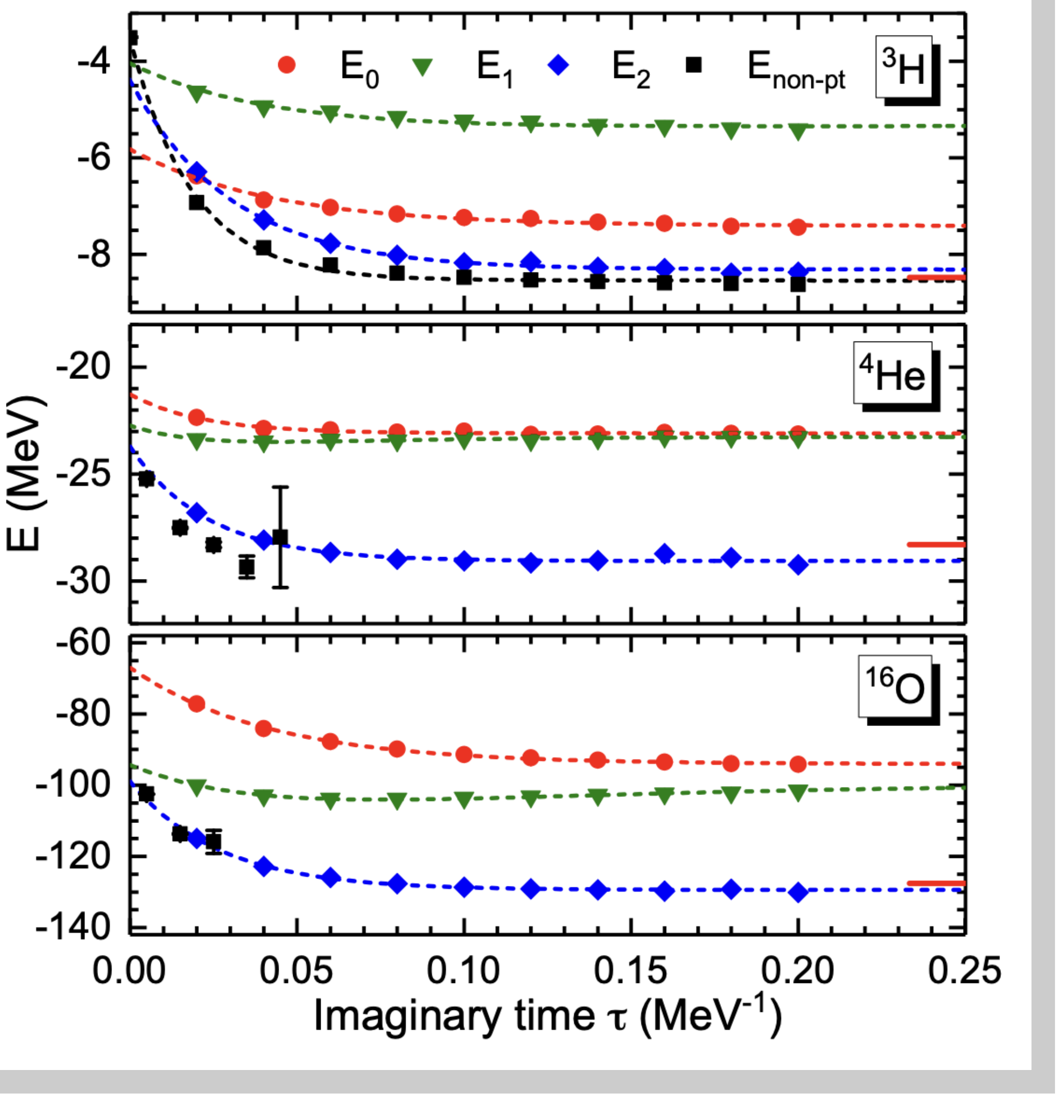
Lattice quantum Monte Carlo: up to 2nd order



- Lattice QMC is QMC (expressed in terms of Euclidean/imaginary time)
- Applied to several nuclei
- Hamiltonian expanded around the Wigner SU(4) limit
- Due to nature of approach, interaction is cast into transfer-matrix form

B.-N. Lu, N. Li, S. Elhatisari, Y.-Z. Ma, D. Lee, U.-G. Meissner, Phys. Rev. Lett. **128**, 242501 (2022)

