Quantum Monte Carlo calculations of properties of nuclei with chiral interactions

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NUCLEI Nuclear Computational Low-Energy Initiative

U.S. DEPARTMENT OF ENERGY

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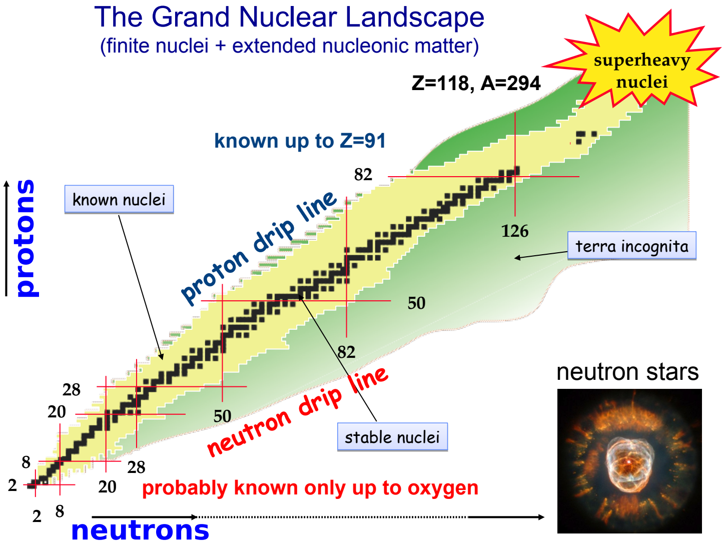
NERSC National Energy Research Scientific Computing Center

The big picture



Outline

- The nuclear Hamiltonian and the method
- Some “issue” of chiral Hamiltonians
- Light nuclei and neutron matter
- Medium nuclei
- 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

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

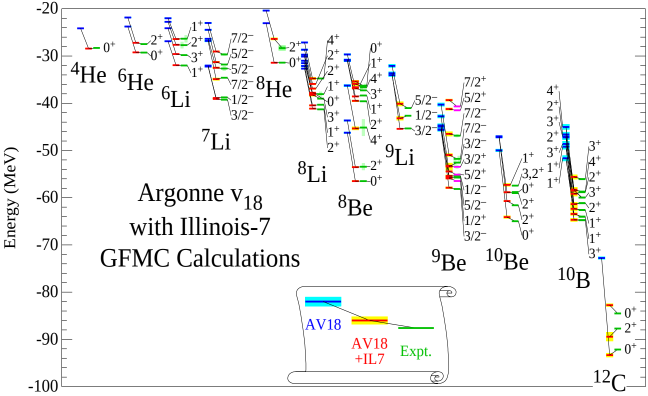
- Importance sampling: $G(R,R',t) \to G(R,R',t)\,\Psi_I(R')/\Psi_I(R)$
- Constrained-path approximation to control the sign problem. Unconstrained-path calculation possible in several cases (exact).

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% (A$\leq$6), 5-6% (12$\leq$A$\leq$16).

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

Light nuclei spectrum computed with GFMC

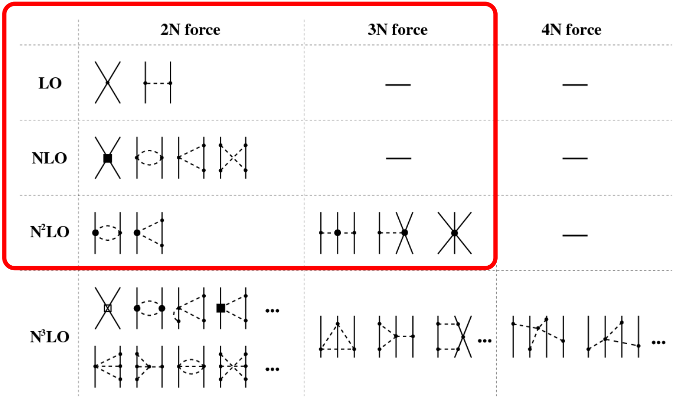


Carlson, et al., Rev. Mod. Phys. 87, 1067 (2015)

Also radii, densities, matrix elements, ...

Unfortunately phenomenological Hamiltonians are not useful to address systematical uncertainties.

Nuclear Hamiltonian



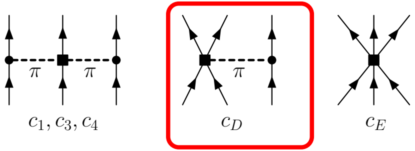
Expansion in powers of Q/Λ, Q$\sim$100 MeV, Λ $\sim$1 GeV.

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!

