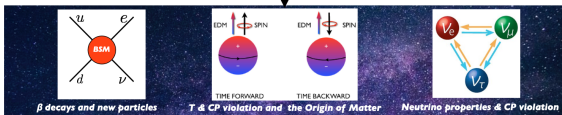


# Nuclear properties from Quantum Monte Carlo with EFT interactions

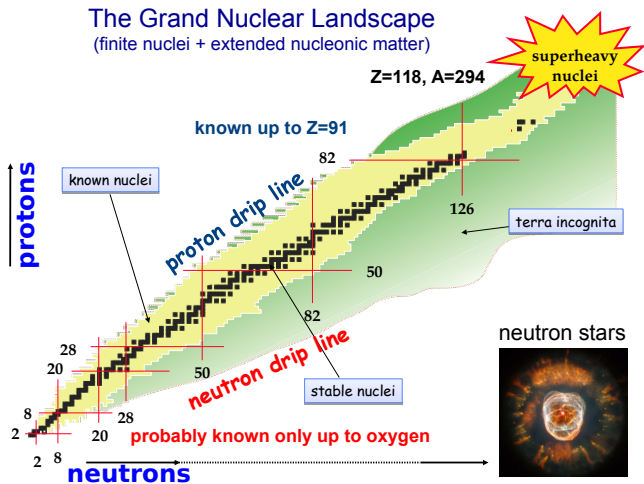
Stefano Gandolfi (Los Alamos National Laboratory)

Lepton Interactions with Nucleons and Nuclei  
Marciana Marina (Isola d'Elba), Sept. 3-8, 2023



National Energy Research  
Scientific Computing Center

# The big picture



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

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

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  $N^2\text{LO}$  (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:

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

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

Propagation performed by

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

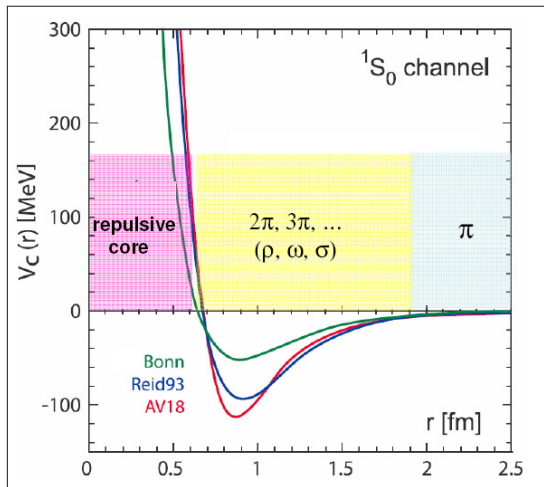
- Importance sampling:  $G(R, R', t) \rightarrow G(R, R', t) \Psi_I(R') / \Psi_I(R)$
- Constrained-path approximation to control the sign problem.  
Unconstrained-path calculation possible in several cases (exact).

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

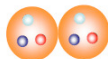


From T. Hatsuda (Oslo 2008)

One-pion exchange  
by Yukawa (1935)



Multi-pions  
by Taketani (1951)

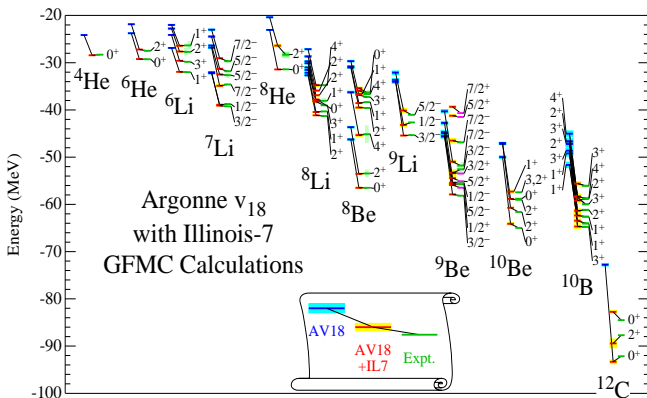


Repulsive core  
by Jastrow (1951)