Beyond the deuteron

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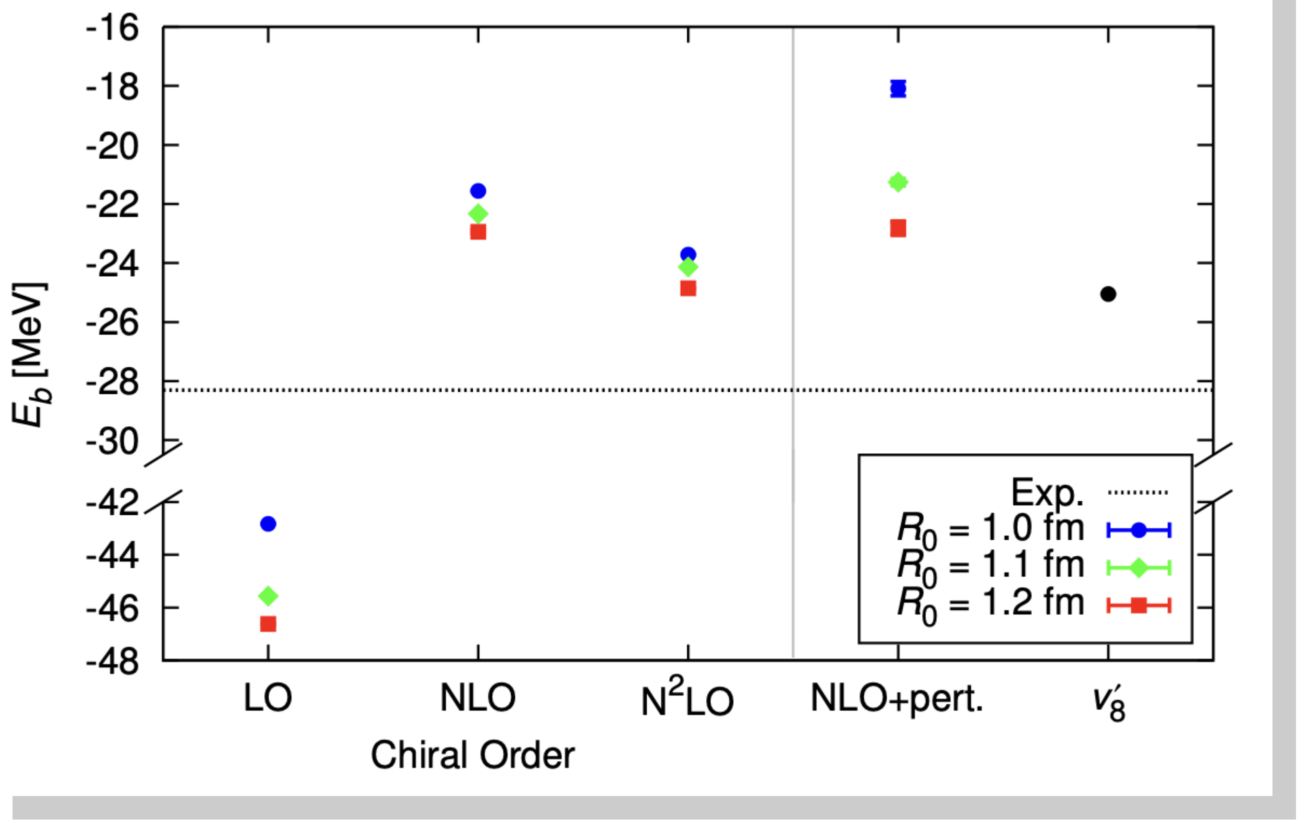
Continuum quantum Monte Carlo: up to 1st order

4He (no TNI)

Three zeroth-order Hamiltonians (and three cutoffs).

Again, speed of convergence appears to depend on softness of interaction.



J. E. Lynn, I. Tews, J. Carlson, E. Epelbaum, S. Gandolfi, A. Gezerlis, K. E. Schmidt, A. Schwenk, I. Tews, Phys. Rev. Lett. **113**, 192501 (2014)

Setting the stage

Desiderata: *approach should be able to*

- straightforwardly go beyond a two-body problem
- use a non-perturbative many-body technique to treat an interaction perturbatively
- straightforwardly handle different momentum cutoffs

R. Curry, J. E. Lynn, K. E. Schmidt, A. Gezerlis, arXiv:2302.07285

Our approach

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Inspired by generic quantum Monte Carlo

$$\lim_{\tau\to\infty}\psi(\tau)=\lim_{\tau\to\infty}\exp[-(\hat{H}_0-E_T)\tau]\psi_T\propto\psi_0^{(0)}$$

Consider the quantity $I(\mathcal{T})=\int_0^{\mathcal{T}} d\tau\left\langle\psi_0^{(0)}\middle|V' e^{-[\hat{H}_0-E_0^{(0)}]\tau}V'\middle|\psi_0^{(0)}\right\rangle$

Recast as

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

With limiting value $I(\mathcal{T}\to\infty)=(E_0^{(1)})^2\mathcal{T}-E_0^{(2)}$

So we can extract the 2nd-order correction from the imaginary time propagation without doing a sum!

