Properties of homogeneous and inhomogeneous neutron matter

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Homogeneous neutron matter
Inhomogeneous neutron matter

W. Nazarewicz – UNEDF
Neutron drops

Why study neutron drops?
Are 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)
• The model and the method

• **Inhomogeneous neutron matter: Skyrme vs ab-initio.**
  • Energy
  • Density and radii

• **Homogeneous neutron matter**
  • Role of three-neutron force
  • Symmetry energy
  • Neutron star structure

• 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 (Argonne AV8’) fitted on scattering data. Sum of operators:

\[ v_{ij} = \sum O_{ij}^{P=1,8} v^P(r_{ij}), \quad O_{ij}^{P} = (1, \vec{\sigma}_i \cdot \vec{\sigma}_j, S_{ij}, \vec{L}_{ij} \cdot \vec{S}_{ij}) \times (1, \vec{\tau}_i \cdot \vec{\tau}_j) \]

Urbana–Illinois \( V_{ijk} \) models processes like

\[ \begin{array}{c}
\pi^- \pi^- \Delta \\
\pi^- \pi^- \Delta \\
\Delta \pi^- \pi^- \\
\end{array} \]

\[ + \text{ short-range correlations (spin/isospin independent).} \]
Nuclear Hamiltonian

Argonne NN interaction

Wiringa, Stoks, Schiavilla (1995)
Light nuclei spectrum computed with GFMC

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

Carlson, Pieper, Wiringa, many papers
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

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

$G(R, R', t)$ is an approximate propagator (small-time limit). We iterate the above integral equation many times in the small time-step limit. → parallel codes and supercomputers.

For a given microscopic Hamiltonian, this method solves the ground–state within a systematic uncertainty of 1–2% in a non-perturbative way.
Quantum Monte Carlo

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, local) 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!
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:**

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

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!
Neutron drops

Now let’s study **inhomogeneous neutron matter**. We confine neutrons by adding an external potential:

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

\( V_{\text{ext}} \) is a Wood-Saxon or Harmonic well:

\[ V_{WS} = -\frac{V_0}{1 + \exp[(r - R)/a]} \]

\[ V_{HO} = \frac{1}{2} m\omega^2 r^2 \]

\[ \text{implies different geometries and densities.} \]
Neutron drops, harmonic oscillator well

External well: harmonic oscillator with $\hbar \omega = 5, 10 \text{ MeV}$.

Skyrme systematically overbind neutron drops.
Neutron drops, harmonic oscillator well

Fixing Skyrme force:

The correction is very similar in all the Skyrme forces we considered.
Neutron drops, adjusted Skyrme force

Note: bulk term of Skyrme fit neutron matter.

We add the **missing repulsion** by adjusting the gradient term $G_d[\nabla \rho_n]^2$, the pairing and spin-orbit terms.

Neutron drops, adjusted Skyrme force

Neutrons in the Wood-Saxon well are also better reproduced by the adjusted SLY4.

Neutron drops: radii

Correction to radii using the adjusted-SLY4.

Neutron drops: radial density

Neutron radial density:

\[ \rho(r) \text{ (fm}^{-1}) \]

\[ \omega = 5 \text{ MeV} \]
\[ \omega = 10 \text{ MeV} \]

SLY4-adj

SLY4

\[ N=8 \]
\[ N=14 \]

Neutron drops

Ab-initio calculations meant as experimental data:

\[
\frac{E_{\text{tot}}}{N^{4/3}} \quad \text{(MeV)}
\]

Neutron drops: comparison

Comparison using the softer Minnesota interaction:

Gradient term

Where is the gradient term important?

Just few examples:

- Medium large neutron-rich nuclei
- Phases in the crust of neutron stars
- Isospin-asymmetry energy of nuclear matter

Note: in the pasta phase the volume vs surface energy process is critical.
Role of the gradient?
Neutron matter and the puzzle of the three-body force

Note: AV8’+UIX and (almost) AV8’ are stiff enough to support observed neutron stars. → How to reconcile with nuclei???
Neutron matter

Assumptions:

- The two-nucleon interaction reproduces well (elastic) \( pp, np \) and \( nn \) scattering data up to high energies (\( E_{lab} \sim 600\text{MeV} \)).

- 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). Difficult to study in light nuclei.
Symmetry energy

Nuclear matter EOS:

\[ E(\rho, x) = E_{SNM}(\rho) + E_{sym}^{(2)}(\rho)(1 - 2x)^2 + \cdots \]

where

\[ \rho = \rho_n + \rho_p, \quad x = \frac{\rho_p}{\rho} \]

\[ E_0 = -16 \text{ MeV} \]

\[ \rho_0 = 0.16 \text{ fm}^{-3} \]
Neutron matter

We consider different forms of three-neutron interaction by only requiring a particular value of $E_{sym}$ at saturation.

different 3N:

- $V_{2\pi} + \alpha V_R$
- $V_{2\pi} + \alpha V_R^\mu$
  (several $\mu$)
- $V_{2\pi} + \alpha \tilde{V}_R$
- $V_{3\pi} + \alpha V_R$
Neutron matter and symmetry energy

We then try to change the neutron matter energy at saturation:

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

Neutron matter and symmetry energy

From the EOS, we can fit the symmetry energy around $\rho_0$ using

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

Very weak dependence to the model of 3N force for a given $E_{\text{sym}}$. Role of NN will be investigated next.
Neutron star structure

EOS used to solve the TOV equations.