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

# Light nuclei spectrum with phenomenological Hamiltonians



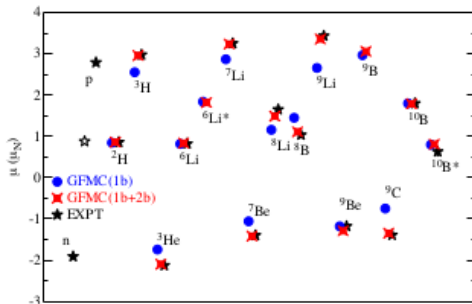
Carlson, et al., Rev. Mod. Phys. 87, 1067 (2015)

Also radii, densities, transitions, ...

**But** 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.



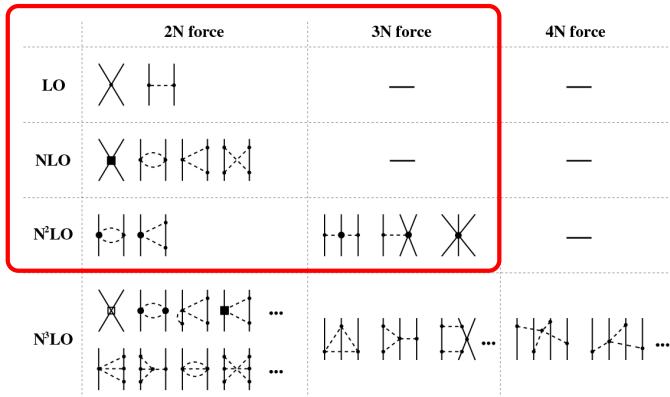
Pastore et al, PRC 2013

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

**But** phenomenological currents are not useful to address systematical uncertainties.



# Nuclear Hamiltonian



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

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,  $\Lambda_b$  is the cutoff, and calculate:

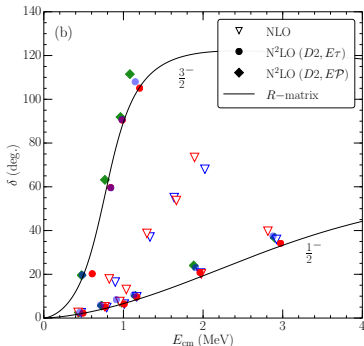
$$\Delta(N2LO) = \max\left(Q^4|\hat{O}_{LO}|, Q^2|\hat{O}_{LO} - \hat{O}_{NLO}|, Q|\hat{O}_{NLO} - \hat{O}_{N2LO}\right)$$

Epelbaum, Krebs, Meissner (2014).

# $^4\text{He}$ binding energy and p-wave $n$ - $^4\text{He}$ scattering

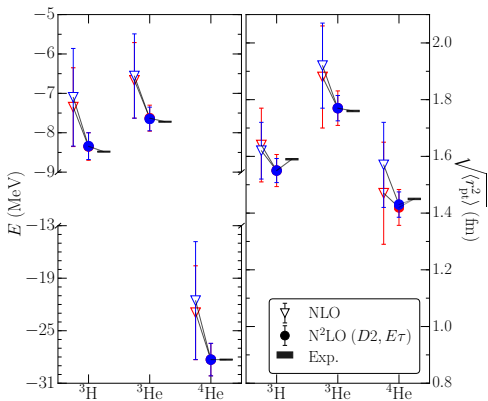
Regulator:  $\delta(r) = \frac{1}{\pi\Gamma(3/4)R_0^3} \exp(-(r/R_0)^4)$

Fit:  $^4\text{He}$  binding energy and  $n$ - $^4\text{He}$  scattering.



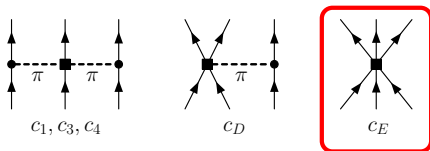
Lynn, Tews, Carlson, Gandolfi, Gezerlis, Schmidt, Schwenk PRL (2016).