R. Curry, J. E. Lynn, K. E. Schmidt, A. Gezerlis, arXiv:2302.07285

Our approach

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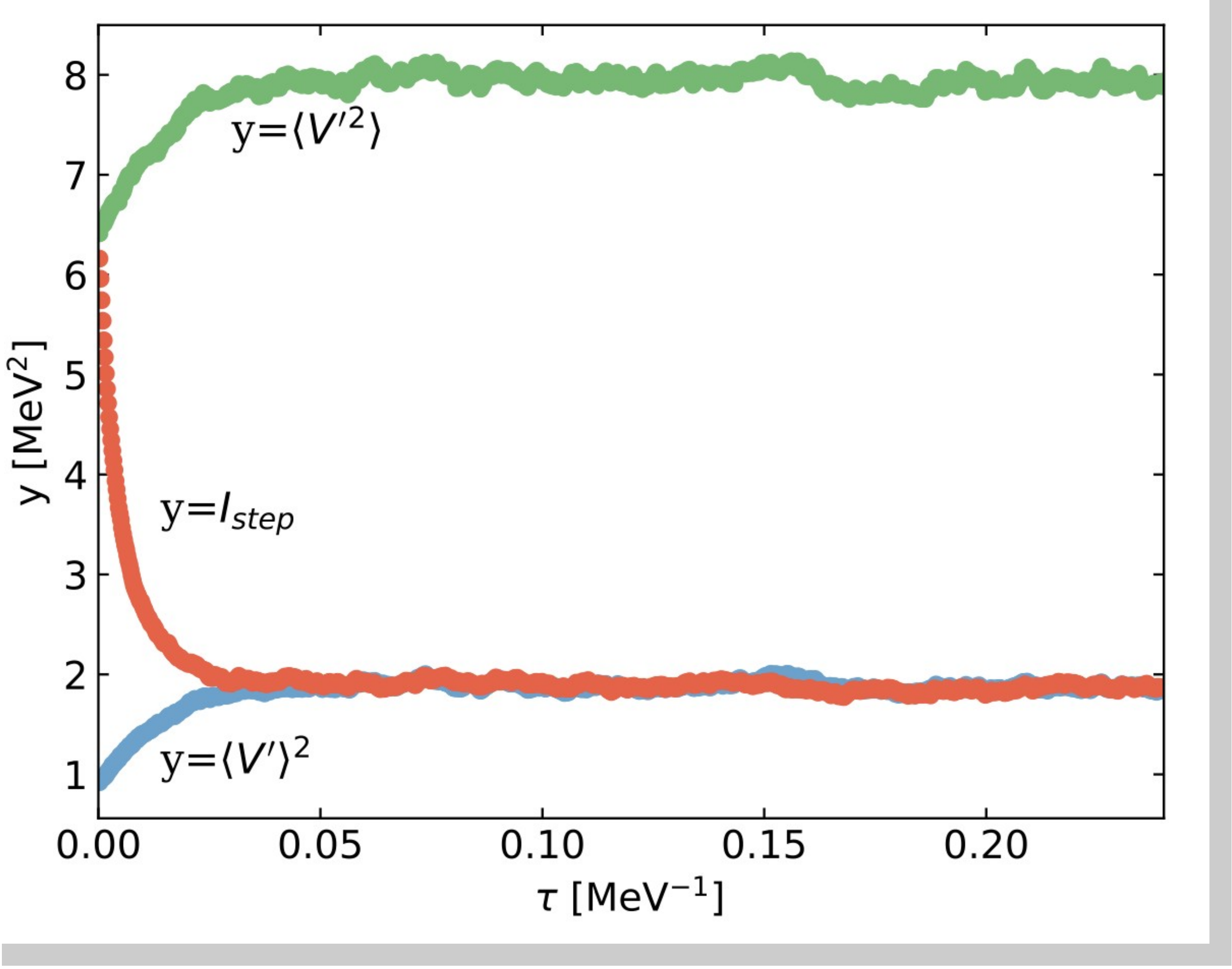
Plot the step-by step evolution of $I(\mathcal{T}) = \int_0^{\mathcal{T}} d\tau \left\langle \psi_0^{(0)} \middle| V' e^{-[\hat{H}_0 - E_0^{(0)}]\tau} V' \middle| \psi_0^{(0)} \right\rangle$



Start at trial values, end up at ground-state values

R. Curry, J. E. Lynn, K. E. Schmidt, A. Gezerlis, arXiv:2302.07285

Applications

- Two particles in a trap (Gaussian perturbation)
- Few neutrons in a trap (charge-independence breaking perturbation)
- Many neutrons in a box (order-by-order perturbation)