Chiral three-body forces, issue (I)?



In the Fourier transformation of V_D two possible operator structures arise:

$$V_{D1} = \frac{g_A c_D m_\pi^2}{96\pi\Lambda_\chi F_\pi^4} \sum_{i<j<k} \sum_{cyc} \tau_i \cdot \tau_k \left[X_{ik}(r_{kj})\delta(r_{ij}) + X_{ik}(r_{ij})\delta(r_{kj}) - \frac{8\pi}{m_\pi^2} \sigma_i \cdot \sigma_k \delta(r_{ij})\delta(r_{kj}) \right]$$

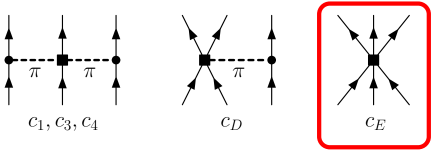
$$V_{D2} = \frac{g_A c_D m_\pi^2}{96\pi\Lambda_\chi F_\pi^4} \sum_{i<j<k} \sum_{cyc} \tau_i \cdot \tau_k \left[X_{ik}(r_{ik}) - \frac{4\pi}{m_\pi^2} \sigma_i \cdot \sigma_k \delta(r_{ik}) \right] \left[\delta(r_{ij}) + \delta(r_{kj}) \right]$$

$$X_{ij}(r) = T(r) S_{ij} + Y(r) \sigma_i \cdot \sigma_j$$

Navratil (2007), Tews et al PRC (2016), Lynn et al PRL (2016).

Equivalent only in the limit of an infinite cutoff. Implications in real life?

Chiral three-body forces, issue (II)?



Equivalent forms of operators entering in V_E (Fierz-rearrangement):

$$1, \quad \sigma_i \cdot \sigma_j, \quad \tau_i \cdot \tau_j, \quad \sigma_i \cdot \sigma_j \tau_i \cdot \tau_j, \quad \sigma_i \cdot \sigma_j \tau_i \cdot \tau_k, \quad [(\sigma_i \times \sigma_j) \cdot \sigma_k][(\tau_i \times \tau_j) \cdot \tau_k]$$

Epelbaum et al (2002). We investigated the following choices:

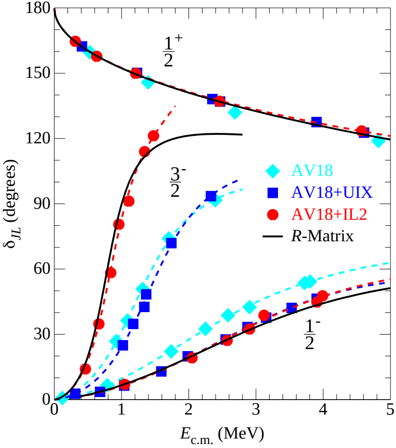
$$V_{E\tau} = \frac{c_E}{\Lambda_\chi F_\pi^4} \sum_{i<j<k} \sum_{\text{cyc}} \tau_i \cdot \tau_k \delta(r_{kj}) \delta(r_{ij})$$

$$V_{E1} = \frac{c_E}{\Lambda_\chi F_\pi^4} \sum_{i<j<k} \sum_{\text{cyc}} \delta(r_{kj}) \delta(r_{ij})$$

Qualitative differences expected, i.e. consider ^{4}He vs neutron matter!

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. (vs A=3, 4)

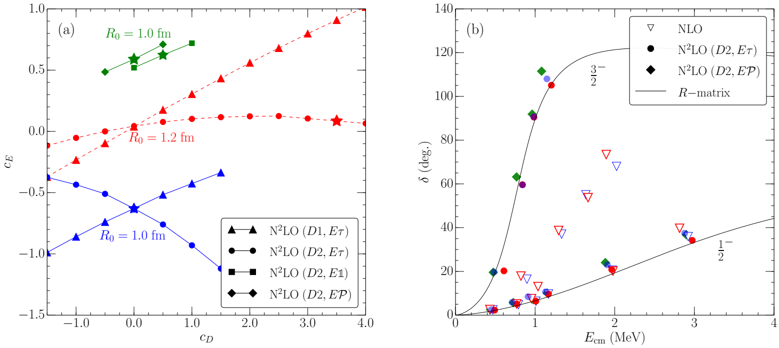


GFMC neutron-^{4}He results using Argonne Hamiltonians.