Accurate measurement of $E_{\text{sym}}$ would put a constraint to the radius of neutron stars, OR observation of $M$ and $R$ would constrain $E_{\text{sym}}$!

$M = 1.97 \, M_{\odot}$ observed – Demorest et al., Nature (2010).
Neutron stars

Observations of the mass-radius relation are available:


We can use neutron star observations to ’measure’ the EOS and constrain $E_{sym}$ and $L$. 
We model neutron star matter as

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

(form suggested by QMC simulations),

and a high density model for $\rho > \rho_t$

i) two polytropes


By changing $\rho_t$ and the high density model we can understand systematic errors in $E_{NSM}$ parametrization.

We also add a correction to account for the proton fraction present in neutron stars.
Observations

What can we learn by fitting our model to observations?

- Symmetry energy and its slope:
  \[ E_{\text{sym}} = a + b + 16, \quad L = 3(a\alpha + b\beta) \]

- Strength of 3N:

<table>
<thead>
<tr>
<th>3N force</th>
<th>( E_{\text{sym}} ) (MeV)</th>
<th>L (MeV)</th>
<th>a (MeV)</th>
<th>( \alpha )</th>
<th>b (MeV)</th>
<th>( \beta )</th>
</tr>
</thead>
<tbody>
<tr>
<td>none</td>
<td>30.5</td>
<td>31.3</td>
<td>12.7</td>
<td>0.49</td>
<td>1.78</td>
<td>2.26</td>
</tr>
<tr>
<td>( V_{2\pi} + V_{R}^{\mu=300} )</td>
<td>32.0</td>
<td>40.6</td>
<td>12.8</td>
<td>0.488</td>
<td>3.19</td>
<td>2.20</td>
</tr>
<tr>
<td>( V_{2\pi} + V_{R}^{\mu=600} )</td>
<td>32.0</td>
<td>41.3</td>
<td>12.8</td>
<td>0.488</td>
<td>3.19</td>
<td>2.20</td>
</tr>
<tr>
<td>( V_{3\pi} + V_{R} )</td>
<td>32.1</td>
<td>41.3</td>
<td>12.7</td>
<td>0.476</td>
<td>3.34</td>
<td>2.22</td>
</tr>
<tr>
<td>( V_{3\pi} + V_{R} )</td>
<td>32.0</td>
<td>44.0</td>
<td>13.0</td>
<td>0.49</td>
<td>3.21</td>
<td>2.47</td>
</tr>
<tr>
<td>( V_{2\pi} + V_{R} )</td>
<td>33.7</td>
<td>52.9</td>
<td>13.3</td>
<td>0.512</td>
<td>4.38</td>
<td>2.39</td>
</tr>
<tr>
<td>( V_{3\pi} + V_{R} )</td>
<td>33.8</td>
<td>56.2</td>
<td>13.0</td>
<td>0.50</td>
<td>4.71</td>
<td>2.49</td>
</tr>
<tr>
<td>UIX</td>
<td>35.1</td>
<td>63.6</td>
<td>13.4</td>
<td>0.514</td>
<td>5.62</td>
<td>2.436</td>
</tr>
</tbody>
</table>

Note: \( a \) and \( \alpha \) don’t depend too much to the model of 3N!
Neutron star observations

32 < \( E_{\text{sym}} < 34 \text{ MeV} \), \( 43 < L < 52 \text{ MeV} \)
Steiner, Gandolfi (2012).
Local N$^2$LO potential

Bands: short-range cutoff $R_0$ varied from 400 to 600 MeV
Neutron matter with QMC/EFT

Gezerlis, Tews, Epelbaum, SG, Hebeler, Nogga, Schwenk (2013)
Inclusion of TNI in progress.
Conclusions

- Isovector parts of Skyrme forces can be better constrained by ab-initio calculations.
- Effect of three-neutron forces to high-density neutron matter is (reasonably) under control.
- $E_{\text{sym}}$ strongly constrain $\mathcal{L}$. Weak dependence to the model of 3N.
- Uncertainty of the radius of neutron stars mainly due $E_{\text{sym}}$ rather than 3N.
- Neutron star observations becoming competitive with terrestrial experiments.
- QMC calculations using chiral forces now possible.

Thanks for the attention