Nuclear magnetic moments from chiral EFT

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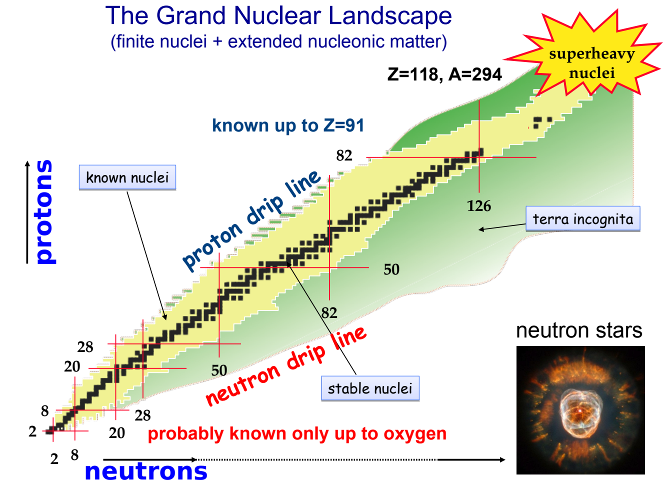
NUCLEI Nuclear Computational Low-Energy Initiative

U.S. DEPARTMENT OF ENERGY

www.computingnuclei.org

NERSC National Energy Research Scientific Computing Center



Plus Electro-weak transitions, response functions, reactions, etc.

Outline

- The nuclear Hamiltonian and the method
- Nuclear energies and charge radii
- Nuclear and neutron matter EOS
- Electro-magnetic currents and nuclear magnetic moments
- Conclusions

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.

V_{ijk} typically constrained to reproduce light systems (A=3,4).

- "Phenomenological/traditional" interactions (Argonne/Illinois)
- Local chiral forces up to N^{2}LO (Gezerlis, et al. PRL 111, 032501 (2013), PRC 90, 054323 (2014), Lynn, et al. PRL 116, 062501 (2016)).

Quantum Monte Carlo

Propagation in imaginary time:

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

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

Propagation performed by

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

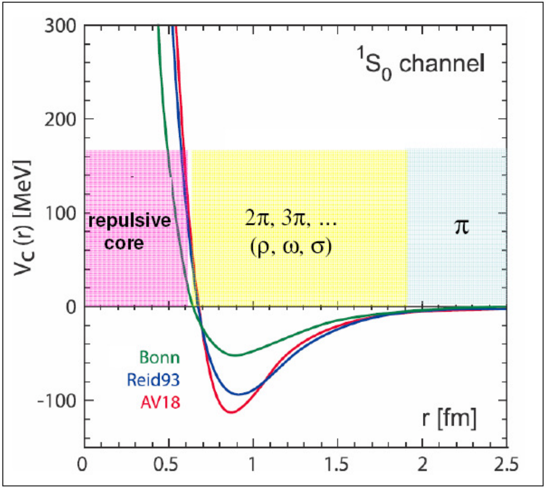
- Importance sampling: $G(R,R',t) \to G(R,R',t)\,\Psi_I(R')/\Psi_I(R)$
- Constrained-path approximation to control the sign problem. Unconstrained-path calculation possible in several cases (exact).

GFMC includes all spin-states of nucleons in the w.f., nuclei up to A=12
AFDMC samples spin states, bigger systems, less accurate than GFMC

Ground–state obtained in a **non-perturbative way.** Systematic uncertainties within 2-3 %.

See Carlson, et al., Rev. Mod. Phys. 87, 1067 (2015)

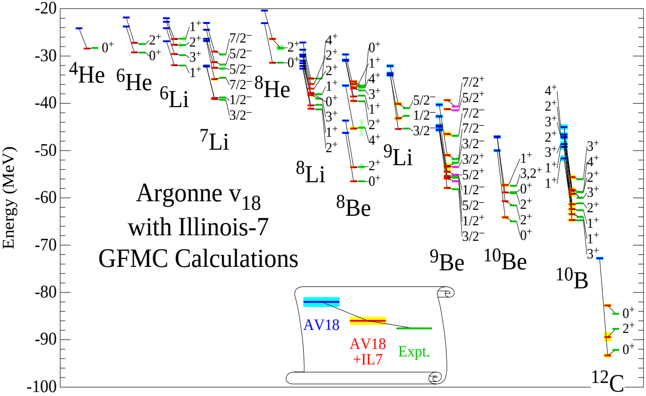
Traditional approach (credit D. Furnstahl, T. Papenbrock)



From T. Hatsuda (Oslo 2008)

Argonne v_{18}, CD-BONN, ...

