Simulations and Symmetries: Cold Atoms, QCD and Few-Hadron systems,
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Motivations

The model and the method

Equation of state of zero temperature nuclear and neutron matter

Neutron drops

Conclusions and perspectives
Why study nuclear matter? Why zero temperature?

Large density: nuclei $\rightarrow$ nuclear matter.

*Neutron matter:* simpler system to model a neutron star.
Neutron drops

Why study neutron drops?
Are not they nothing more than a pure simple toy model?

Neutron drops are interesting because:

- Provide a strong benchmark for microscopic calculations
- Model neutron-rich nuclei
- Calibrate Skyrme models for neutron-rich systems (useful to check $\nabla \rho$ terms in different geometries)
Quantum Monte Carlo methods (GFMC and AFDMC) provide very accurate results for nuclear systems.

NN scattering data and few-body theory → nuclear Hamiltonians. Few-body → many-body ⇒ experiments/observations?

EOS of nuclear and neutron matter relevant for nuclear astrophysics (neutron stars and supernovae).

Neutron drops can be useful to calibrate mean-field theories, and produce new predictions of neutron-rich nuclei (FRIB).
HAMILTONIAN AND METHOD
Hamiltonian

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

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

NN and TNI are usually written as sums of operators:

\[
v_{ij} = \sum_{p=1}^{M} v_p(r_{ij}) O^{(p)}(i,j)
\]

\(O^{(p)}\) operators including spin, isospin, tensor and others. Main contribution given by one-pion exchange (OPE) and spin-orbit:

\[
O_p^{1,8} = (1, \vec{\sigma}_i \cdot \vec{\sigma}_j, S_{ij}, \vec{L}_{ij} \cdot \vec{S}_{ij}) \times (1, \vec{\tau}_i \cdot \vec{\tau}_j).
\]

\(V_{ij}\) fitted on scattering data.
Urbana Three-Nucleon-Interaction model:

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

where the \( X \) operators have the same structure of OPE terms of NN.

Parameters of various TNI forces fitted on light nuclei \(^1\).

\(^1\)Pieper et al., Phys. Rev. C 64, 014001 (2001)
Different approach to include TNI (Friedman-Lagaris-Pandharipande): modify the NN interaction by adding density-dependent terms to NN:

\[
\nu_{DD6}' = \nu_{OPE}^p + \nu_I^p e^{-\gamma_1 \rho} + \nu_S^p + \text{TNA}(\rho),
\]

\[
\text{TNA}(\rho) = 3\gamma_2 \rho^2 e^{-\gamma_3 \rho} \left[ 1 - \frac{2}{3} \left( \frac{\rho_n - \rho_p}{\rho_n + \rho_p} \right)^2 \right]
\]

The modified NN takes into account the contribution of TNI in the \( l = 0 \) channel. TNA is a phenomenological attractive part (includes missing binding energy).

\[^2\text{Lagaris and Pandharipande, Nucl. Phys. A359, 349 (1981),}\]
Quantum Monte Carlo

Evolution of Schrödinger equation in imaginary time $t$:

$$
\psi(R, t) = e^{-(H - E_T)t} \psi(R, 0)
$$

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

Propagation performed by

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

where $G(R, R', t)$ is an approximate propagator known in the small-time limit:

$$
G(R, R', \Delta t) = \langle R | e^{-H\Delta t} | R' \rangle
$$

Then we need to iterate many times the above integral equation in the small time-step limit.
Because the Hamiltonian is state dependent, all spin/isospin states of nucleons must be included in the wave-function.
Example of just the 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 propagator like

\[
e^{-v(r)\sigma_1 \cdot \sigma_2 \Delta t}
\]

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:

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

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.
The trial wave-function used for the projection has the following general form:

\[
\psi_T(R, S) = \Phi_J(R) \cdot A[\phi_i(\vec{r}_j, s_j)]
\]  

(1)

where \( R = (\vec{r}_1...\vec{r}_A), \ S = (s_1...s_A) \) and \( \{\phi_i\} \) is a single-particle base. \( \Phi_J(R) \) is a Jastrow factor. It contains spin/isospin correlations in GFMC, and it is scalar in AFDMC:

\[
GFMC: \quad \Phi_J(R) = \prod_{i<j} (f_c(r_{ij}) + f_\sigma(r_{ij})\sigma_i \cdot \sigma_j + ... )
\]

\[
AFDMC: \quad \Phi_J(R) = \prod_{i<j} f(r_{ij})
\]