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

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

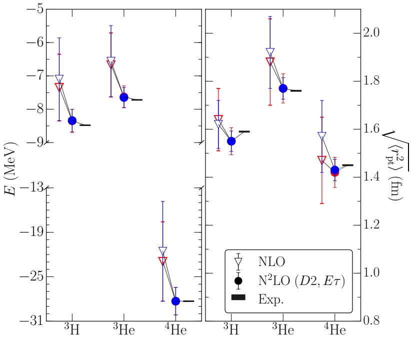
Cutoff R_0 taken consistently with the two-body interaction.



No fit can be obtained for $R_0 = 1.2$ fm and V_{D1} - Issue (I)

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

A=3, 4 nuclei at N2LO



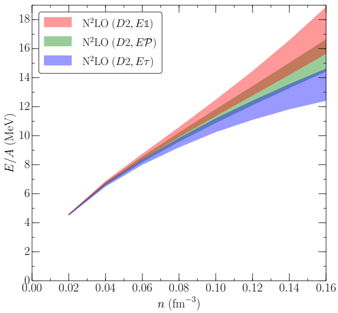
Error quantification: define $Q = \max\left(\frac{p}{\Lambda_b}, \ \frac{m_\pi}{\Lambda_b}\right)$ and calculate:

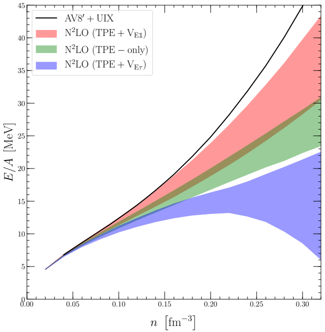
$$\Delta(N2LO) = \max\left(Q^4|\hat{O}_{LO}|, \ Q^2|\hat{O}_{LO} - \hat{O}_{NLO}|, \ Q|\hat{O}_{NLO} - \hat{O}_{N2LO}\right)$$

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.



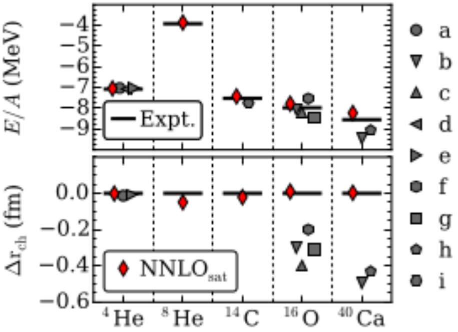


Lynn, Tews, Carlson, Gandolfi, Gezerlis, Schmidt, Schwenk, PRL (2016).
Tews, Carlson, Gandolfi, Reddy, arXiv:1801.01923 (2018).

Significant dependence to the choice of V_E - Issue (II)
Probably even worse for the softer cutoff!

Heavier nuclei

What about heavier nuclei?



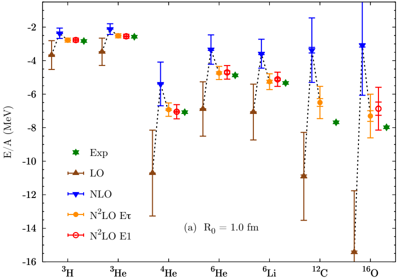
Many chiral Hamiltonians cannot predict both energies and radii.

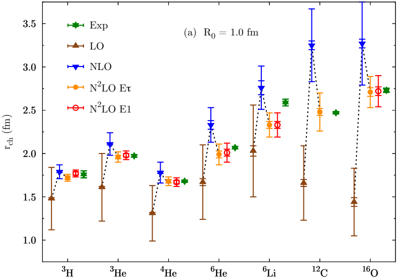
Strategy: include medium nuclei properties in the fit (but sacrifice nucleon-nucleon data)?

Ekström, Hagen, et al., Phys. Rev. C 91, 051301(R) (2015)

AFDMC calculations

Energies and charge radii, cutoff 1.0 fm:





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

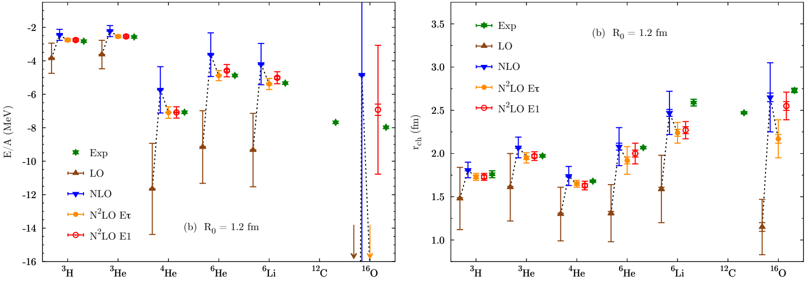
Qualitative good description of both energies and radii.

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

Different V_E operators give similar results.