Light nuclei spectrum with phenomenological Hamiltonians



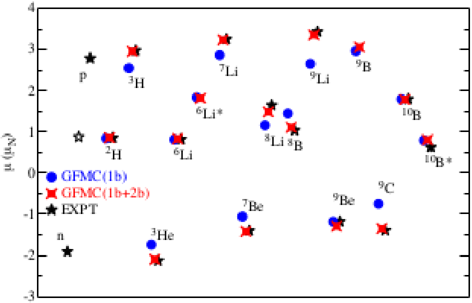
Carlson, et al., Rev. Mod. Phys. 87, 1067 (2015)

Also radii, densities, ...

Unfortunately phenomenological Hamiltonians are not useful to address systematical uncertainties.

Nuclear magnetic with phenomenological currents

Magnetic moments provide a good benchmark to test electro-magnetic currents at low (zero) momentum.

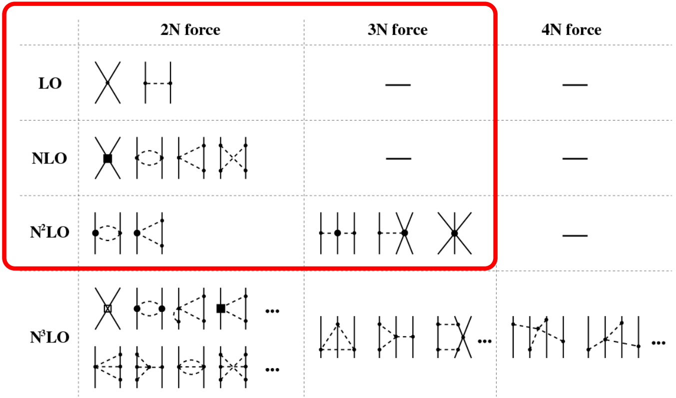


Pastore *et* al, PRC 2013

Also matrix elements, $\beta-$decays, response functions, ...

Unfortunately phenomenological currents are not useful to address systematical uncertainties.

Nuclear Hamiltonian



Expansion in powers of Q/Λ, Q$\sim$100 MeV, Λ $\sim$1 GeV.

Long-range physics given by pion-exchanges (no free parameters).

Short-range physics: contact interactions (LECs) to fit.

Operators need to be regulated $\rightarrow$ cutoff dependency!

Order's expansion provides a way to quantify uncertainties!

Truncation error estimate

Error quantification (one possible scheme), friendly (easy) one. Define

$$Q = \max\left(\frac{p}{\Lambda_b}, \ \frac{m_\pi}{\Lambda_b}\right),$$

where p is a typical nucleon's momentum or k_F for matter, Λ_b is the cutoff, and calculate:

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

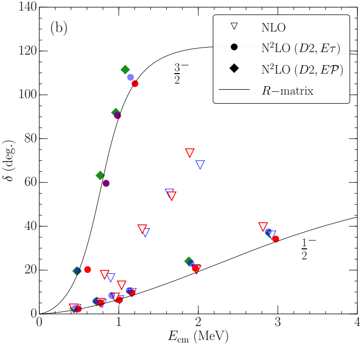
Epelbaum, Krebs, Meissner (2014).

^{4}He binding energy and p-wave n-^{4}He scattering

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

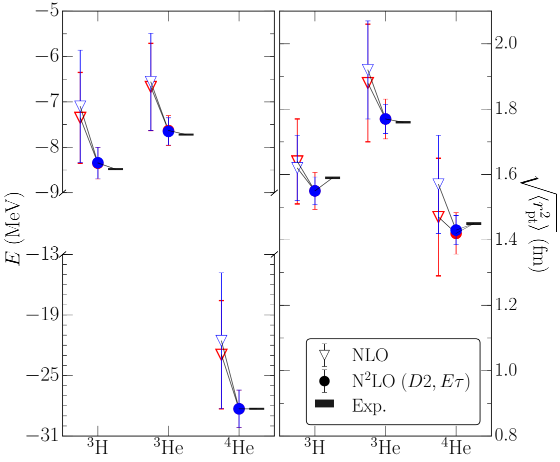
Cutoff R_0 taken consistently with the two-body interaction.