According to the problem correct boundary conditions to the trial wave-function must be imposed.
NUCLEAR AND NEUTRON MATTER
SYMMETRIC NUCLEAR MATTER

We re-adjusted the DDI parameters combined with the NN AV6’ to reproduce following properties of SNM:

- $\rho_0 = 0.16 \text{ fm}^{-3}$
- $E(\rho_0) = -16 \text{ MeV}$
- the compressibility $K \approx 240 \text{ MeV}$
The density-dependent Hamiltonian used to compute the EOS of neutron matter, and compared to that given by Hamiltonian AV8’+UIX. ³

Green line: PNM, AV8’ (two-body interaction only)

Black line: PNM, AV8’+UIX (explicit three-body force)

Red line: PNM, AV6’+DDI (density-dependent term)

Blue line: SNM, AV6’+DDI

The EOS of neutron matter is now sensibly softer than the previous one. Of course this effect is due to the different treatment of three-body force.

Using the AV6’+DDI Hamiltonian, the resulting symmetry energy is parametrized by

\[ E_{\text{sym}}(\rho) = c \left( \frac{\rho}{\rho_0} \right)^\gamma. \]  

(2)

By fitting our results we have

\[ c = 31.3 \text{MeV} \]
\[ \gamma = 0.64 \]  

(3)

Typical values for these parameters are

\[ c \approx 31 - 33 \text{MeV} \quad \text{and} \quad \gamma \approx 0.55 - 0.69 \]

\[ c = 31.6 \text{MeV} \quad \text{and} \quad \gamma \approx 0.69 - 1.05 \]  

(4)

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Neutron matter

Comparison of equation of state of neutron matter using different Hamiltonians:

Hebeler-Schwenk: EFT approach\(^6\)

\(^6\)K. Hebeler, A. Schwenk, arXiv:0911.0483
We can impose the $\beta$-equilibrium, so

$$n \rightarrow p + e^- + \bar{\nu}$$  \hspace{1cm} (5)

and require that chemical potentials are conserved

$$\mu_n = \mu_p + \mu_e$$  \hspace{1cm} (6)

The resulting proto-neutron EOS can be used as a model of neutron star

Note: by now we do not consider the effects of hyperons.
TOV equation solved to analyze the static structure of a compact star

The EOS computed using AV8’+UIX Hamiltonian or AV6’+DDI give sensible different star structure.  


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Neutron drops
Neutron drops

Hamiltonian:

\[
H = -\frac{\hbar^2}{2m} \sum_{i=1}^{A} \nabla_i^2 + \sum_{i<j} v_{ij} + \sum_{i<j<k} V_{ijk} + \sum_i V_{\text{ext}}(r_i) \tag{7}
\]

\(V_{\text{ext}}\) confines neutrons.

We used Wood-Saxon or Harmonic well.
Comparison of GFMC and AFDMC energies. 
Hamiltonian: AV8’ + U1X + Wood-Saxon well, V0=-35.5 MeV, R=3 MeV, a=1.1

<table>
<thead>
<tr>
<th>N</th>
<th>$J^\pi$</th>
<th>GFMC</th>
<th>AFDMC</th>
<th>% diff.</th>
</tr>
</thead>
<tbody>
<tr>
<td>8</td>
<td>0$^+$</td>
<td>-103.9(1)</td>
<td>-104.9(1)</td>
<td>.9(1)</td>
</tr>
<tr>
<td>9</td>
<td>1/2$^+$</td>
<td>-107.8(1)</td>
<td>-108.6(1)</td>
<td>.8(1)</td>
</tr>
<tr>
<td>10</td>
<td>0$^+$</td>
<td>-113.4(1)</td>
<td>-113.9(1)</td>
<td>.4(2)</td>
</tr>
<tr>
<td>11</td>
<td>5/2$^+$</td>
<td>-116.9(2)</td>
<td>-117.8(2)</td>
<td>.8(2)</td>
</tr>
<tr>
<td>12</td>
<td>0$^+$</td>
<td>-123.6(3)</td>
<td>-123.4(2)</td>
<td>-.2(3)</td>
</tr>
<tr>
<td>13</td>
<td>5/2$^+$</td>
<td>-125.9(3)</td>
<td>-126.3(3)</td>
<td>.3(3)</td>
</tr>
<tr>
<td>14</td>
<td>0$^+$</td>
<td>-131.6(7)</td>
<td>-132.5(3)</td>
<td>.6(6)</td>
</tr>
</tbody>
</table>

Agreement generally better than 1%.
Neutron drops: Wood-Saxon well

Comparison of *ab-initio* and Skyrme models.