AFDMC calculations

Energies and charge radii, cutoff 1.2 fm:



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

Qualitative good description up to A=6.

Different V_E operators give very different results for ^{16}O.

Energy contribution

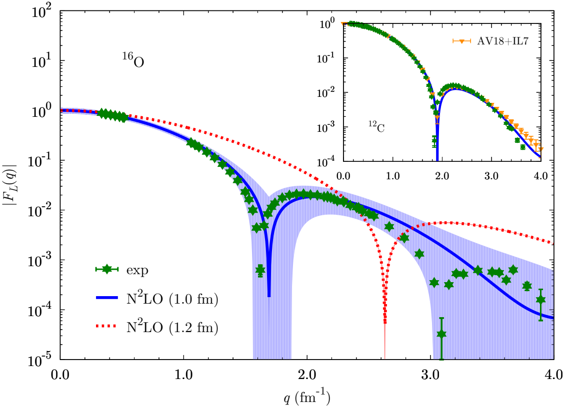
Expectation value of the N^2LO energy contributions ^{16}O:

Potential	$E_{\rm kin} + v_{ij}$	V_{ijk}	$V^{2\pi,P}$	$V^{2\pi,S}$	V_D	V_E
2b, 1.0	$-134(2)$					
$E\tau$, 1.0	$-130(2)$	$-44(1)$	$-55(1)$	0.85(1)	0	8.50(4)
$E1$, 1.0	$-131(2)$	$-41(1)$	$-54(1)$	0.72(1)	$-4.03(5)$	15.7(1)
2b, 1.2	$-151(3)$					
$E\tau$, 1.2	$-156(7)$	$-202(3)$	$-101(2)$	$-0.72(9)$	$-94(2)$	$-5.43(3)$
$E1$, 1.2	$-152(2)$	$-26(1)$	$-34(1)$	0.94(1)	4.53(8)	1.90(1)

LECs c_D and c_E for different cutoffs and parametrizations of the three-body force (other strengths are the same):

V_{ijk}	R_0 (fm)	c_D	c_E
$E\tau$	1.0	0.0	-0.63
$E1$	1.0	0.5	0.62
$E\tau$	1.2	3.5	0.09
$E1$	1.2	-0.75	0.025

Charge form factor



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

Hard interaction reproduces exp.

Conclusions

- Quantum Monte Carlo calculations for larger nuclei is now possible (at least up to A=16, work in progress...)
- Chiral EFT provides a way to constrain nuclear interactions and estimate systematic uncertainties

But...

- Effect of the cutoff important to explore
- Effect of using different ("equivalent") operators important to explore. Some working better. How to choose?

Acknowledgments:
J. Carlson (LANL), D. Lonardoni (LANL and FRIB), J. Lynn, A. Schwenk (Darmstadt), I. Tews (INT), A. Gezerlis (Guelph), K.E. Schmidt (ASU)

Extra slides

Quantum Monte Carlo

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

Propagation performed by

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- 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:

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

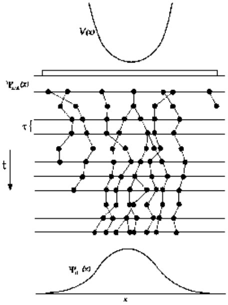
Algorithm for each time-step:

- 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:

$$\begin{aligned} V &= \sum_{i<j} [v_\sigma(r_{ij})\vec{\sigma}_i \cdot \vec{\sigma}_j + v_t(r_{ij})(3\vec{\sigma}_i \cdot \hat{r}_{ij}\vec{\sigma}_j \cdot \hat{r}_{ij} - \vec{\sigma}_i \cdot \vec{\sigma}_j)] = \\ &= \sum_{i,j} \sigma_{i\alpha} A_{i\alpha;j\beta} \sigma_{j\beta} = \frac{1}{2}\sum_{n=1}^{3N} O_n^2 \lambda_n \end{aligned}$$