Fit: ^4He binding energy and n-^4He scattering.



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

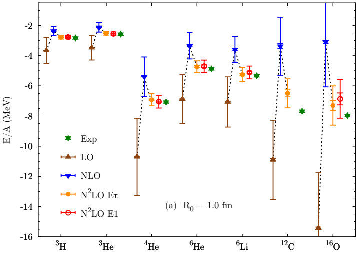
A=3, 4 nuclei at N2LO

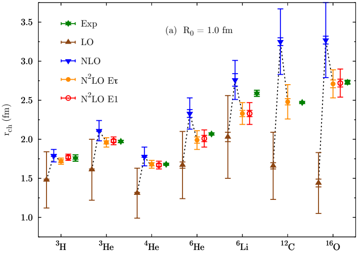


Lynn, Tews, Carlson, Gandolfi, Gezerlis, Schmidt, Schwenk PRL (2016).

AFDMC calculations

Energies and charge radii, cutoff 1.0 fm:





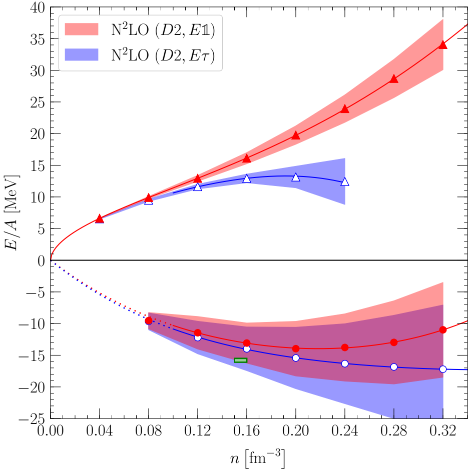
Lonardoni, et al., PRL (2018), PRC (2018).

Qualitative good description of both energies and radii.

Good convergence (although uncertainties still large if LO included).

Different V_E operators give similar results. For a softer cutoff (not shown) things are worse.

Nuclear and neutron matter EOS

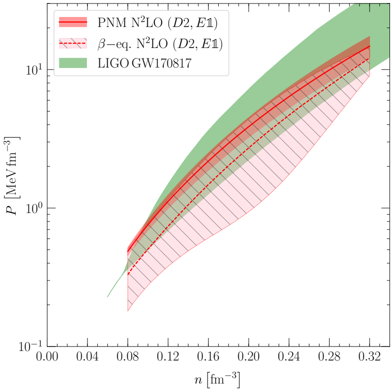


Lonardoni, et al., Phys. Rev. Research 2, 022033(R) (2020).

Symmetric nuclear matter less dependent upon the choice of V_E (cf. nuclei). E_τ is very bad for neutron matter.

Nuclear and neutron matter EOS

Pressure of pure neutron matter and $\beta-$equilibrated matter.



Lonardoni, et al., Phys. Rev. Research 2, 022033(R) (2020).

Very good agreement with LIGO posterior from GW.