R. Curry, J. E. Lynn, K. E. Schmidt, A. Gezerlis, arXiv:2302.07285

Application 1

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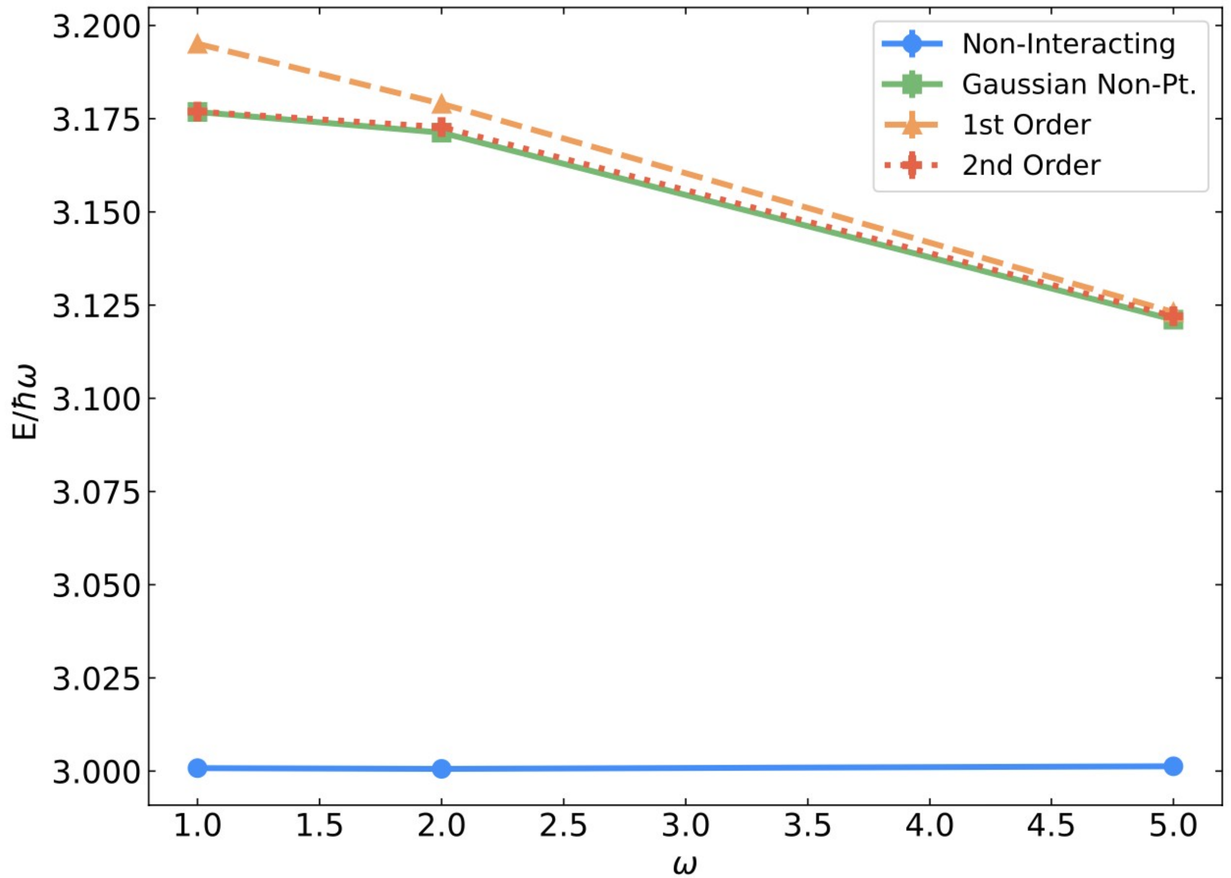
Two particles in a trap (Gaussian perturbation)



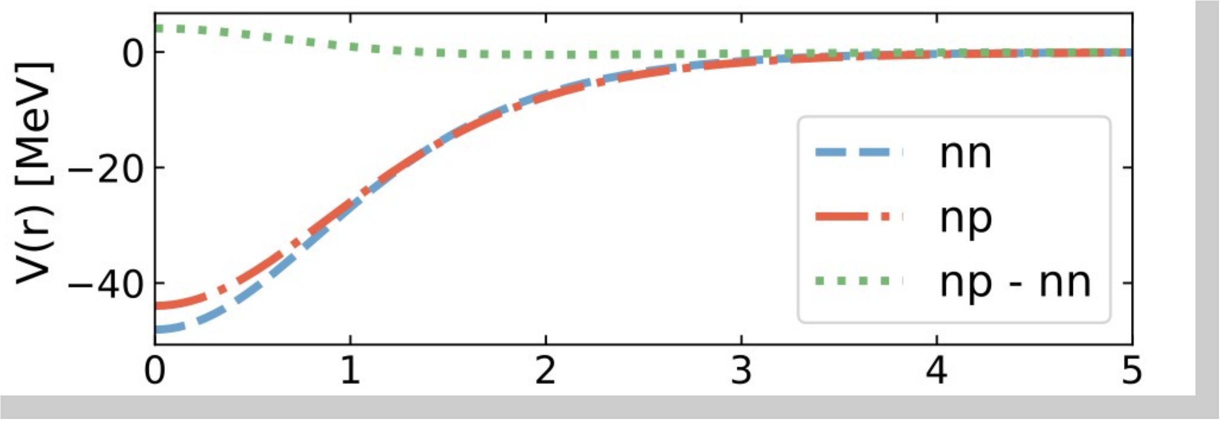
$$V' = a e^{-q^2 (\boldsymbol{r}_2 - \boldsymbol{r}_1)^2}$$

2nd order gets us to non-perturbative value

R. Curry, J. E. Lynn, K. E. Schmidt, A. Gezerlis, arXiv:2302.07285

Application 2

Few neutrons in a trap (charge-independence breaking perturbation)



