From few to many neutrons using Quantum Monte Carlo techniques

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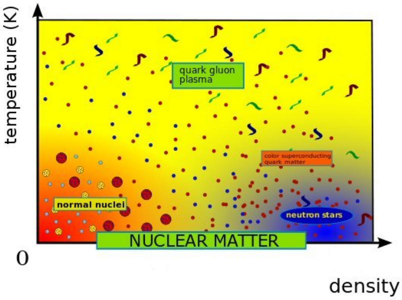
Outline

- Motivations
- The model and the method
- Equation of state of zero temperature nuclear and neutron matter
- Neutron drops
- Conclusions and perspectives

Outline

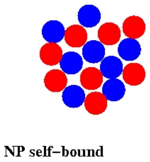
Why study nuclear matter? Why zero temperature?

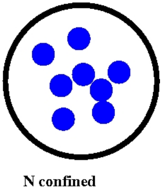


Large density: nuclei → *nuclear matter*.
Neutron matter: simpler system to model a neutron star.

Neutron drops

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



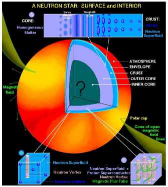


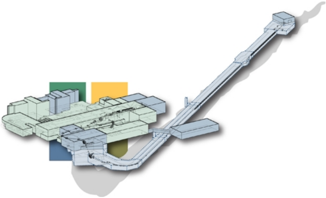
Neutron drops are interesting because:

- 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)

Motivations

- Quantum Monte Carlo methods (GFMC and AFDMC) provide very accurate results for nuclear systems.
- NN scattering data and few-body theory $\rightarrow$ nuclear Hamiltonians. Few-body $\rightarrow$ many–body $\Rightarrow$ 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).

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

NN and TNI are usually written as sums of operators:

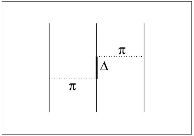
$$v_{ij} = \sum_{p=1}^{M} v_p(r_{ij}) O^{(p)}(i,j)$$

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

$$O_{ij}^{p=1,8} = (1, \vec{\sigma}_i \cdot \vec{\sigma}_j, S_{ij}, \vec{L}_{ij} \cdot \vec{S}_{ij}) \times (1, \vec{\tau}_i \cdot \vec{\tau}_j)\,.$$

V_{ij} fitted on scattering data.

Urbana Three-Nucleon-Interaction model:



$+$ Phenomenological repulsive term.

For example the Fujita-Miyazawa diagram gives:

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

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)

TNI density-dependent interaction

Different approach to include TNI (Friedman-Lagaris-Pandharipande): modify the NN interaction by adding density-dependent terms to NN: [2]

$$
\begin{aligned}
v^p_{DD6'} &= v^p_{OPE} + v^p_I e^{-\gamma_1 \rho} + v^p_S + \mathrm{TNA}(\rho)\,, \\
\mathrm{TNA}(\rho) &= 3\gamma_2 \rho^2 e^{-\gamma_3 \rho} \left[1 - \frac{2}{3} \left(\frac{\rho_n - \rho_p}{\rho_n + \rho_p} \right)^2 \right]
\end{aligned}
$$

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

[2] Lagaris and Pandharipande, Nucl. Phys. A359, 349 (1981).

Quantum Monte Carlo

Evolution of Schrodinger 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.

GFMC and AFDMC

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:

$$\psi = \begin{pmatrix} a_{\uparrow\uparrow\uparrow} \\ a_{\uparrow\uparrow\downarrow} \\ a_{\uparrow\downarrow\uparrow} \\ a_{\uparrow\downarrow\downarrow} \\ a_{\downarrow\uparrow\uparrow} \\ a_{\downarrow\uparrow\downarrow} \\ a_{\downarrow\downarrow\uparrow} \\ a_{\downarrow\downarrow\downarrow} \end{pmatrix}$$

A 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:

$$\psi = \mathcal{A}\left[\xi_{s_1}\begin{pmatrix} a_1 \\ b_1 \end{pmatrix}\xi_{s_2}\begin{pmatrix} a_2 \\ b_2 \end{pmatrix}\xi_{s_3}\begin{pmatrix} a_3 \\ b_3 \end{pmatrix}\right]$$

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 deal to large systems (up to $A \approx 100$).
Operators (except the energy) are very hard to be computed.

