Progresses in Quantum Monte Carlo calculations of nuclei and nuclear matter

Stefano Gandolfi

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Marciana Marina, Isola d’Elba, June 23-27, 2014

www.computingnuclei.org
Homogeneous neutron matter

Progresses in Quantum Monte Carlo calculations of nuclei and nuclear matter
Outline

- The model and the method
- Nuclei
- Equation of state of neutron matter
- Symmetry energy and neutron stars
- Nuclear matter
- 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. 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 AV6’ (no LS), AV7’ (no LS-\( \tau \)), AV8’.

Local chiral forces up to N\(^2\)LO has the same spin/isospin operatorial structure than AV7’ - Gezerlis, Tews, et al. PRL (2013).
Phase shifts, Argonne AV6', AV7' and AV8'

Nuclear Hamiltonian

Stefano Gandolfi (LANL)  Progresses in Quantum Monte Carlo calculations of nuclei and nuclear matter
### Progresses in Quantum Monte Carlo calculations of nuclei and nuclear matter

#### Nuclear Hamiltonian

<table>
<thead>
<tr>
<th>Level</th>
<th>Order</th>
<th>Diagrams</th>
</tr>
</thead>
<tbody>
<tr>
<td>LO</td>
<td>$O\left(\frac{Q}{\Lambda_b}\right)^0$</td>
<td><img src="image1" alt="Diagram" /></td>
</tr>
<tr>
<td>NLO</td>
<td>$O\left(\frac{Q}{\Lambda_b}\right)^2$</td>
<td><img src="image2" alt="Diagram" /></td>
</tr>
<tr>
<td>N2LO</td>
<td>$O\left(\frac{Q}{\Lambda_b}\right)^3$</td>
<td><img src="image3" alt="Diagram" /></td>
</tr>
<tr>
<td>N3LO</td>
<td>$O\left(\frac{Q}{\Lambda_b}\right)^4$</td>
<td><img src="image4" alt="Diagram" /></td>
</tr>
</tbody>
</table>

- **Chiral EFT** is an expansion in powers of $Q/\Lambda_b$.

  $Q \sim m_\pi \sim 100$ MeV;

  $\Lambda_b \sim 800$ MeV.

- **Long-range physics**: given explicitly (no parameters to fit) by pion-exchanges.

- **Short-range physics**: parametrized through contact interactions with low-energy constants (LECs) fit to low-energy data.

- **Many-body forces** enter systematically and are related via the same LECs.

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*Slide by Joel Lynn, Scidac NUCLEI meeting 2014.*
Urbana–Illinois $V_{ijk}$ models processes like

\[ \pi \pi \Delta \]

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

Chiral forces at $N^2$LO:
Quantum Monte Carlo

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

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: \( G(R, R', t) \to G(R, R', t) \frac{\Psi_I(R')}{\Psi_I(R)} \)
- Constrained-path approximation to control the sign problem.
- A new improved sampling of \( G(R, R', t) \) required to dramatically reduce the time-step dependence.

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

\[
\psi = \begin{pmatrix}
a_{↑↑↑} \\
a_{↑↑↓} \\
a_{↑↓↑} \\
a_{↑↓↓} \\
a_{↓↑↑} \\
a_{↓↑↓} \\
a_{↓↓↑} \\
a_{↓↓↓}
\end{pmatrix}
\]

A correlation like

\[1 + f(r)\mathbf{\sigma}_1 \cdot \mathbf{\sigma}_2\]

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

AFDMC wave-function:

\[
\psi = A \left[ \xi_{s_1} \left( \begin{array}{c} a_1 \\ b_1 \end{array} \right) \xi_{s_2} \left( \begin{array}{c} a_2 \\ b_2 \end{array} \right) \xi_{s_3} \left( \begin{array}{c} a_3 \\ b_3 \end{array} \right) \right]
\]

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

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

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!
Simple wave function used so far

\[ \langle R, S | \Psi_T \rangle = \langle R, S | \prod_{i<j} f_c(r_{ij}) | \Phi \rangle \]

good for pure neutron systems, tensor correlations in \( T=1 \) are small.

However, the \( T=0 \) tensor force is very strong, and it’s hard to generate
the many-body correlations from the above wave function. Improvement:

\[ \langle R, S | \Psi_T \rangle = \langle R, S | \prod_{i<j} f_c(r_{ij}) \left[ 1 + \sum_{i<j,p} f_p(r_{ij}) O^p_{ij} \right] | \Phi \rangle \]

where \( O^p \) are spin/isospin dependent correlations. About 12-15
parameters to variationally optimize.