Like in Application 1, this is a small perturbation

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Application 2

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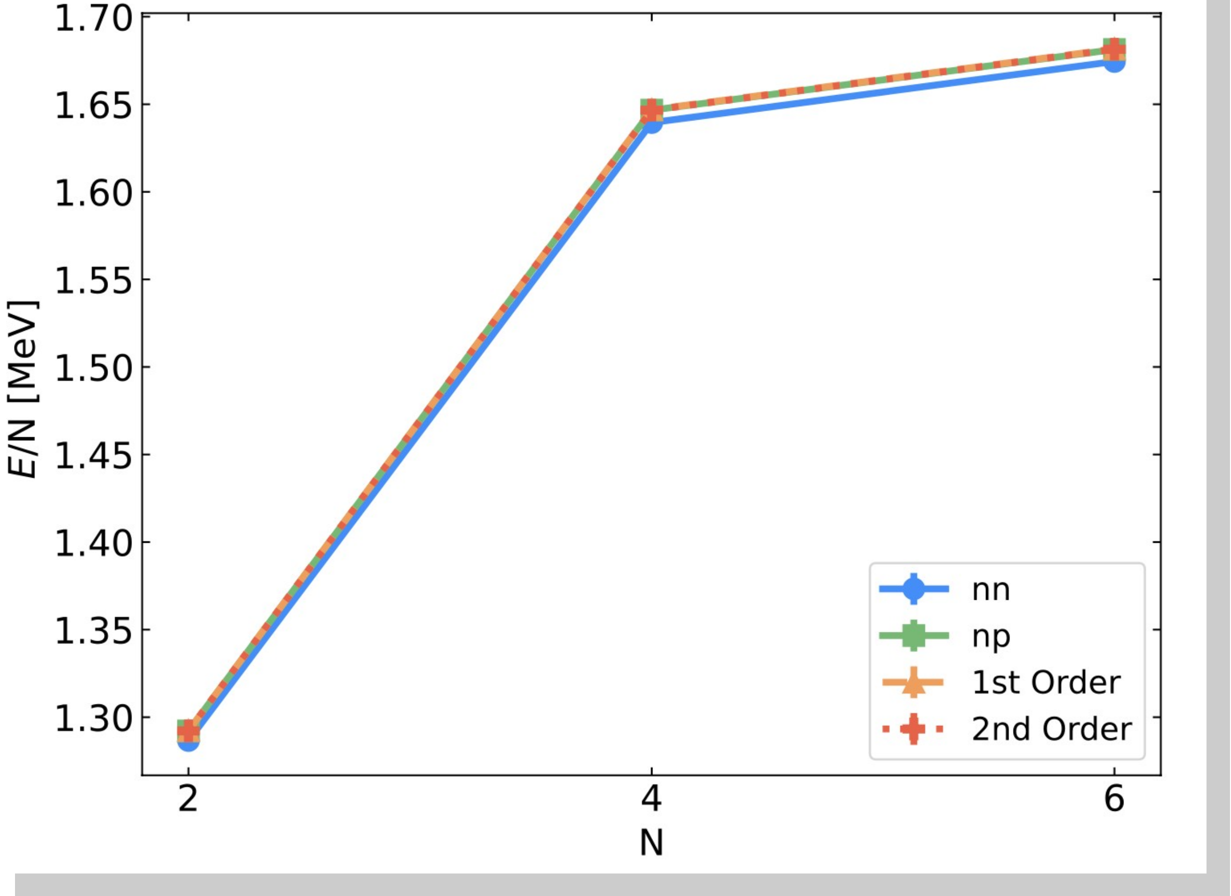
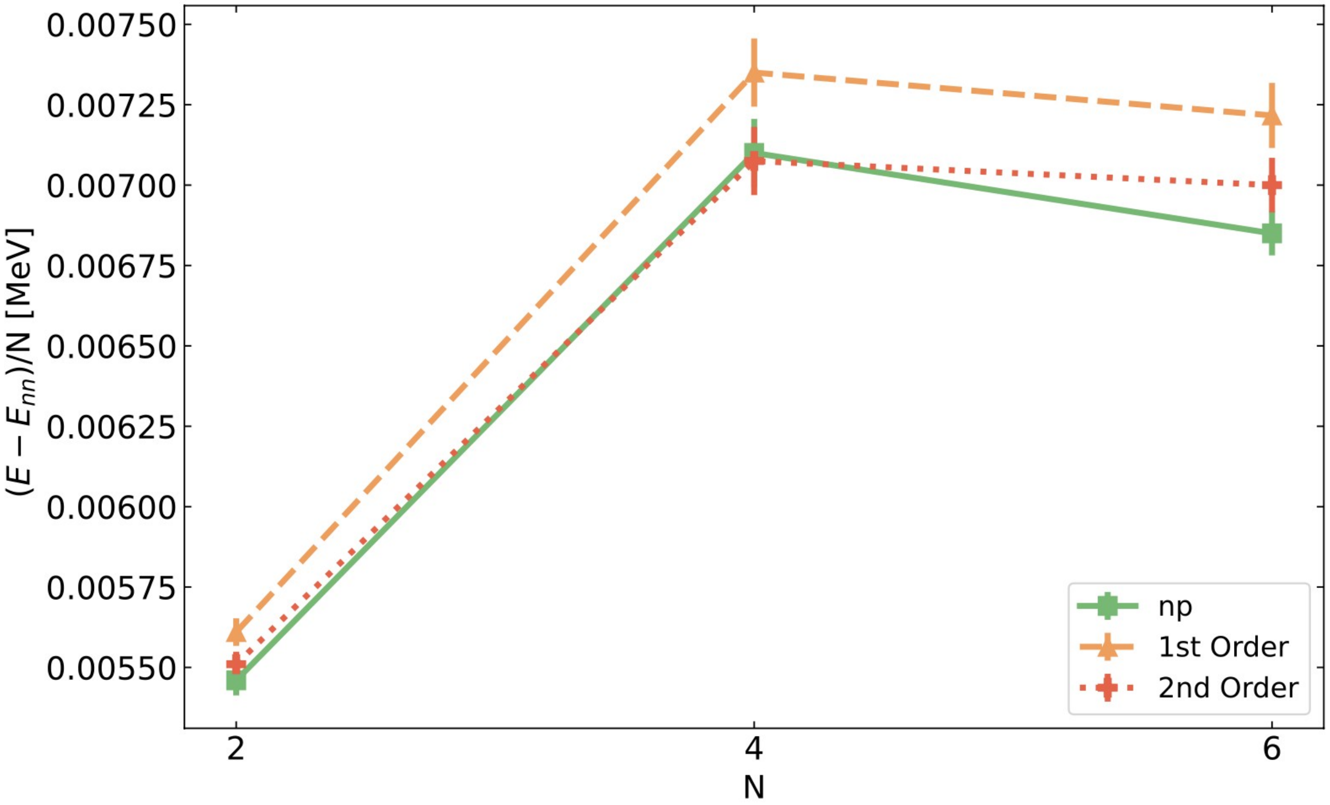