# A=3, 4 nuclei at N2LO



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

# Chiral three-body forces, contact



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

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

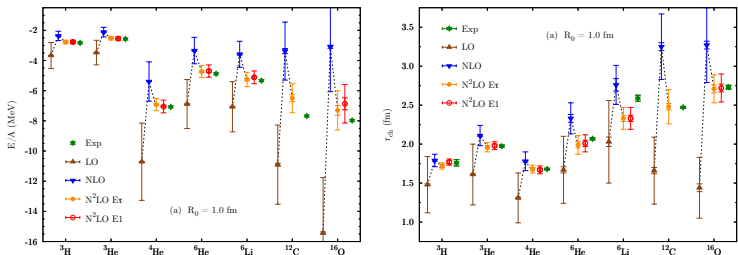
Epelbaum et al (2002). We investigated the following choices:

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

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

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

Energies and charge radii, **cutoff  $R_0=1.0$  fm:**



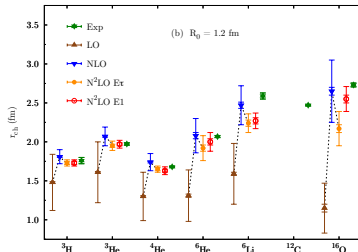
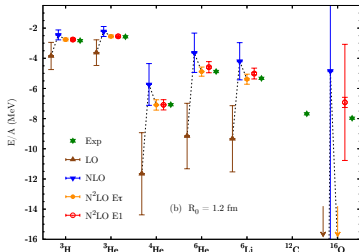
Lonardoni, et al., PRL (2018), PRC (2018).

Qualitative good description of both energies and radii.

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

**Different  $V_E$  operators give similar results.**

Energies and charge radii, **cutoff  $R_0 = 1.2$  fm:**



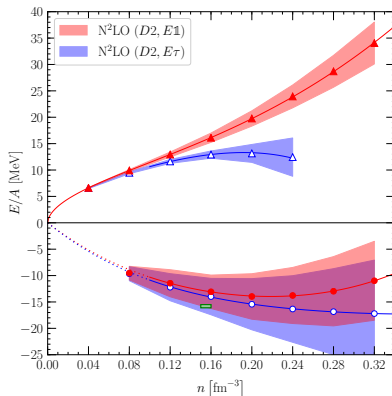
Lonardonì, et al., PRL (2018), PRC (2018).

Qualitative good description up to  $A=6$ .

**Different  $V_E$  operators give very different results for  $^{16}\text{O}$ .**

# Nuclear and neutron matter EOS

Cutoff  $R_0=1.0$  fm



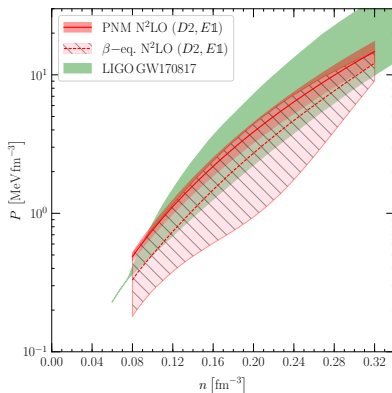
Lonardoni, et al., Phys. Rev. Research 2, 022033(R) (2020).

Symmetric nuclear matter less dependent upon the choice of  $V_E$  (cf. nuclei).  $E_\tau$  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.

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

	Single-nucleon	Two-nucleon	Three-nucleon
$Q^{-3}$		—	—
$Q^{-1}$			—
$Q^0$		—	—
$Q^1$		<p>depend on <math>d_{8,9,18,21,22}</math>    parameter-free</p> <p>parameter-free</p> <p>depend on <math>C_{2,4,5,7}</math> and <math>L_{1,2}</math>    depend on <math>C_T</math> (known)</p>	<p>depend on <math>C_T</math> (known)</p>

# Electro-magnetic currents

Within chiral EFT, there are different ways to construct the currents (different expansions).