Note: w.f. much more computationally demanding, not as good as
GFMC, but its overlap with the ground-state is much higher.
Light nuclei spectrum computed with GFMC

Argonne v18 with UIX or Illinois-7 GFMC Calculations
1 June 2011

Carlson, Pieper, Wiringa, many papers
<table>
<thead>
<tr>
<th>Hamiltonian</th>
<th>AFDMC</th>
<th>GFMC</th>
</tr>
</thead>
<tbody>
<tr>
<td>AV6'</td>
<td>-27.09(3)</td>
<td>-26.85(2)</td>
</tr>
<tr>
<td>AV7'</td>
<td>-25.7(2)</td>
<td>-26.2(1)</td>
</tr>
<tr>
<td>N²LO ($R_0=1.0$ fm)</td>
<td>-24.41(3)</td>
<td>-24.56(1)</td>
</tr>
<tr>
<td>N²LO ($R_0=1.2$ fm)</td>
<td>-25.77(2)</td>
<td>-25.75(1)</td>
</tr>
</tbody>
</table>

Gandolfi, Lovato, Carlson, Schmidt, arXiv:1406.3388

Binding energies for $^4$He using different two-body interactions. Agreement within 2%.
### Nuclei

<table>
<thead>
<tr>
<th></th>
<th>AV6'</th>
<th>AV7'</th>
<th>exp</th>
</tr>
</thead>
<tbody>
<tr>
<td>$^4$He</td>
<td>-27.09(3)</td>
<td>-25.7(2)</td>
<td>-28.295</td>
</tr>
<tr>
<td>$^{16}$O</td>
<td>-115.6(3)</td>
<td>-90.6(4)</td>
<td>-127.619</td>
</tr>
<tr>
<td>$^{40}$Ca</td>
<td>-322(2)</td>
<td>-209(1)</td>
<td>-342.051</td>
</tr>
</tbody>
</table>

Gandolfi, Lovato, Carlson, Schmidt, arXiv:1406.3388

About 10 to 40% of binding energy missing.

**Preliminary:** $^{16}$O binding energy with chiral potentials:

<table>
<thead>
<tr>
<th></th>
<th>$R_0=1.2$ fm</th>
<th>$R_0=1.0$ fm</th>
</tr>
</thead>
<tbody>
<tr>
<td>LO</td>
<td>-1210.1(3)</td>
<td>-269.9(4)</td>
</tr>
<tr>
<td>NLO</td>
<td>-87.4(2)</td>
<td>-35.9(7)</td>
</tr>
<tr>
<td>$N^2$LO</td>
<td>-116.1(2)</td>
<td>-91.1(3)</td>
</tr>
</tbody>
</table>
Light nuclei spectrum computed with GFMC


Note: three-body terms not yet included.
Assumptions/observations:

- EOS of neutron matter useful to study the symmetry energy and its slope at saturation.
- The two-nucleon interaction reproduces well scattering data.
- The three-neutron force \((T = 3/2)\) very weak in light nuclei, while \(T = 1/2\) is the dominant part (but zero in neutron matter). No direct \(T = 3/2\) experiments available!
What is the Symmetry energy?

Assumption from experiments:

\[ E_{\text{SNM}}(\rho_0) = -16 \text{MeV} , \quad \rho_0 = 0.16 \text{fm}^{-3} , \quad E_{\text{sym}} = E_{\text{PNM}}(\rho_0) + 16 \]

At \( \rho_0 \) we access \( E_{\text{sym}} \) by studying PNM.
Equation of state of neutron matter using Argonne forces:

\[ E_{\text{sym}} = 35.1 \text{ MeV (AV8'+UIX)} \]
\[ E_{\text{sym}} = 33.7 \text{ MeV} \]
\[ E_{\text{sym}} = 32 \text{ MeV} \]
\[ E_{\text{sym}} = 30.5 \text{ MeV (AV8')} \]

Gandolfi, Carlson, Reddy, PRC (2012)
From the EOS, we can fit the symmetry energy around $\rho_0$ using

$$E_{\text{sym}}(\rho) = E_{\text{sym}} + \frac{L}{3} \left( \rho - 0.16 \right) + \cdots$$

Very weak dependence to the model of 3N force for a given $E_{\text{sym}}$. Chiral Hamiltonians give compatible results.
Equation of state of neutron matter using NN chiral forces:

For a finite cutoff, there are ”additional” $V_D$ and $V_E$ diagrams that contribute in pure neutron matter.

They have been often neglected in existing neutron matter calculations!