1st order is already good, so it's hard to see what's going on

R. Curry, J. E. Lynn, K. E. Schmidt, A. Gezerlis, arXiv:2302.07285

Few neutrons in a trap (charge-independence breaking perturbation)



2nd order gets us to non-perturbative value

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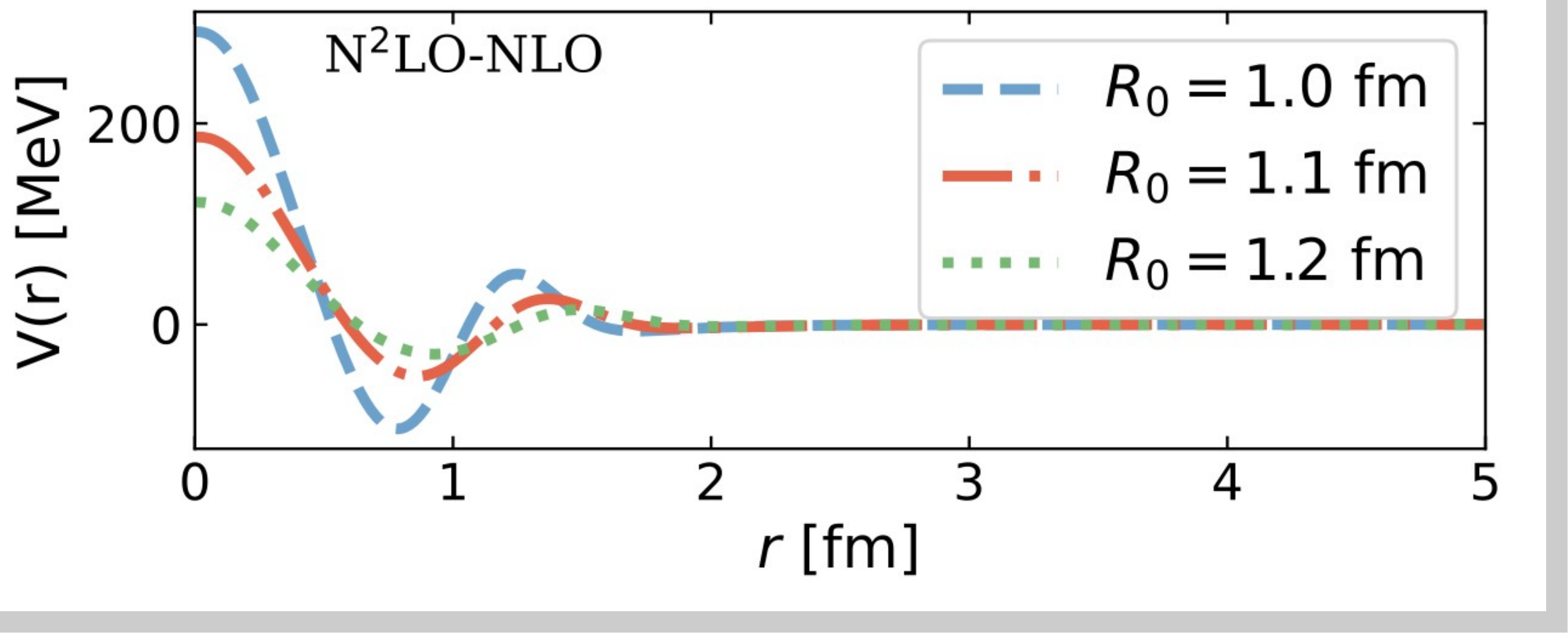
Application 3

