Momentum distributions and pair distribution functions

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www.computingnuclei.org

Nucleon-nucleon correlations

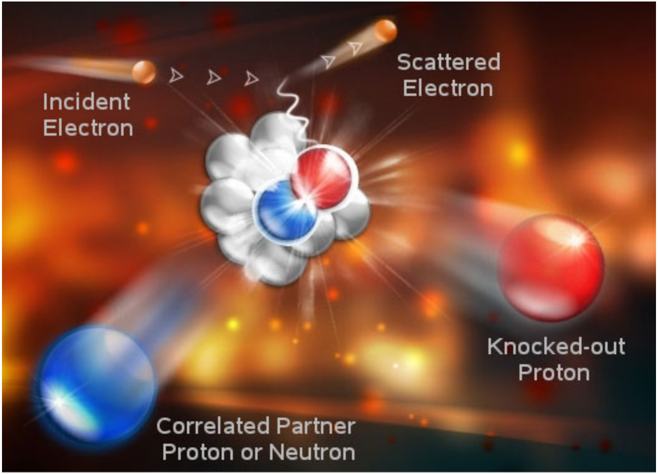
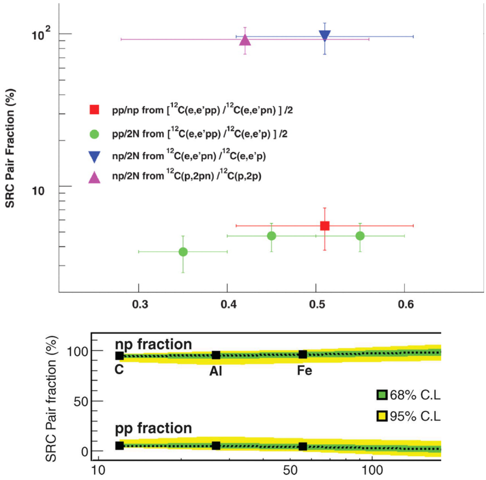


Illustration of back-to-back proton-neutron pairs in Jefferson Lab Experiment, Subedi *et al.*, Science (2008)

Nucleon-nucleon correlations



Ratio of np to pp pairs in light (upper panel) and heavy (lower panel) nuclei, Subedi *et al.*, Science (2008), Hen *et al.*, Science (2014)

Nucleon-nucleon correlations

Overarching questions:

- What is the origin of nucleon-nucleon correlations?
- Are nucleons more correlated at low- or high-momenta?
- Can we extract information from momentum distributions?
- Can we extract information from pair correlation functions?
- Which are observables and data related to those correlations?

In this talk **I am not giving answers**, but showing what we can calculate!

- One-body momentum distributions
- Two-body momentum distributions
- Contact parameter in cold atoms but not in nuclei

Nuclear Hamiltonian

Most common models: non-relativistic nucleons interacting with an effective nucleon-nucleon force (NN) and three-nucleon interaction (TNI).

$$H = -\frac{\hbar^2}{2m}\sum_{i=1}^{A}\nabla_i^2 + \sum_{i<j} v_{ij} + \sum_{i<j<k} V_{ijk}$$

v_{ij} NN, Argonne, chiral EFT, CD-Bonn, etc.

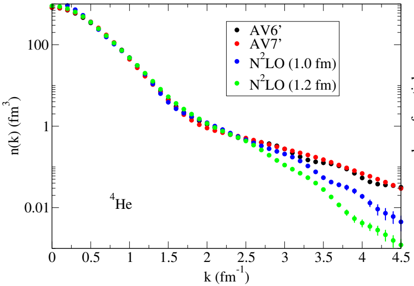
V_{ijk} TNI Urbana, Illinois, chiral EFT, etc.

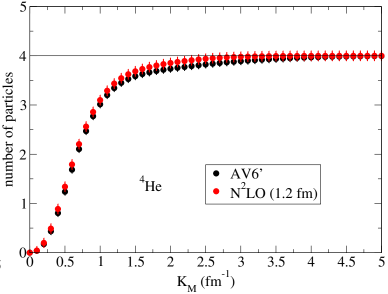
Many-body methods: GFMC, AFDMC, CC, SCGF, ...

Momentum distribution - ^{4}He

Preliminary!

AFDMC calculations:

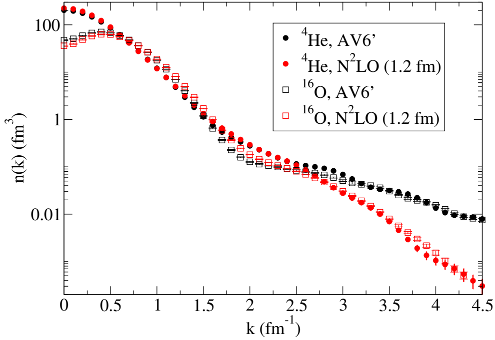




Useful to "check" the contact(s)?

Preliminary!