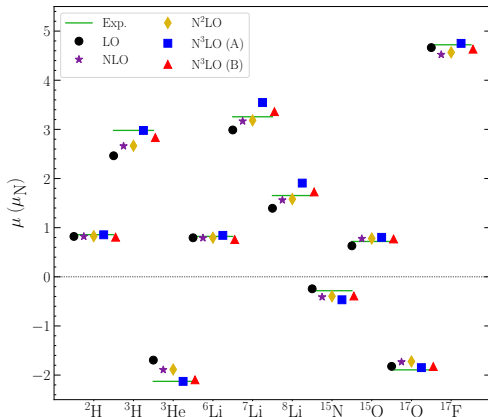
Hamiltonian	Pisa/Norfolk	Bochum
$Q^0$ LO	$Q^{-2}$ LO	$Q^{-3}$ LO
$Q^1$ –	$Q^{-1}$ NLO	$Q^{-2}$ –
$Q^2$ NLO	$Q^0$ N2LO	$Q^{-1}$ NLO
$Q^3$ N2LO	$Q^1$ N3LO	$Q^0$ N2LO
		$Q^1$ N3LO
	2 LECS (contact)	2 LECS (contact)
	1 LEC (OPE)	

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.

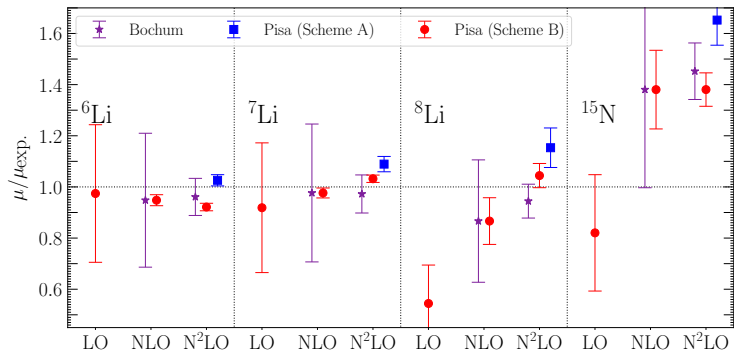


J. D. Martin, S. J. Novario, D. Lonardoni, J. Carlson, S. Gandolfi, I. Tews, arXiv:2301.08349.

# Nuclear magnetic moments

Order by order calculation. Each order correspond to the same order in the Hamiltonian and currents.

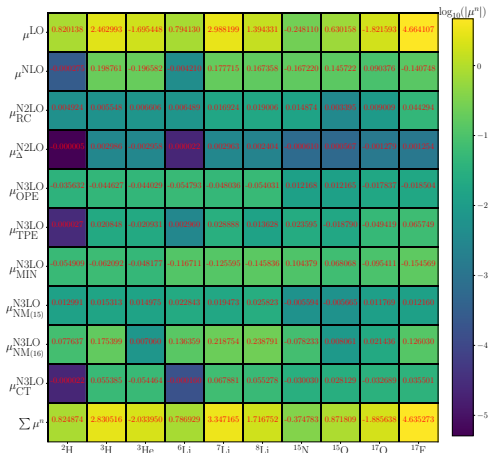
Bochum LECs are fit to all nuclei (B).



Different currents that are fit with the same scheme (B) give same results within error bars.

# Nuclear magnetic moments

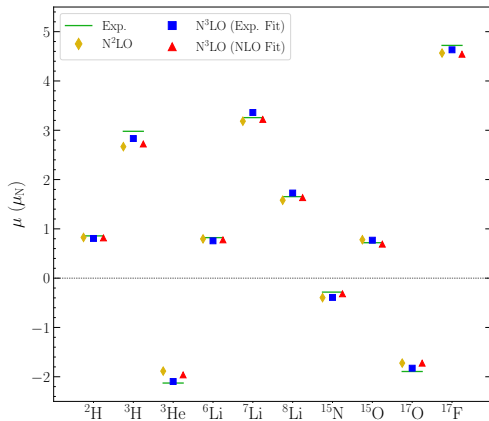
Magnetic moments, single contributions (Pisa).