Wave function

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

$$\psi_T(R,S) = \Phi_J(R) \cdot A[\phi_i(\vec{r}_j, s_j)] \tag{1}$$

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:

$$GFMC: \quad \Phi_J(R) = \prod_{i<j} \left(f_c(r_{ij}) + f_\sigma(r_{ij}) \sigma_i \cdot \sigma_j + \dots \right)$$

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

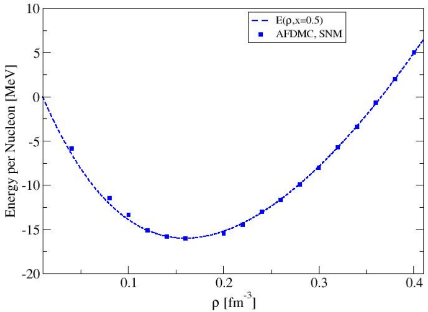
According to the problem correct boundary conditions to the trial wave-function must be imposed.

NUCLEAR AND NEUTRON MATTER

SYMMETRIC NUCLEAR MATTER

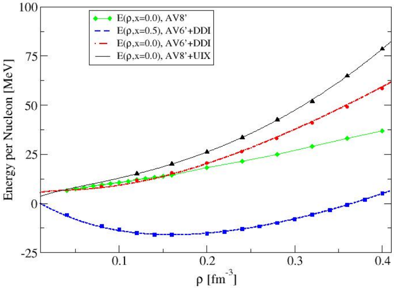
We re-adjusted the DDI parameters combined with the NN AV6' to reproduce following properties of SNM:

- $\rho_0 = 0.16$ fm^{-3}
- $E(\rho_0) = -16$ MeV
- the compressibility K ≈240 MeV



Neutron and Nuclear matter

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.

[3] SG *et al.*, Mon. Not. R. Astron. Soc. 404, L35 (2010).

Symmetry energy

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

$$E_{sym}(\rho) = c\,(\rho/\rho_0)^\gamma \ . \tag{2}$$

By fitting our results we have

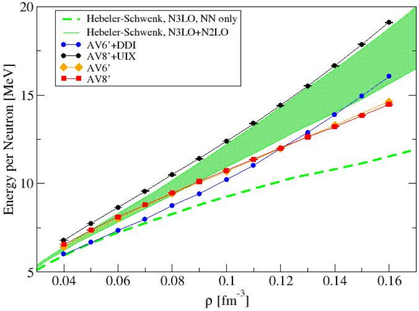
$$\begin{aligned} c &= 31.3 MeV \\ \gamma &= 0.64 \end{aligned} \tag{3}$$

Typical values for these parameters are

$$\begin{aligned} c \approx 31 - 33 MeV \quad &\text{and} \quad \gamma \approx 0.55 - 0.69^4 \\ c = 31.6 MeV \quad &\text{and} \quad \gamma \approx 0.69 - 1.05^5 \end{aligned} \tag{4}$$

[4] D.V. Shetty, S.J. Yennello, and G.A. Souliotis, *Phys. Rev. C* 76, 024606 (2007)
[5] Aaron Worley, Plamen G. Krastev, and Bao-An Li, *ApJ* 685, 390 (2008)

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



Hebeler-Schwenk: EFT approach[6]

[6] K. Hebeler, A. Schwenk, arXiv:0911.0483

β–equilibrium

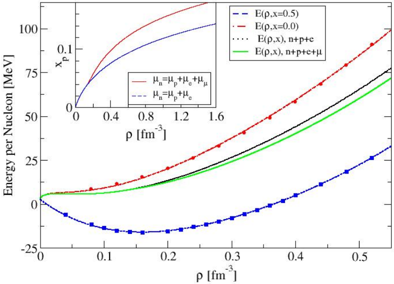
We can impose the β-equilibrium, so

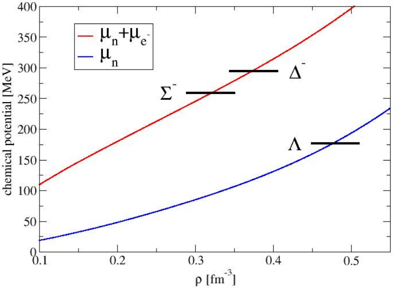
$$n \rightarrow p + e^- + \bar{\nu} \quad (5)$$