By rescaling the momentum distributions of ^{4}He and ^{16}O, at large momenta they seem universal:

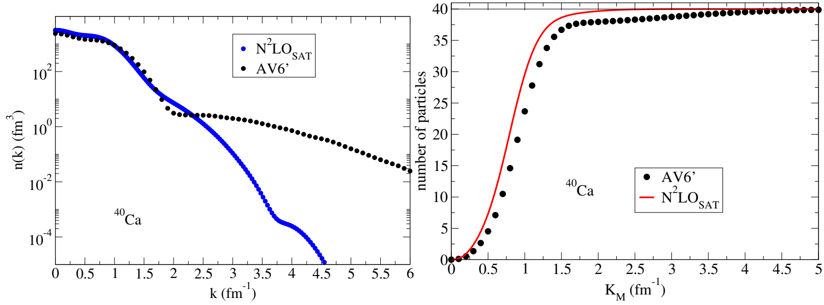


Again, useful to "check" the contact(s)?

Momentum distribution - ^{40}Ca

Preliminary!

AFDMC calculations using AV6' compared to Coupled-Cluster using $N2LO_{SAT}$:

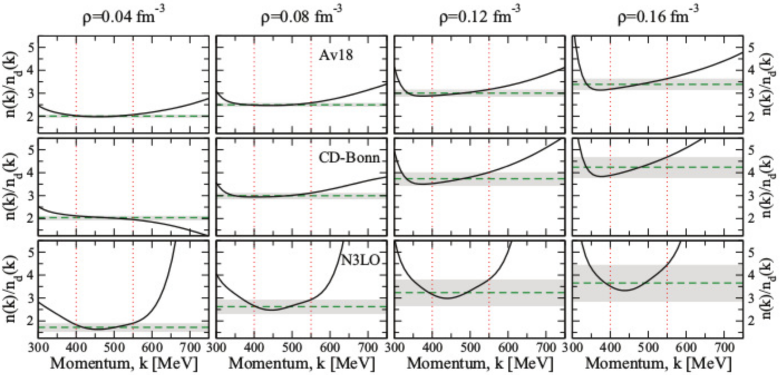


CC calculations provided by G. Hagen (ORNL).

Implications???

Symmetric nuclear matter

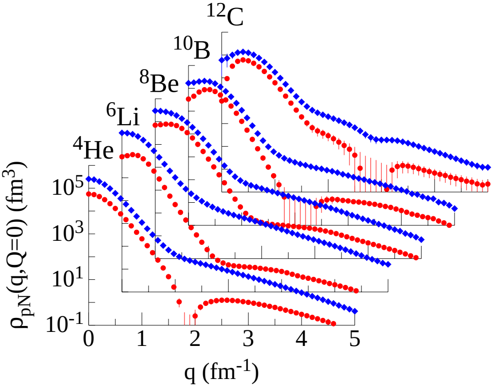
Self Consistent Green's Function calculations of nuclear matter:



Rios, Polls, Dickhoff, PRC (2014)

Two-body momentum distributions in light nuclei

VMC calculations using AV18+UIX:

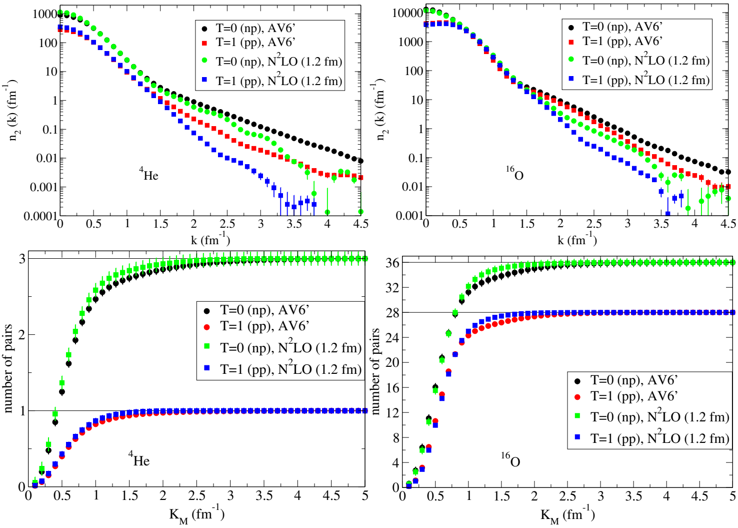


Carlson, *et al.*, RMP (2015).

Blue symbols are T=0 pairs, and red symbols are T=1 pairs.

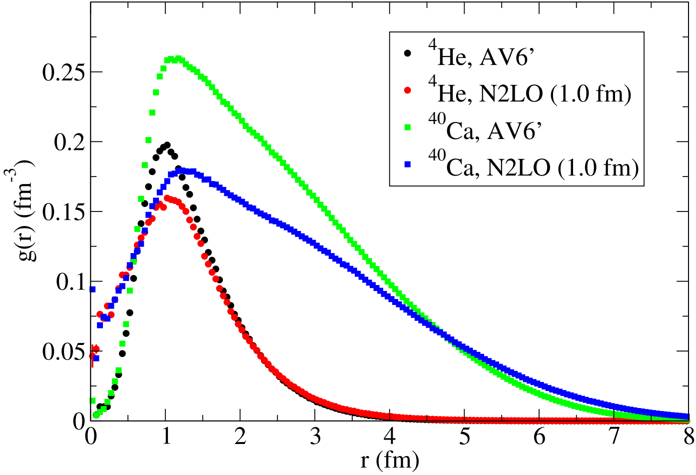
Strong dominance of T=0 pairs!

Preliminary! AFDMC calculations using different NN interactions (Q integrated):



Pair distribution functions

Preliminary! AFDMC calculations using different NN interactions:



Very similar at the origin, but more statistics needed.