All the above terms have been written in coordinate space, and included into AFDMC.
Neutron matter with chiral forces

Preliminary! Contribution of ”additional” $V_D$ and $V_E$ terms:

Note: Contribution of FM ($2\pi$ exchange) about 0.9 MeV with AV8′
Neutron matter with chiral forces

Preliminary!

Equation of state of neutron matter at $N^2\text{LO}$.

Note: the "real" $V_D$ and $V_E$ terms are not included yet.
Neutron matter with chiral forces

Preliminary!

Equation of state of neutron matter, a comparison.

![Graph showing the energy per neutron as a function of density for different models of neutron interactions.](image-url)
TOV equations:

\[
\frac{dP}{dr} = -\frac{G[m(r) + 4\pi r^3 P/c^2][\epsilon + P/c^2]}{r[r - 2Gm(r)/c^2]},
\]

\[
\frac{dm(r)}{dr} = 4\pi \epsilon r^2,
\]
Accurate measurement of $E_{\text{sym}}$ would put a constraint to the radius of neutron stars, OR observation of $M$ and $R$ would constrain $E_{\text{sym}}$!
Observations of the mass-radius relation are becoming available:


Neutron star observations can be used to 'measure' the EOS and constrain $E_{\text{sym}}$ and $L$. 
Neutron star matter

Neutron star matter model:

\[ E_{NSM} = a \left( \frac{\rho}{\rho_0} \right)^\alpha + b \left( \frac{\rho}{\rho_0} \right)^\beta, \quad \rho < \rho_t \]

(form suggested by QMC simulations),

and a high density model for \( \rho > \rho_t \)

i) two polytropes

ii) polytrope+quark matter model

Direct way to extract \( E_{sym} \) and \( L \) from neutron stars observations:

\[ E_{sym} = a + b + 16, \quad L = 3(a\alpha + b\beta) \]
Here an 'astrophysical measurement'

32 < $E_{sym}$ < 34 MeV, 43 < $L$ < 52 MeV

Steiner, Gandolfi, PRL (2012).
Symmetry energy

Hebeler, Schwenk, EPJA (2014)
EOS of symmetric nuclear matter using Argonne AV6’ and AV7’:

Gandolfi, Lovato, Carlson, Schmidt, arXiv:1406.3388
Preliminary results!

EOS of symmetric nuclear matter with chiral forces:

\[ \rho \text{ (fm}^{-3}\text{)} \]

\[ \text{energy per nucleon (MeV)} \]

\[ N^2\text{LO (no V3)} \]

\[ R_0=1.0 \text{ fm} \]

\[ R_0=1.2 \text{ fm} \]

\[ N\text{LO} \]

\[ R_0=1.0 \text{ fm} \]

\[ R_0=1.2 \text{ fm} \]
Why neutron and nuclear matter behave so differently?
Perturbative vs non-perturbative?
Phase shifts?
Importance of the (not included yet) V3?
Asymmetric nuclear matter, AV6’:

Gandolfi, Lovato, Carlson, Schmidt, arXiv:1406.3388

Quadratic dependence to isospin-asymmetry look fine.
QMC methods useful to study nuclear systems in a coherent framework: same Hamiltonians and same many-body machinery

- Chiral potentials show some convergence in nuclei (but three-body terms not included yet)
- Three-neutron force is the (strong) bridge between $E_{sym}$ and neutron star structure.
- Calculations of medium nuclei and nuclear matter is in progress. Role of three-body forces need investigation.
- Nuclear and neutron matter have very different behavior with chiral forces. We need to understand why!
Acknowledgments

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Extra slides
Neutron matter EOS

![Graph showing energy per neutron (MeV) vs. density (fm$^{-3}$) for different models: AV8'+UIX, AV8'/AV7', AV6'.]
Gandolfi, Lovato, Carlson, Schmidt, arXiv:1406.3388
Phase shifts, Argonne AV6’, AV7’ and AV8’
Phase shifts, LO, NLO and $N^2$LO with $R_0 = 1.0$ and 1.2 fm:
Nuclear Hamiltonian

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

- $^3P_2$
- $^3F_2$
- $\epsilon_2$
- $^1D_2$
- $^3D_2$
- $^1F_3$

Stefano Gandolfi (LANL)
Progresses in Quantum Monte Carlo calculations of nuclei and nuclear matter
Nuclear Hamiltonian

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

![Graphs showing phase shifts vs lab. energy for different partial waves and energies.](image-url)
Phase shifts, LO, NLO and N$^2$LO with $R_0=1.0$ and 1.2 fm:
Three-body forces

Urbana–Illinois $V_{ijk}$ models processes like

\[
\begin{align*}
\pi & \Delta \pi \\
\pi & \pi \\
\pi & \pi \\
\Delta & \pi \Delta \\
\end{align*}
\]

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

Chiral forces at $N^2$LO:

\[
\begin{align*}
\pi & \pi \\
c_1, c_3, c_4 \\
\pi & \pi \\
c_D \\
\pi & \pi \\
c_E \\
\end{align*}
\]
What about three-body forces?