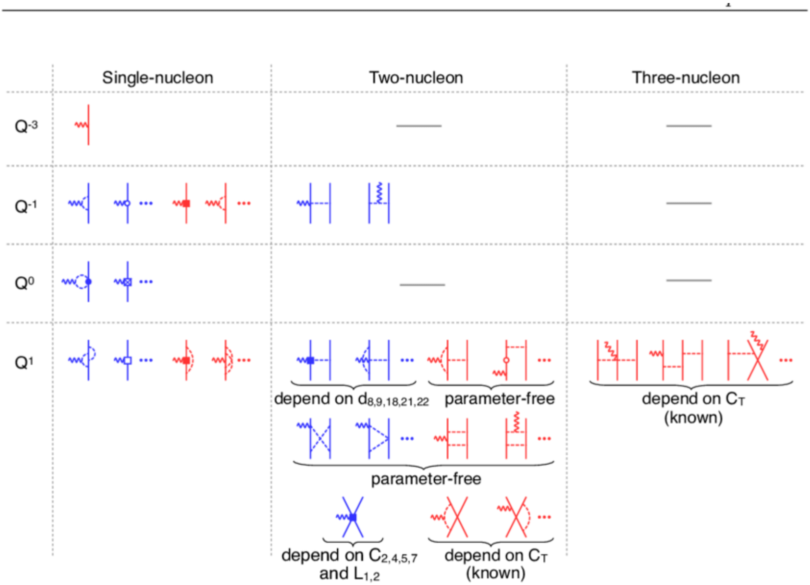
Magnetic moments

Nuclear magnetic moments for a nucleus A can be calculated as:

$$F_M(q;A) = -i\frac{2m}{q}\langle A;JJ_z|j_y(q\hat{x})|A;JJ_z\rangle\,,$$
$$\mu_A = f_M(0;A)$$

where $\vec{j}$ are electro-magnetic currents (see next slides) with one-, two-, (more)-body operators.

Electro-magnetic currents



Electro-magnetic currents

But, within chiral EFT, there are different ways to construct the currents, different expansions.

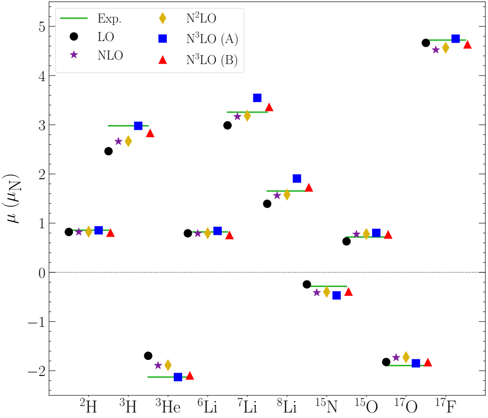
Hamiltonian	Pisa/Norfolk/WUSTL	Bochum
Q^0 LO	Q^{-2} LO	Q^{-3} LO
Q^1 –	Q^{-1} NLO	Q^{-2} –
Q^2 NLO	Q^0 N2LO	Q^{-1} NLO
Q^3 N2LO	Q^1 N3LO	Q^0 N2LO
		Q^1 N3LO
	2 LECS (contact)	2 LECS (contact)
	1 LEC (OPE)	

Understanding which currents to use, chiral order, regulators, continuity equation, etc., is still work in progress.

Here, same regulator as in the Hamiltonian, cutoff R_0=1.0 *fm*.

Nuclear magnetic moments

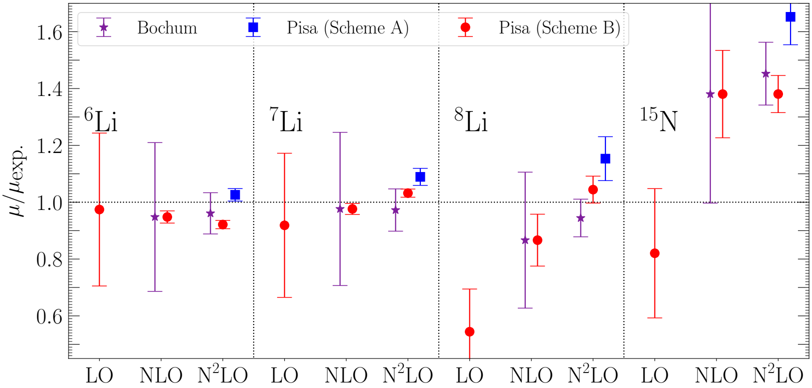
Fit: up to A=3 (A) or including all nuclei (B), Pisa.