For the last time ... useful to "check" the contact(s)?

Contact parameter

Tan universal relations: **Tan's** contact

$$\frac{E}{E_{FG}} = \xi - \frac{\zeta}{k_F a} - \frac{5\nu}{3(k_F a)^2} + \dots, \qquad \frac{C}{N k_F} = \frac{6}{5}\pi\zeta$$

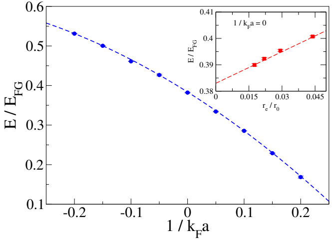
$$N(k) \to \frac{8}{10\pi}\zeta\frac{k_F^4}{k^4} = \frac{2}{3\pi^2}\frac{C}{N k_F}\frac{k_F^4}{k^4}$$

$$g_{\uparrow\downarrow}(r) \to \frac{9\pi}{20}\zeta(k_F r)^{-2} = \frac{3}{8}\frac{C}{N k_F}(k_F r)^{-2}$$

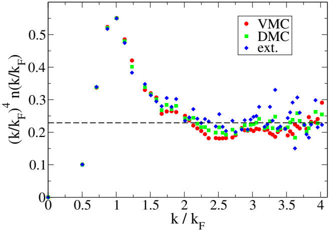
$$S_{\uparrow\downarrow}(k) \to \frac{3\pi}{10}\zeta\frac{k_F}{k} = \frac{1}{4}\frac{C}{N k_F}\frac{k_F}{k}$$

Shina Tan, Ann. Phys. (2008).

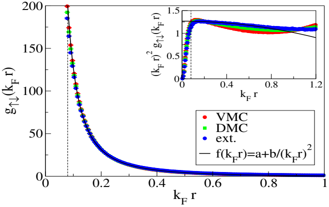
Contact parameter



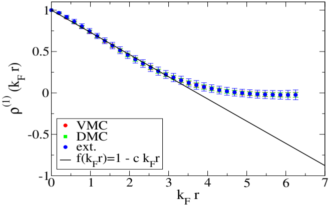
Equation of state



Momentum distribution



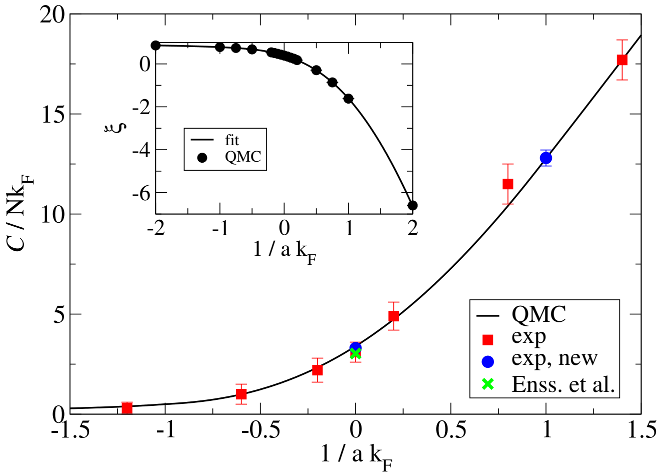
Pair distribution function



One-body density matrix

$C/Nk_F = 3.39(1)$, Gandolfi, Schmidt, Carlson, PRA 83, 041601 (2011).

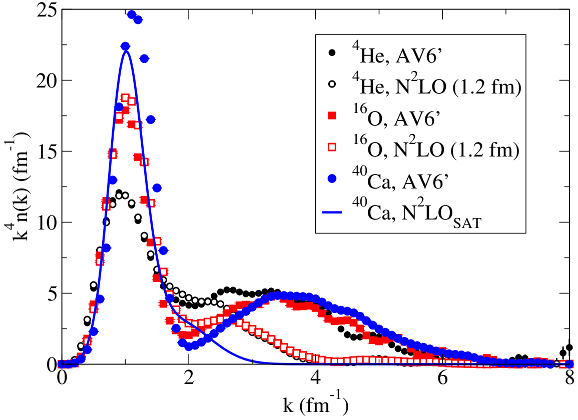
Contact parameter



Hoinka, Lingham, Fenech, Hu, Vale, Drut, Gandolfi, PRL 110, 055305 (2013).

Contact parameter in nuclei?

Preliminary!



Some flat region for harder interactions that is “maybe” universal for different A (but not using different interactions).

Summary

Thank you!

Discussion ...