The full inclusion of three-body forces for nuclei/nuclear matter in AFDMC is not possible. Ideas:

- Reduce $V_3 \rightarrow V_2(\rho)$ in the AFDMC propagator, and calculate perturbatively:
  \[
  \delta_3 = \frac{\langle \psi | V_3 - V_2(\rho) | \psi \rangle}{\langle \psi | \psi \rangle}
  \]

- ”Partially” include three-body terms in the propagator: some of them can be treated exactly. Example, Fujita-Miyazawa:

  \[
  O_{2\pi} = \sum_{\text{cyc}} \left\{ \{ X_{ij}, X_{jk} \} \{ \tau_i \cdot \tau_j, \tau_j \cdot \tau_k \} + \frac{1}{4} [X_{ij}, X_{jk}] [\tau_i \cdot \tau_j, \tau_j \cdot \tau_k] \right\}
  \]

  \[
  \Rightarrow O_{2\pi}^{\text{eff}} = \alpha \sum_{\text{cyc}} \left\{ \{ X_{ij}, X_{jk} \} \{ \tau_i \cdot \tau_j, \tau_j \cdot \tau_k \} \right\}
  \]

  and calculate the difference perturbatively.
Quantum Monte Carlo

We want to solve:

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

In the limit of \( t \to \infty \) it approaches to the lowest energy eigenstate (not orthogonal to \( \psi(R,0) \)).

Propagation performed by

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

- Importance sampling: \( G(R, R', t) \to G(R, R', t) \frac{\Psi_I(R')}{\Psi_I(R)} \)
- Constrained-path approximation to control the sign problem.

For a given (local) Hamiltonian, these methods solve the ground–state within a systematic uncertainty of 1–2% in a non-perturbative way.
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!
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:**

\[ \psi = \begin{pmatrix} a_{↑↑↑} \\ a_{↑↑↓} \\ a_{↑↓↑} \\ a_{↑↓↓} \\ a_{↓↑↑} \\ a_{↓↑↓} \\ a_{↓↓↑} \\ a_{↓↓↓} \end{pmatrix} \]

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:**

\[ \psi = \mathcal{A} \left[ \xi_{s_1} \left( \begin{array}{c} a_1 \\ b_1 \end{array} \right) \xi_{s_2} \left( \begin{array}{c} a_2 \\ b_2 \end{array} \right) \xi_{s_3} \left( \begin{array}{c} a_3 \\ b_3 \end{array} \right) \right] \]

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 deal to large 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:

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

\[ = \sum_{i,j} \sigma_i \alpha A_{i\alpha,j\beta} \sigma_j \beta = \frac{1}{2} \sum_{n=1}^{3N} O_n^2 \lambda_n \]

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:

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

Computational cost \( \approx (3N)^3 \).
Three-body forces, Urbana, Illinois, and local chiral N^2LO can be exactly included in the case of neutrons.

For example:

\[
O_{2\pi} = \sum_{cyc} \left\{ X_{ij}, X_{jk} \right\} \left\{ \tau_i \cdot \tau_j, \tau_j \cdot \tau_k \right\} + \frac{1}{4} \left[ X_{ij}, X_{jk} \right] \left[ \tau_i \cdot \tau_j, \tau_j \cdot \tau_k \right]
\]

\[
= 2 \sum_{cyc} \left\{ X_{ij}, X_{jk} \right\} = \sigma_i \sigma_k f (r_i, r_j, r_k)
\]

The above form can be included in the AFDMC propagator.
New load-balancing implemented to increase the efficiency.

AFDMC scaling @ Mira (ANL)
32,768 configurations, 25 steps, 28 nucleons in a periodic box, $\rho=0.16\,\text{fm}^{-3}$

Note: MPI (unbalanced) only so far. Similar scaling on Edison (NERSC).
AFDMC efficiency

Edison, NERSC:

Time to propagate 96,000 configurations for 100 steps
28 nucleons in a periodic box, $\rho = 0.16 \text{ fm}^{-3}$

Note: MPI only so far.