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

$$V_a^{2\pi,PW} = A_a^{2\pi,PW} \sum_{i<j<k} \sum_{cyc} \{\vec{\tau}_i \cdot \vec{\tau}_k, \vec{\tau}_j \cdot \vec{\tau}_k\} \{\sigma_i^\alpha \sigma_k^\gamma, \sigma_k^\mu \sigma_j^\beta\} \mathcal{X}_{i\alpha k\gamma} \mathcal{X}_{k\mu j\beta}$$

$$= 4A_a^{2\pi,PW} \sum_{i<j} \vec{\tau}_i \cdot \vec{\tau}_j \sigma_i^\alpha \sigma_j^\beta \sum_{k\neq i,j} \mathcal{X}_{i\alpha k\gamma} \mathcal{X}_{k\gamma j\beta}\,, \tag{1}$$

$$V_c^{2\pi,PW} = A_c^{2\pi,PW} \sum_{i<j<k} \sum_{cyc} [\vec{\tau}_i \cdot \vec{\tau}_k, \vec{\tau}_j \cdot \vec{\tau}_k][\sigma_i^\alpha \sigma_k^\gamma, \sigma_k^\mu \sigma_j^\beta] \mathcal{X}_{i\alpha k\gamma} \mathcal{X}_{k\mu j\beta}$$

$$= -4A_c^{2\pi,PW} \sum_{i<j<k} \sum_{cyc} \tau_i^\eta \tau_j^\xi \tau_k^\phi \epsilon_{\eta\xi\phi} \sigma_i^\alpha \sigma_j^\beta \sigma_k^\nu \epsilon_{\nu\gamma\mu} \mathcal{X}_{i\alpha k\gamma} \mathcal{X}_{k\mu j\beta} \tag{2}$$

$$= A_c^{2\pi,PW} \sum_{i<j<k} \sum_{cyc} [\vec{\tau}_i \cdot \vec{\tau}_k, \vec{\tau}_j \cdot \vec{\tau}_k][\sigma_i^\alpha \sigma_k^\gamma, \sigma_k^\mu \sigma_j^\beta] \left(X_{i\alpha k\gamma} - \delta_{\alpha\gamma} \frac{4\pi}{m_\pi^3} \Delta(r_{ik})\right) \left(X_{k\mu j\beta} - \delta_{\mu\beta} \frac{4\pi}{m_\pi^3} \Delta(r_{kj})\right) \tag{3}$$

$$= V_c^{\Delta\Delta} + V_c^{\Delta\delta} + V_c^{\delta\delta} \tag{4}$$

$$V^{2\pi,SW} = A^{2\pi,SW} \sum_{i<j<k} \sum_{cyc} \mathcal{Z}_{ik\alpha} \mathcal{Z}_{jk\alpha} \sigma_i^\alpha \sigma_j^\beta \vec{\tau}_i \cdot \vec{\tau}_j$$

$$= A^{2\pi,SW} \sum_{i<j} \sigma_i^\alpha \sigma_j^\beta \vec{\tau}_i \cdot \vec{\tau}_j \sum_{k\neq i,j} \mathcal{Z}_{ik\alpha} \mathcal{Z}_{jk\alpha} \tag{5}$$

$$V_D = A_D \sum_{i<j} \sigma_i^\alpha \sigma_j^\beta \vec{\tau}_i \cdot \vec{\tau}_j \sum_{k\neq i,j} \mathcal{X}_{i\alpha j\beta} [\Delta(r_{ik}) + \Delta(r_{jk})] \tag{6}$$

$$V_E = A_E \sum_{i<j} \vec{\tau}_i \cdot \vec{\tau}_j \sum_{k\neq i,j} \Delta(r_{ik}) \Delta(r_{jk}) \tag{7}$$

Three-body forces

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

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

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

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

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

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.

Variational wave function

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

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

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

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.

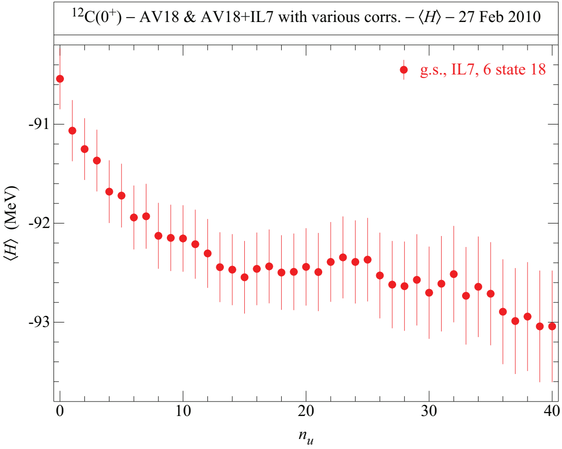
If Ψ is complex:

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

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

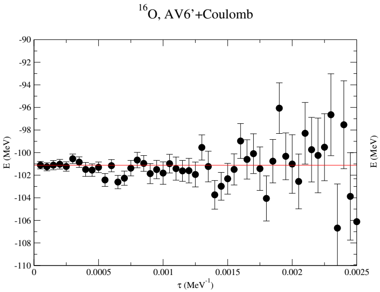
GFMC unconstrained-path propagation:



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.