Extra slides

Nuclear Hamiltonian

Model: non-relativistic nucleons interacting with an effective nucleon-nucleon force (NN) and three-nucleon interaction (TNI).

$$H = -\frac{\hbar^2}{2m}\sum_{i=1}^{A}\nabla_i^2 + \sum_{i<j} v_{ij} + \sum_{i<j<k} V_{ijk}$$

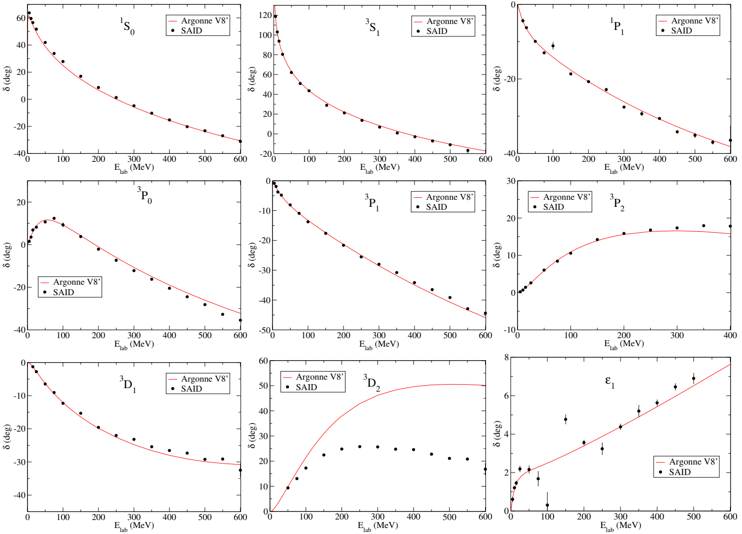
v_{ij} NN fitted on scattering data. Sum of operators:

$$v_{ij} = \sum O_{ij}^{p=1,8} v^p(r_{ij}), \quad O_{ij}^p = (1, \vec{\sigma}_i \cdot \vec{\sigma}_j, S_{ij}, \vec{L}_{ij} \cdot \vec{S}_{ij}) \times (1, \vec{\tau}_i \cdot \vec{\tau}_j)$$

Argonne AV8'.

Local chiral forces up to N^2LO has the similar spin/isospin operatorial structure of AV8' - Gezerlis, Tews, et al. PRL (2013), PRC (2014)

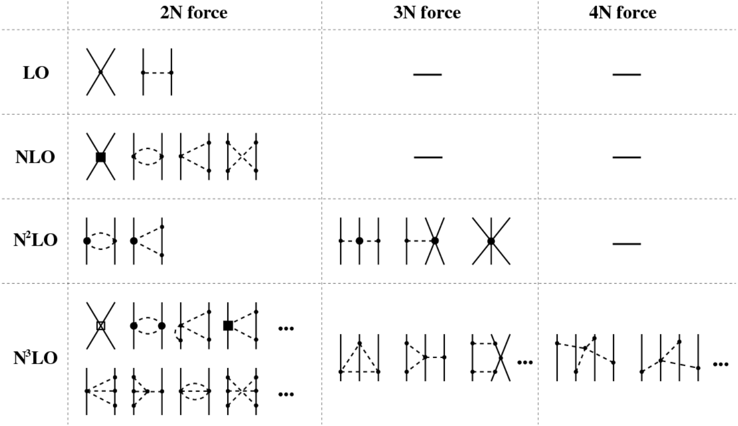
Phase shifts, AV8'



Difference AV8′-AV18 less than 0.2 MeV per nucleon up to A=12.

Nuclear Hamiltonian

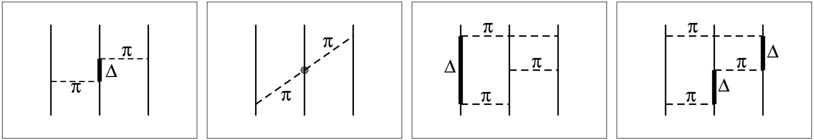
Chiral EFT interactions



Short range operators need to be regulated → cutoff dependency!

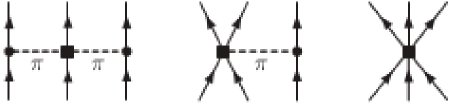
Three-body forces

Urbana–Illinois V_{ijk} models processes like



$+$ short-range correlations (spin/isospin independent).

Chiral forces at N^{2}LO:



c_1, c_3, c_4 c_D c_E

Nuclear Hamiltonians

Advantages:

- Argonne interactions fit phase shifts up to high energies: accurate up to high densities. Provide a very good description of several observables in light nuclei.
- Interactions derived from chiral EFT can be systematically improved. Changing the cutoff probes the physics and energy scales entering into observables. They are generally softer, and make most of the calculations easier to converge.

Disadvantages:

- Phenomenological interactions are phenomenological, not clear how to improve their quality. Systematic uncertainties hard to quantify.
- Chiral interactions describe low-energy (momentum) physics: bad for high densities. How do they work at large momenta, (i.e. e and ν scattering)?

Important to consider both and compare predictions

Scattering data and neutron matter

The energy of scattering data included in the fit gives an idea of the validity of the interaction in dense matter.

Two neutrons have

$$k \approx \sqrt{E_{lab}\, m/2}\,, \qquad \to k_F$$

that correspond to

$$k_F \to \rho \approx (E_{lab}\, m/2)^{3/2}/2\pi^2\,.$$

E_{lab}=150 MeV corresponds to about 0.12 fm^{-3}.