Many neutrons in a box (order-by-order perturbation)



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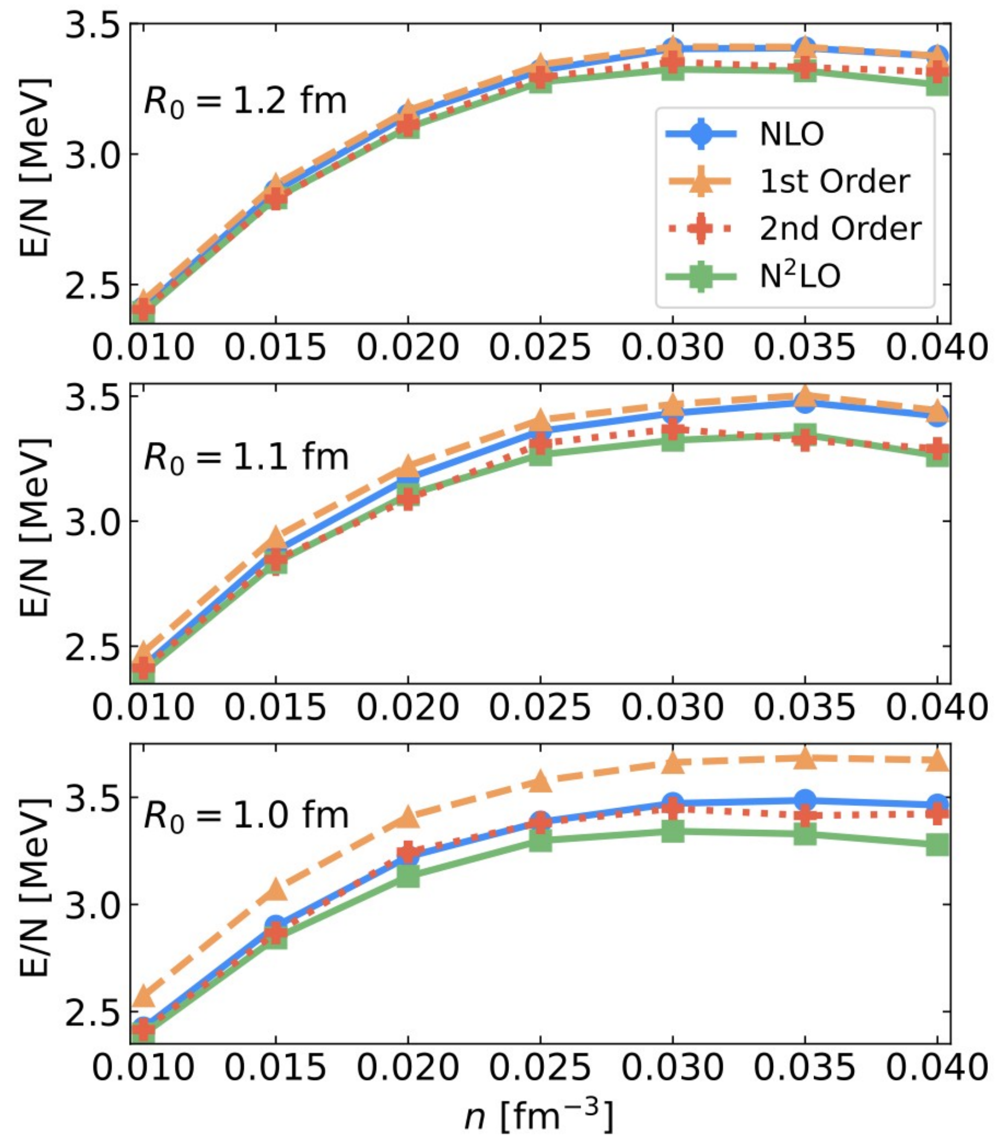

- 66 neutrons
- combination of DMC and PT
- three different cutoffs

(recall our desiderata)