and require that chemical potentials are conserved

$$\mu_n = \mu_p + \mu_e \quad (6)$$

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

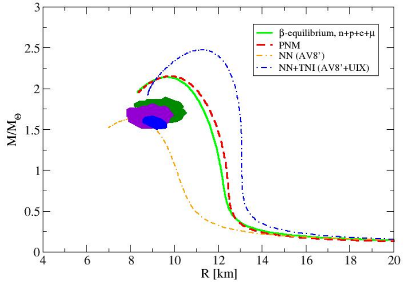


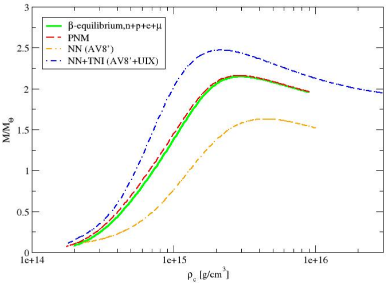


Note: by now we do not consider the effects of hyperons.

Neutron star structure

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. [7]

Observations: Özel, Baym and Güver, arXiv:1002.3153 (2010).

[7] SG *et al.*, Mon. Not. R. Astron. Soc. 404, L35 (2010).

Neutron drops

Neutron drops

Hamiltonian:

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

V_{ext} confines neutrons.

We used Wood-Saxon or Harmonic well.

Neutron drops: Wood-Saxon well

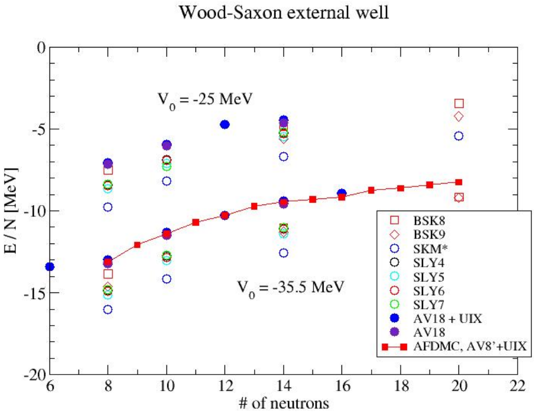
Comparison of GFMC and AFDMC energies.
Hamiltonian: AV8' + UIX + Wood-Saxon well, V0=-35.5 MeV, R=3 MeV, a=1.1

N	J^π	GFMC	AFDMC	% diff.
8	0^+	-103.9(1)	-104.9(1)	.9(1)
9	$1/2^+$	-107.8(1)	-108.6(1)	.8(1)
10	0^+	-113.4(1)	-113.9(1)	.4(2)
11	$5/2^+$	-116.9(2)	-117.8(2)	.8(2)
12	0^+	-123.6(3)	-123.4(2)	-.2(3)
13	$5/2^+$	-125.9(3)	-126.3(3)	.3(3)
14	0^+	-131.6(7)	-132.5(3)	.6(6)

Agreement generally better than 1%.

Neutron drops: Wood-Saxon well

Comparison of *ab-initio* and Skyrme models.



Skyrmes systematically overbind neutron drops.

Neutron drops: Harmonic oscillator well

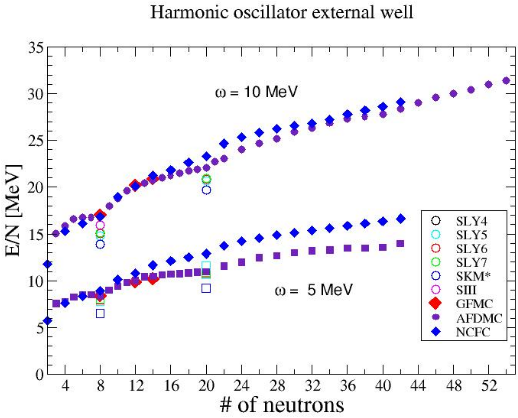
Comparison of GFMC and AFDMC energies.
Hamiltonian: AV8' + UIX + Harmonic oscillator well

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

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

Neutron drops: harmonic oscillator well

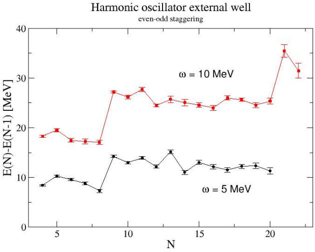
Comparison of *ab-initio* and Skyrme models.

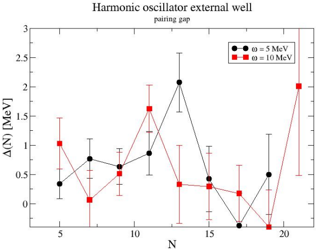


NCFC (No Core Full Configuration) provided by P. Maris and J. Vary.

Neutron drops: harmonic oscillator well

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