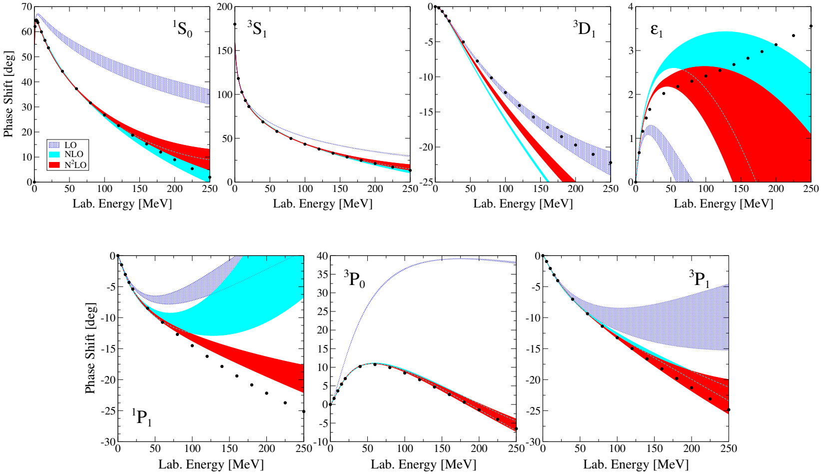
E_{lab}=350 MeV to 0.44 fm^{-3}.

Argonne potentials useful for dense matter well above ρ_0=0.16 fm^{-3}

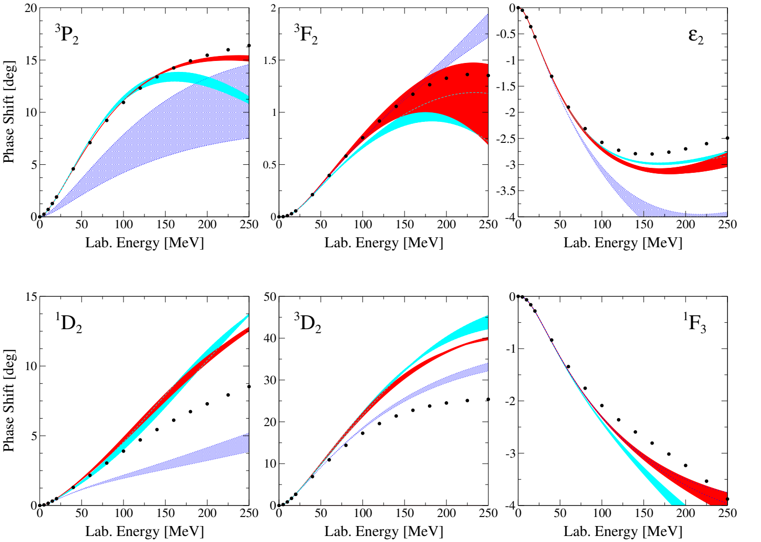
Recent chiral forces fit $30 < E_{lab} < 200$ MeV.

Nuclear Hamiltonian

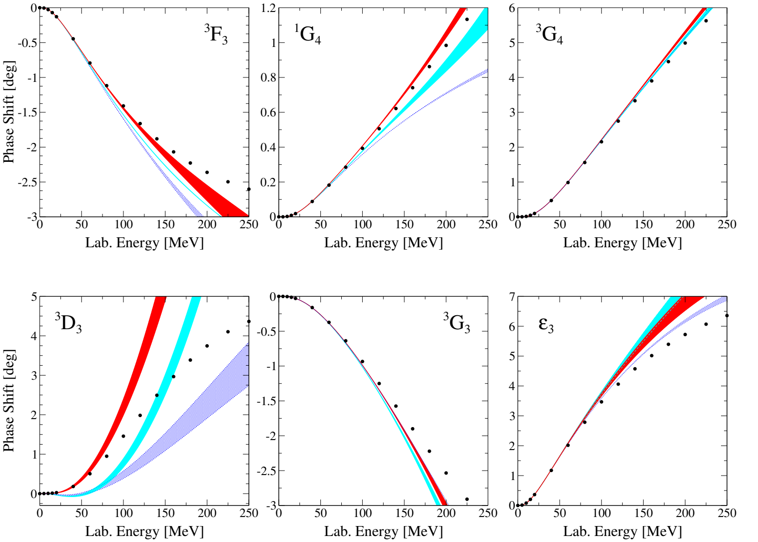
Phase shifts, LO, NLO and N^2LO with R_0=1.0 and 1.2 fm:



Phase shifts, LO, NLO and N^2LO with R_0=1.0 and 1.2 fm:

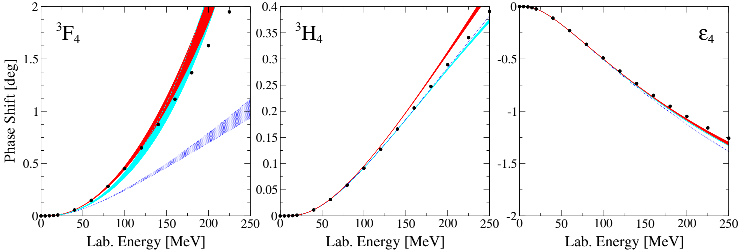


Phase shifts, LO, NLO and N^2LO with R_0=1.0 and 1.2 fm:



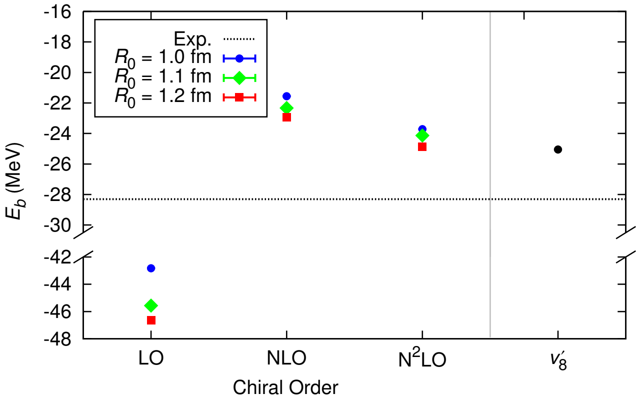
Nuclear Hamiltonian

Phase shifts, LO, NLO and N^2LO with R_0=1.0 and 1.2 fm:



^{4}He energy with chiral two-body interactions.