R. Curry, J. E. Lynn, K. E. Schmidt, A. Gezerlis, arXiv:2302.07285

Setting the stage

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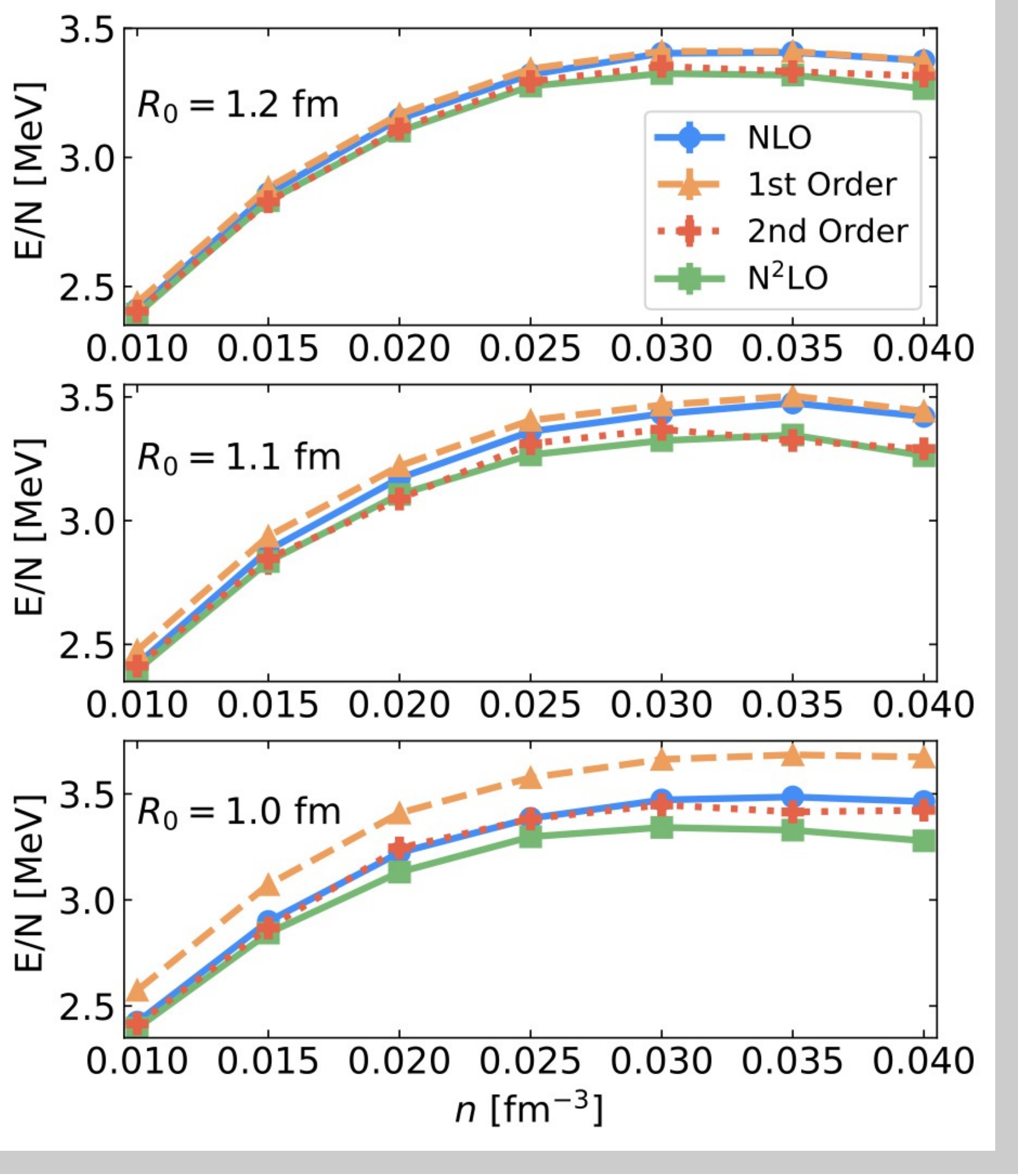
R. Curry, J. E. Lynn, K. E. Schmidt, A. Gezerlis, arXiv:2302.07285

Application 3

Many neutrons in a box (order-by-order perturbation)

Once again,
speed of convergence
depends on softness
of interaction.

(*The end is in the beginning and yet you go on*.)



R. Curry, J. E. Lynn, K. E. Schmidt, A. Gezerlis,
arXiv:2302.07285

Conclusions

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- Exciting time in terms of interplay between nuclear interactions and many-body approaches
- Non-perturbative and perturbative approaches are being fruitfully combined
- Detailed probe of well-behavedness of interactions with different cutoffs at the many-body level

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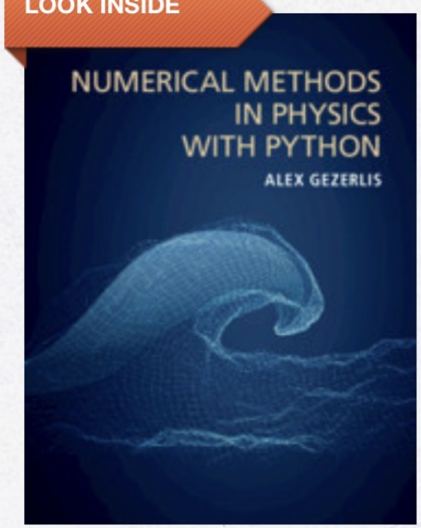

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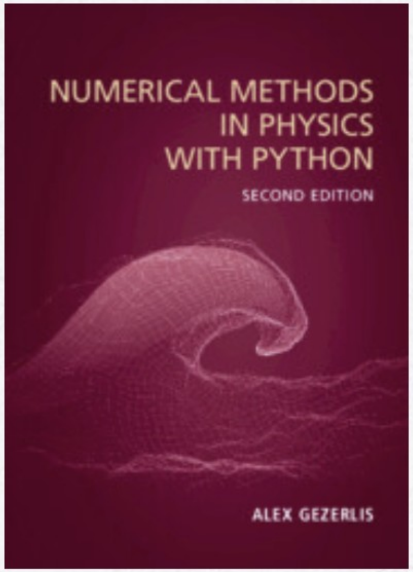

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2nd Edition

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