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

# Nuclear magnetic moments

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



Qualitatively similar results.



- 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:

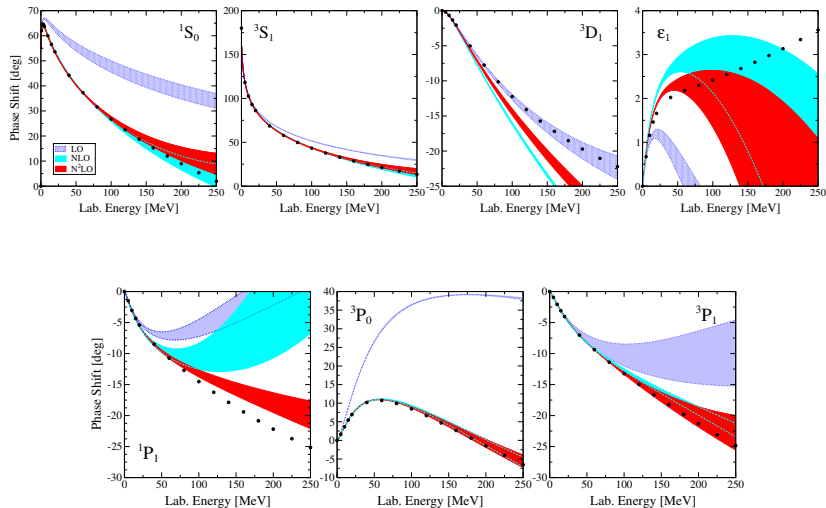
J. Martin, S. Novario,

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

# Extra slides

# Nuclear Hamiltonian

Phase shifts, LO, NLO and N<sup>2</sup>LO with  $R_0=1.0$  and  $1.2$  fm:



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

# Energy contribution

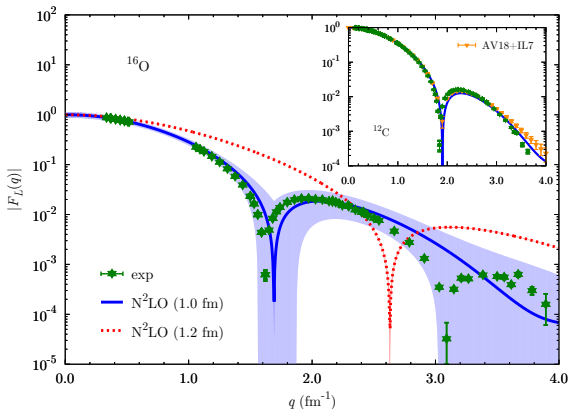
Expectation value of the N<sup>2</sup>LO energy contributions <sup>16</sup>O:

Potential	$E_{\text{kin}} + v_{ij}$	$V_{ijk}$	$V^{2\pi,P}$	$V^{2\pi,S}$	$V_D$	$V_E$
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., arXiv:1709.09143, and in preparation.

Hard interaction reproduces exp.

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

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

Propagation performed by

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

- Importance sampling:  $G(R, R', t) \rightarrow G(R, R', t) \Psi_I(R') / \Psi_I(R)$
- 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 %.

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:

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

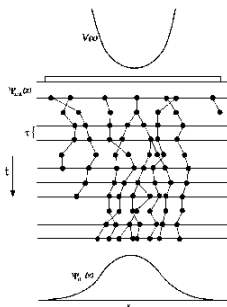
Algorithm for each time-step:

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

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

$$\text{int}[w + \xi]$$

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!

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<sup>2</sup>LO can be exactly included in the case of neutrons.

For example:

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

The above form can be included in the AFDMC propagator.