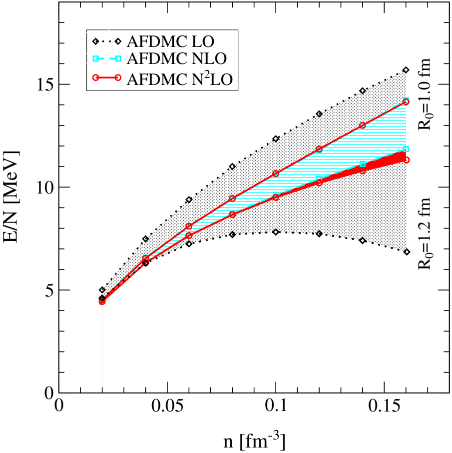
Binding energy of ^{4}He with only two-body interactions:



Lynn, Carlson, Epelbaum, Gandolfi, Gezerlis, Schwenk, PRL (2014).

Neutron matter

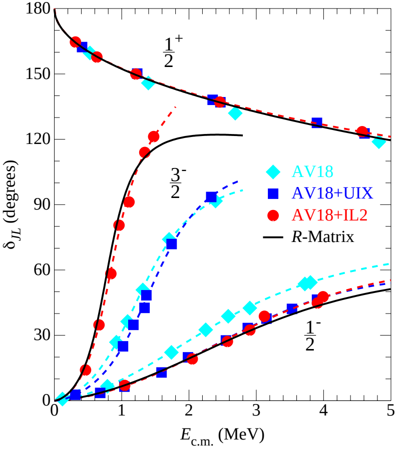
Equation of state of neutron matter using NN chiral forces:



Gezerlis, Tews, *et al.*, PRL (2013), PRC (2014)

Chiral three-body forces

Coefficients c_D and c_E fit to reproduce the binding energy of ^{4}He and neutron-^{4}He scattering. $\rightarrow$ more information on T=3/2 part of three-body interaction.

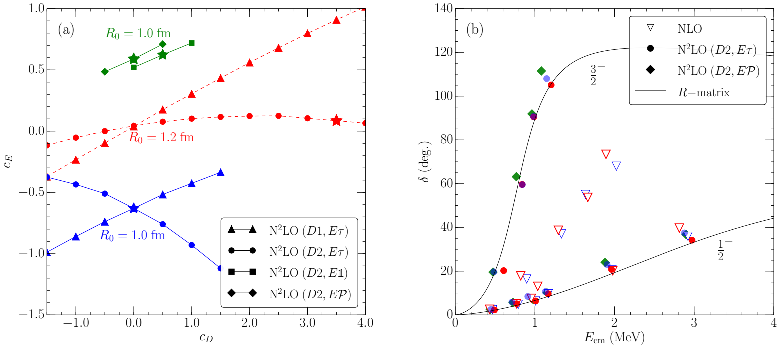


GFMC neutron-^{4}He results using Argonne Hamiltonians.

Nollett, Pieper, Wiringa, Carlson, Hale, PRL (2007).

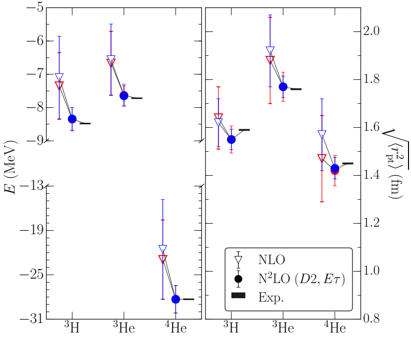
Regulator: $\delta(r) = \frac{1}{\pi\Gamma(3/4)R_0^3} \exp[-(r/R_0)^4]$

Cutoff R_0 taken consistently with the two-body interaction.



No fit to both observables can be obtained for $R_0 = 1.2$ fm and V_{D1}

Lynn, Tews, Carlson, Gandolfi, Gezerlis, Schmidt, Schwenk PRL (2016).



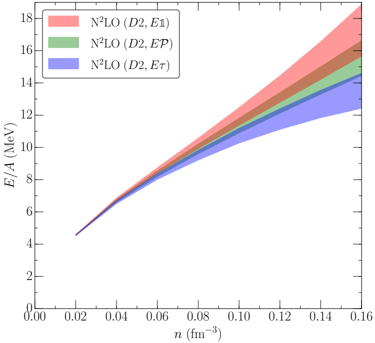
Error quantification: define $Q = \max\left(\frac{p}{\Lambda_b}, \; \frac{m_\pi}{\Lambda_b}\right)$ and calculate:

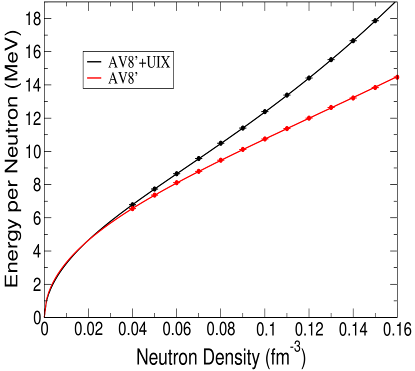
$$\Delta(N2LO) = \max\left(Q^4|\hat{O}_{LO}|, \; Q^2|\hat{O}_{LO} - \hat{O}_{NLO}|, \; Q|\hat{O}_{NLO} - \hat{O}_{N2LO}|\right)$$

Epelbaum, Krebs, Meissner (2014).