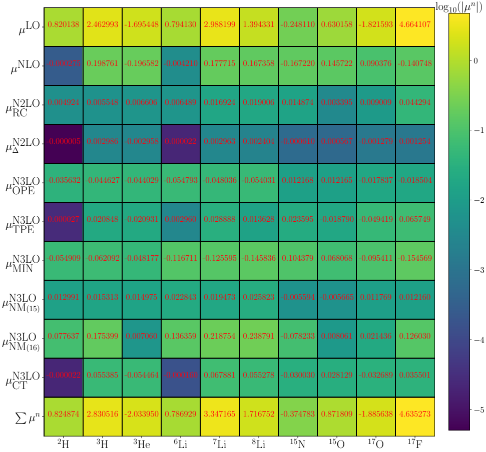
J. D. Martin, S. J. Novario, D. Lonardoni, J. Carlson, S. Gandolfi, I. Tews, arXiv:2301.08349.

Nuclear magnetic moments

Order by order calculation. Same order in the Hamiltonian and currents. Bochum LECs are fit to all nuclei (B).



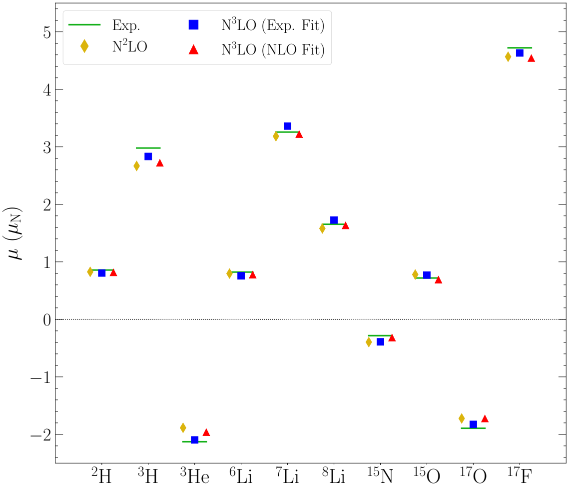
Magnetic moments, single contributions (Pisa).



In several cases, the contribution of N3LO terms is larger than N2LO and NLO.

Nuclear magnetic moments

Fit to have $|N^3LO| \ll |N^2LO|$ vs exp. (Pisa).



Conclusions

- Chiral EFT provides a way to constrain nuclear interactions and currents, and to estimate systematic uncertainties
- Nuclear energies, radii and EOS well reproduced by the hard interaction.
- Overall good description of nuclear magnetic moments. Best fitting strategy not clear yet.
- Convergence with the chiral expansion not clear.

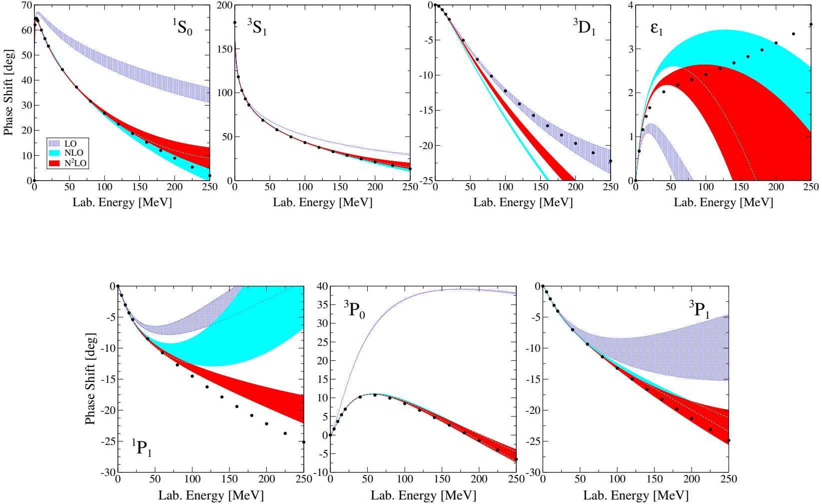
Acknowledgments:

J. Martin, S. Novario,

J. Carlson, I. Tews (LANL), R. Schiavilla (JLAB/ODU), H. Krebs (Bochum)

Extra slides

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



Gezerlis, et al. PRC 90, 054323 (2014)

Quantum Monte Carlo

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

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

Propagation performed by

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

- Importance sampling: $G(R,R',t) \to G(R,R',t)\,\Psi_I(R')/\Psi_I(R)$
- 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:

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

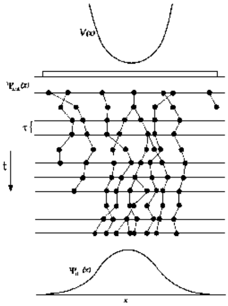
Algorithm for each time-step:

- 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.