Skyrmes systematically overbind neutron drops.
Comparison of GFMC and AFDMC energies.
Hamiltonian: AV8’ + UIX + Harmonic oscillator well

<table>
<thead>
<tr>
<th>N</th>
<th>$J^\pi$</th>
<th>$\hbar \omega = 5\text{MeV}$</th>
<th>$\hbar \omega = 10\text{MeV}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>8</td>
<td>0$^+$</td>
<td>GFMC 67.00(1) AFDMC 67.0(2) % diff. .0(3)</td>
<td>GFMC 135.80(4) AFDMC 134.8(1) % diff. -.7(1)</td>
</tr>
<tr>
<td>9</td>
<td>1/2$^+$</td>
<td>GFMC 80.90(4) AFDMC 81.2(1) % diff. .4(2)</td>
<td>GFMC 163.7(1) AFDMC 163.1(2) % diff. -.4(2)</td>
</tr>
<tr>
<td>9</td>
<td>5/2$^+$</td>
<td>GFMC 81.20(3) AFDMC 81.6(2) % diff. .5(3)</td>
<td>GFMC 163.2(1) AFDMC 162.0(2) % diff. -.8(1)</td>
</tr>
<tr>
<td>10</td>
<td>0$^+$</td>
<td>GFMC 92.1(1) AFDMC 94.2(2) % diff. 2.2(2)</td>
<td>GFMC 188.1(3) AFDMC 188.1(3)</td>
</tr>
<tr>
<td>12</td>
<td>0$^+$</td>
<td>GFMC 118.1(1) AFDMC 120.3(3) % diff. 1.8(2)</td>
<td>GFMC 242.0(6) AFDMC 240.3(1) % diff. -.7(2)</td>
</tr>
<tr>
<td>13</td>
<td>5/2$^+$</td>
<td>GFMC 131.5(1) AFDMC 135.4(3) % diff. 2.9(2)</td>
<td>GFMC 267.6(6) AFDMC 266.0(6) % diff. -.6(3)</td>
</tr>
<tr>
<td>13</td>
<td>1/2$^+$</td>
<td>GFMC 130.8(1) AFDMC 135.9(3) % diff. 3.8(2)</td>
<td>GFMC 268.0(5) AFDMC 266.4(2) % diff. -.6(2)</td>
</tr>
<tr>
<td>14</td>
<td>0$^+$</td>
<td>GFMC 142.2(2) AFDMC 146.4(3) % diff. 2.9(2)</td>
<td>GFMC 291.9(2) AFDMC 291.1(2) % diff. -.3(1)</td>
</tr>
</tbody>
</table>

- $\hbar \omega = 5 \text{ MeV}$, differences probably due to pairing effects
- $\hbar \omega = 10 \text{ MeV}$, agreement better than 1%
- $5/2^+ - 1/2^+$ ordering well reproduced in 3 of 4 cases
Neutron drops: harmonic oscillator well

Comparison of \textit{ab-initio} and Skyrme models.

Harmonic oscillator external well

NCFC (No Core Full Configuration) provided by P. Maris and J. Vary.
Even-odd staggering and pairing gap.

\[ \Delta(N) = E(N) - E(N-1) \]

\[ \Delta(N) = E(N) - \frac{E(N-1) + E(N+1)}{2} \]
CONCLUSIONS AND PERSPECTIVES
Conclusions

- The study of neutron and nuclear matter using realistic Hamiltonians is now possible within QMC techniques.
- EOS of nuclear and neutron matter revisited.
- Properties of confined neutrons in different geometries now possible up to $N \sim 50$. Skyrme can be now adjusted to deal with large neutron-rich nuclei.
- Computation of spin-orbit splitting and excitation energies in progress.
Thanks for your attention