Neutron matter at N2LO

EOS of pure neutron matter at N2LO, R_0=1.0 fm.
Error quantification estimated as previously.





Lynn, Tews, Carlson, Gandolfi, Gezerlis, Schmidt, Schwenk PRL (2016).

Quantum Monte Carlo

Projection in imaginary-time t:

$$H\,\psi(\vec{r}_1\ldots\vec{r}_N) = E\,\psi(\vec{r}_1\ldots\vec{r}_N) \qquad \psi(t) = e^{-(H-E_T)t}\psi(0)$$

Ground-state extracted in the limit of $t\to\infty$.

Propagation performed by

$$\psi(R,t) = \langle R|\psi(t)\rangle = \int dR'\,G(R,R',t)\psi(R',0)$$

- $dR' \to dR_1\,dR_2\ldots,\ G(R,R',t) \to G(R_1,R_2,\delta t)\,G(R_2,R_3,\delta t)\ldots$
- Importance sampling: $G(R,R',\delta t) \to G(R,R',\delta t)\,\Psi_I(R')/\Psi_I(R)$
- Constrained-path approximation to control the sign problem. Unconstrained calculation possible in several cases (exact).

Ground–state obtained in a **non-perturbative way.** Systematic uncertainties within 1-2 %.

Overview

Recall: propagation in imaginary-time

$$e^{-(T+V)\Delta\tau}\psi \approx e^{-T\Delta\tau}e^{-V\Delta\tau}\psi$$

Kinetic energy is sampled as a diffusion of particles:

$$e^{-\nabla^2\Delta\tau}\psi(R) = e^{-(R-R')^2/2\Delta\tau}\psi(R) = \psi(R')$$

The (scalar) potential gives the weight of the configuration:

$$e^{-V(R)\Delta\tau}\psi(R) = w\psi(R)$$

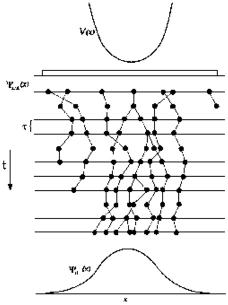
Algorithm for each time-step:

- do the diffusion: $R' = R + \xi$
- compute the weight w
- compute observables using the configuration R' weighted using w over a trial wave function ψ_T.

For spin-dependent potentials things are much worse!

Branching

The configuration weight w is efficiently sampled using the branching technique:



Configurations are replicated or destroyed with probability

$$int[w + \xi]$$

Note: the re-balancing is the bottleneck limiting the parallel efficiency.

Because the Hamiltonian is state dependent, all spin/isospin states of nucleons must be included in the wave-function.

Example: spin for 3 neutrons (radial parts also needed in real life):

GFMC wave-function:

$$\psi = \begin{pmatrix} a_{\uparrow\uparrow\uparrow} \\ a_{\uparrow\uparrow\downarrow} \\ a_{\uparrow\downarrow\uparrow} \\ a_{\uparrow\downarrow\downarrow} \\ a_{\downarrow\uparrow\uparrow} \\ a_{\downarrow\uparrow\downarrow} \\ a_{\downarrow\downarrow\uparrow} \\ a_{\downarrow\downarrow\downarrow} \end{pmatrix}$$

A correlation like

$$1 + f(r)\sigma_1 \cdot \sigma_2$$

can be used, and the variational wave function can be very good. Any operator accurately computed.

AFDMC wave-function:

$$\psi = \mathcal{A}\left[\xi_{s_1}\begin{pmatrix} a_1 \\ b_1 \end{pmatrix}\xi_{s_2}\begin{pmatrix} a_2 \\ b_2 \end{pmatrix}\xi_{s_3}\begin{pmatrix} a_3 \\ b_3 \end{pmatrix}\right]$$

We must change the propagator by using the Hubbard-Stratonovich transformation:

$$e^{\frac{1}{2}\Delta t O^2} = \frac{1}{\sqrt{2\pi}}\int dx e^{-\frac{x^2}{2}+x\sqrt{\Delta t}O}$$

Auxiliary fields x must also be sampled. The wave-function is pretty bad, but we can simulate larger systems (up to $A \approx 100$). Operators (except the energy) are very hard to be computed, but in some case there is some trick!

Propagator

We first rewrite the potential as:

$$V = \sum_{i<j} [v_\sigma(r_{ij})\vec{\sigma}_i \cdot \vec{\sigma}_j + v_t(r_{ij})(3\vec{\sigma}_i \cdot \hat{r}_{ij}\vec{\sigma}_j \cdot \hat{r}_{ij} - \vec{\sigma}_i \cdot \vec{\sigma}_j)] =$$

$$= \sum_{i,j} \sigma_{i\alpha} A_{i\alpha;j\beta} \sigma_{j\beta} = \frac{1}{2} \sum_{n=1}^{3N} O_n^2 \lambda_n$$

where the new operators are

$$O_n = \sum_{j\beta} \sigma_{j\beta} \psi_{n,j\beta}$$

Now we can use the HS transformation to do the propagation:

$$e^{-\Delta\tau \frac{1}{2} \sum_n \lambda O_n^2} \psi = \prod_n \frac{1}{\sqrt{2\pi}} \int dx e^{-\frac{x^2}{2} + \sqrt{-\lambda\Delta\tau} x O_n} \psi$$

Computational cost $\approx (3N)^3$.