GFMC and AFDMC

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^2LO 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.

Three-body forces

$$
\begin{aligned}
V_a^{2\pi,PW} &= A_a^{2\pi,PW} \sum_{i<j<k} \sum_{cyc} \{\vec{\tau}_i \cdot \vec{\tau}_k, \vec{\tau}_j \cdot \vec{\tau}_k\}\{\sigma_i^\alpha \sigma_k^\gamma, \sigma_k^\mu \sigma_j^\beta\} \mathcal{X}_{i\alpha k\gamma} \mathcal{X}_{k\mu j\beta} \\
&= 4A_a^{2\pi,PW} \sum_{i<j} \vec{\tau}_i \cdot \vec{\tau}_j \sigma_i^\alpha \sigma_j^\beta \sum_{k\neq i,j} \mathcal{X}_{i\alpha k\gamma} \mathcal{X}_{k\gamma j\beta} \,, \qquad (1) \\
V_c^{2\pi,PW} &= A_c^{2\pi,PW} \sum_{i<j<k} \sum_{cyc} [\vec{\tau}_i \cdot \vec{\tau}_k, \vec{\tau}_j \cdot \vec{\tau}_k][\sigma_i^\alpha \sigma_k^\gamma, \sigma_k^\mu \sigma_j^\beta] \mathcal{X}_{i\alpha k\gamma} \mathcal{X}_{k\mu j\beta} \\
&= -4A_c^{2\pi,PW} \sum_{i<j<k} \sum_{cyc} \tau_i^\eta \tau_j^\xi \tau_k^\phi \epsilon_{\eta\xi\phi} \sigma_i^\alpha \sigma_j^\beta \sigma_k^\nu \epsilon_{\nu\gamma\mu} \mathcal{X}_{i\alpha k\gamma} \mathcal{X}_{k\mu j\beta} \qquad (2) \\
&= A_c^{2\pi,PW} \sum_{i<j<k} \sum_{cyc} [\vec{\tau}_i \cdot \vec{\tau}_k, \vec{\tau}_j \cdot \vec{\tau}_k][\sigma_i^\alpha \sigma_k^\gamma, \sigma_k^\mu \sigma_j^\beta] \left(X_{i\alpha k\gamma} - \delta_{\alpha\gamma} \frac{4\pi}{m_\pi^3} \Delta(r_{ik}) \right) \left(X_{k\mu j\beta} - \delta_{\mu\beta} \frac{4\pi}{m_\pi^3} \Delta(r_{kj}) \right) \qquad (3) \\
&= V_c^{\Delta\Delta} + V_c^{\Delta\delta} + V_c^{\delta\delta} \qquad (4) \\
V^{2\pi,SW} &= A^{2\pi,SW} \sum_{i<j<k} \sum_{cyc} \mathcal{Z}_{ik\alpha} \mathcal{Z}_{jk\alpha} \sigma_i^\alpha \sigma_j^\beta \vec{\tau}_i \cdot \vec{\tau}_j \\
&= A^{2\pi,SW} \sum_{i<j} \sigma_i^\alpha \sigma_j^\beta \vec{\tau}_i \cdot \vec{\tau}_j \sum_{k\neq i,j} \mathcal{Z}_{ik\alpha} \mathcal{Z}_{jk\alpha} \qquad (5) \\
V_D &= A_D \sum_{i<j} \sigma_i^\alpha \sigma_j^\beta \vec{\tau}_i \cdot \vec{\tau}_j \sum_{k\neq i,j} \mathcal{X}_{i\alpha j\beta} [\Delta(r_{ik}) + \Delta(r_{jk})] \qquad (6) \\
V_E &= A_E \sum_{i<j} \vec{\tau}_i \cdot \vec{\tau}_j \sum_{k\neq i,j} \Delta(r_{ik}) \Delta(r_{jk}) \qquad (7)
\end{aligned}
$$