# Three-body forces

$$\begin{aligned}
 V_a^{2\pi, PW} &= A_a^{2\pi, PW} \sum_{i < j < k} \sum_{\text{cyc}} \{ \vec{\tau}_i \cdot \vec{\tau}_k, \vec{\tau}_j \cdot \vec{\tau}_k \} \{ \sigma_i^\alpha \sigma_k^\gamma, \sigma_k^\mu \sigma_j^\beta \} \mathcal{X}_{i\alpha k\gamma} \mathcal{X}_{k\mu j\beta} \\
 &= 4A_a^{2\pi, PW} \sum_{i < j} \vec{\tau}_i \cdot \vec{\tau}_j \sigma_i^\alpha \sigma_j^\beta \sum_{k \neq i, j} \mathcal{X}_{i\alpha k\gamma} \mathcal{X}_{k\gamma j\beta}, \tag{1}
 \end{aligned}$$

$$\begin{aligned}
 V_c^{2\pi, PW} &= A_c^{2\pi, PW} \sum_{i < j < k} \sum_{\text{cyc}} [ \vec{\tau}_i \cdot \vec{\tau}_k, \vec{\tau}_j \cdot \vec{\tau}_k ] [ \sigma_i^\alpha \sigma_k^\gamma, \sigma_k^\mu \sigma_j^\beta ] \mathcal{X}_{i\alpha k\gamma} \mathcal{X}_{k\mu j\beta} \\
 &= -4A_c^{2\pi, PW} \sum_{i < j < k} \sum_{\text{cyc}} \tau_i^\eta \tau_j^\xi \tau_k^\phi \epsilon_{\eta\xi\phi} \sigma_i^\alpha \sigma_j^\beta \sigma_k^\nu \epsilon_{\nu\gamma\mu} \mathcal{X}_{i\alpha k\gamma} \mathcal{X}_{k\mu j\beta} \tag{2}
 \end{aligned}$$

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

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

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

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

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

# 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  $\alpha_i$  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  $\Psi$  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

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

→ 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.

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

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

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

In particular, we included orbitals in  $1S_{1/2}$ ,  $1P_{3/2}$ ,  $1P_{1/2}$ ,  $1D_{5/2}$ ,  $2S_{1/2}$ , and  $1D_{3/2}$ .

# 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  $\Psi$  is complex:

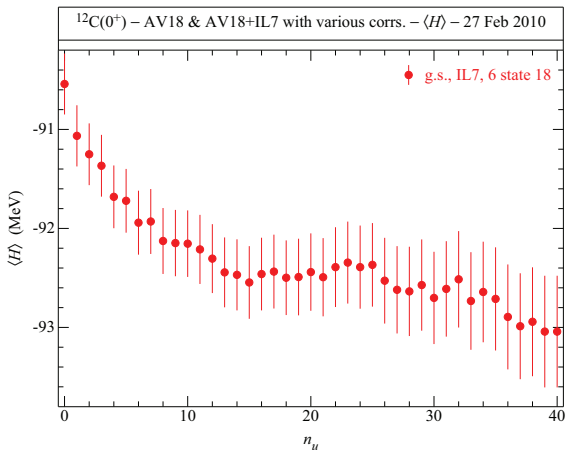
$$|\psi_I(R')||\Psi(R', t + dt)| = \int dR G(R, R', dt) \left| \frac{\psi_I(R')}{\psi_I(R)} \right| |\psi_I(R)||\Psi(R, t)|$$

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



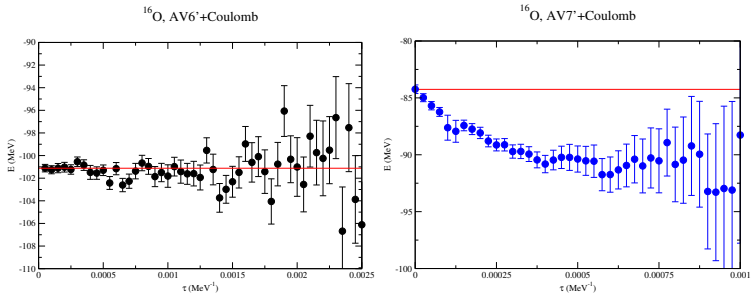
# Unconstrained-path

GFMC unconstrained-path propagation:



Changing the trial wave function gives same results.

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  $\Psi$  to improve the constrained-path.