Three-body forces

Three-body forces, Urbana, Illinois, and local chiral N^{2}LO can be exactly included in the case of neutrons.

For example:

$$\begin{aligned} O_{2\pi} &= \sum_{cyc}\left[\{X_{ij},X_{jk}\}\{\tau_i\cdot\tau_j,\tau_j\cdot\tau_k\}+\frac{1}{4}[X_{ij},X_{jk}][\tau_i\cdot\tau_j,\tau_j\cdot\tau_k]\right] \\ &= 2\sum_{cyc}\{X_{ij},X_{jk}\}=\sigma_i\sigma_k f(r_i,r_j,r_k) \end{aligned}$$

The above form can be included in the AFDMC propagator.

Variational wave function

$$E_0 \leq E = \frac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle} = \frac{\int dr_1 \ldots dr_N \, \psi^*(r_1 \ldots r_N) H \psi^*(r_1 \ldots r_N)}{\int dr_1 \ldots dr_N \, \psi^*(r_1 \ldots r_N) \psi^*(r_1 \ldots r_N)}$$

$\rightarrow$ Monte Carlo integration. Variational wave function:

$$|\Psi_T\rangle = \left[\prod_{i<j} f_c(r_{ij})\right] \left[\prod_{i<j<k} f_c(r_{ijk})\right] \left[1 + \sum_{i<j,p} \prod_k u_{ijk} f_p(r_{ij}) O_{ij}^p\right] |\Phi\rangle$$

where O^p are spin/isospin operators, f_c, u_{ijk} and f_p are obtained by minimizing the energy. About 30 parameters to optimize.

$|\Phi\rangle$ is a mean-field component, usually HF. Sum of many Slater determinants needed for open-shell configurations.

BCS correlations can be included using a Pfaffian.

The Sign problem in one slide

Evolution in imaginary-time:

$$\psi_I(R')\Psi(R', t+dt) = \int dR\, G(R, R', dt) \frac{\psi_I(R')}{\psi_I(R)} \psi_I(R)\Psi(R, t)$$

note: $\Psi(R, t)$ must be positive to be "Monte Carlo" meaningful.

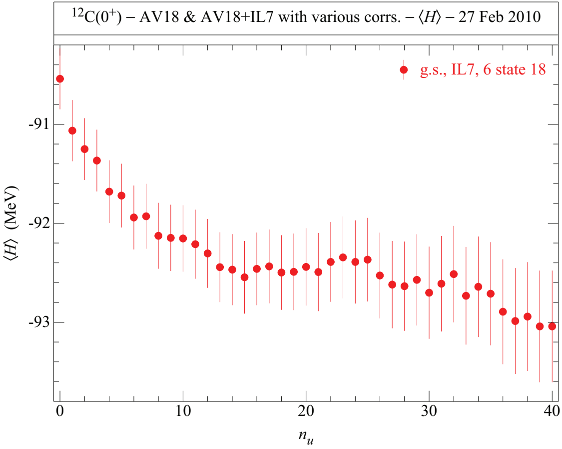
Fixed-node approximation: solve the problem in a restricted space where $\Psi > 0$ (Bosonic problem) $\Rightarrow$ upperbound.

If Ψ is complex:

$$|\psi_I(R')||\Psi(R', t+dt)| = \int dR\, G(R, R', dt) \left|\frac{\psi_I(R')}{\psi_I(R)}\right| |\psi_I(R)||\Psi(R, t)|$$

Constrained-path approximation: project the wave-function to the real axis. Extra weight given by $\cos\Delta\theta$ (phase of $\frac{\Psi(R')}{\Psi(R)}$), $Re\{\Psi\} > 0 \Rightarrow$ not necessarily an upperbound.

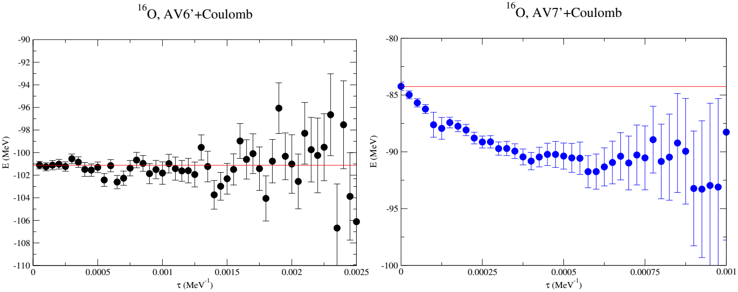
GFMC unconstrained-path propagation:



Changing the trial wave function gives same results.

Unconstrained-path

AFDMC unconstrained-path propagation:



The difference between CP and UP results is mainly due to the presence of LS terms in the Hamiltonian. Same for heavier systems.

Work in progress to improve Ψ to improve the constrained-path.