Three-body forces

$$H' = H - V_c^{2\pi,PW} + \alpha_1 V_a^{2\pi,PW} + \alpha_2 V_D + \alpha_3 V_E \,. \tag{8}$$

The Hamiltonian H' can be exactly included in the AFDMC propagation. The three constants α_i are adjusted in order to have:

$$\begin{aligned} \langle V_c^{\Delta\Delta} \rangle &\approx \langle \alpha_1 V_a^{2\pi,PW} \rangle \\ \langle V_c^{\Delta\delta} \rangle &\approx \langle \alpha_2 V_D \rangle \\ \langle V_c^{\delta\delta} \rangle &\approx \langle \alpha_3 V_E \rangle \end{aligned} \tag{9}$$

Once the ground state Ψ of H' is calculated with AFDMC as explained above, the expectation value of the Hamiltonian H is given by

$$\begin{aligned} \langle H \rangle &= \langle \Psi | H' | \Psi \rangle + \langle \Psi | H - H' | \Psi \rangle \\ &= \langle \Psi | H' | \Psi \rangle + \langle \Psi | V_c^{2\pi,PW} - \alpha_1 V_a^{2\pi,PW} - \alpha_2 V_D - \alpha_3 V_E | \Psi \rangle \end{aligned} \tag{10}$$

Variational wave function

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

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

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

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.

Variational wave function

$$\langle RS|\Psi_V\rangle = \langle RS|\Big[\prod_{i<j} f^c(r_{ij})\Big]\Big[1+\sum_{i<j}F_{ij}+\sum_{i<j<k}F_{ijk}\Big]|\Phi_{JM}\rangle\,,$$

$$\langle RS|\Phi_{JM}\rangle = \sum_n k_n\Big[\sum D\{\phi_\alpha(r_i,s_i)\}\Big]_{JM}\,,$$

$$\phi_\alpha(r_i,s_i) = \Phi_{nlj}(r_i)\left[Y_{lm_l}(\hat{r}_i)\xi_{sm_s}(s_i)\right]_{jm_j}\,,$$

In particular, we included orbitals in $1\mathrm{S}_{1/2}$, $1\mathrm{P}_{3/2}$, $1\mathrm{P}_{1/2}$, $1\mathrm{D}_{5/2}$, $2\mathrm{S}_{1/2}$, and $1\mathrm{D}_{3/2}$.

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.

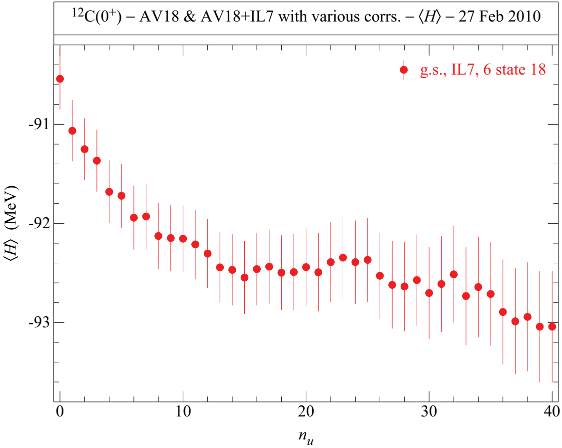
If Ψ is complex:

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

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.

Unconstrained-path

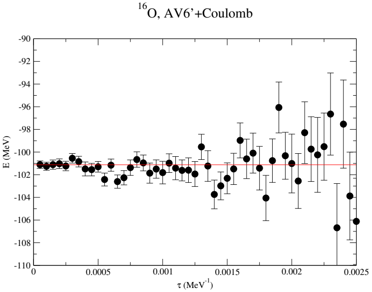
GFMC unconstrained-path propagation:

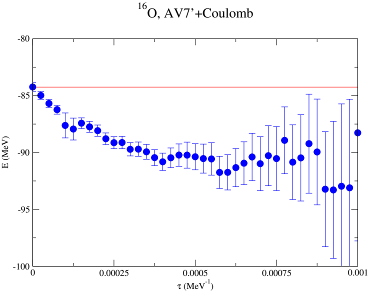


Changing the trial wave function gives same results.

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.