Ab-initio calculation of confined neutrons and implications for Skyrme models

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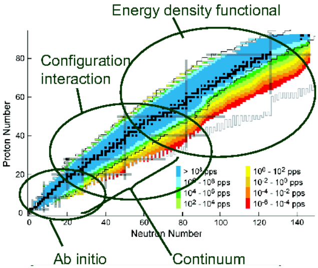
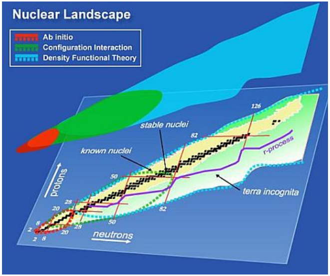
Overview





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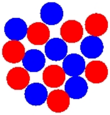
Large nuclei and inhomogeneous matter (pasta phase in neutron stars) can be studied using density functional theory.

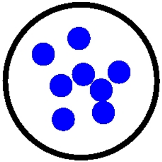
We need some input to build functionals and then compare with measurements and make predictions.

Neutron drops

Why study neutron drops?



NP self–bound



N confined

Neutron drops are interesting because:

- Calibrate Skyrme models for neutron-rich systems (useful to check $\nabla\rho$ terms in different geometries)
- Provide a strong benchmark for microscopic calculations
- Model neutron-rich nuclei

Outline

- The model and QMC methods
- Ab-initio calculations and Skyrme forces
- Comparison between different Hamiltonians, ground– and excited–states
- Conclusions

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 the above integral equation many times in the small time-step limit.

Wave function

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

$$\psi_T(R) = \Phi_J(R) \cdot A[\phi_i(\vec{r}_j)]_{J,M}$$

where $R = (\vec{r}_1 ... \vec{r}_A)$, and $\{\phi_i\}$ is a single-particle basis:

$$\phi_i(\vec{r}_j) = R_{n,l}(r_j) Y_{l,m_l}(\hat{r}_j)$$

$\Phi_J(R)$ is a Jastrow factor, it contains short-range correlations:

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

Nuclear Hamiltonian

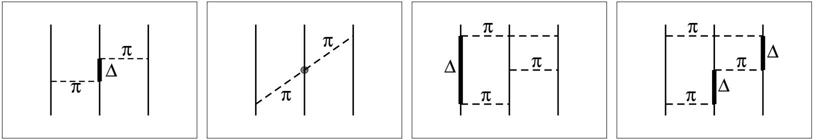
Model: non-relativistic nucleons interacting with an effective nucleon-nucleon force (NN) and three-nucleon interaction (TNI).

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

v_{ij} NN (Argonne AV8') fitted on scattering data. Sum of operators:

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

V_{ijk} models processes like



$+$ Phenomenological repulsive term.

GFMC and AFDMC

Hamiltonian state dependent
$\Longrightarrow$ spin/isospin states must be included in the wave function.

Example of the spin for 3 neutrons (spatial 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

$$\exp\left[-v(r)\sigma_1 \cdot \sigma_2 \Delta t\right]$$

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

AFDMC wave-function:

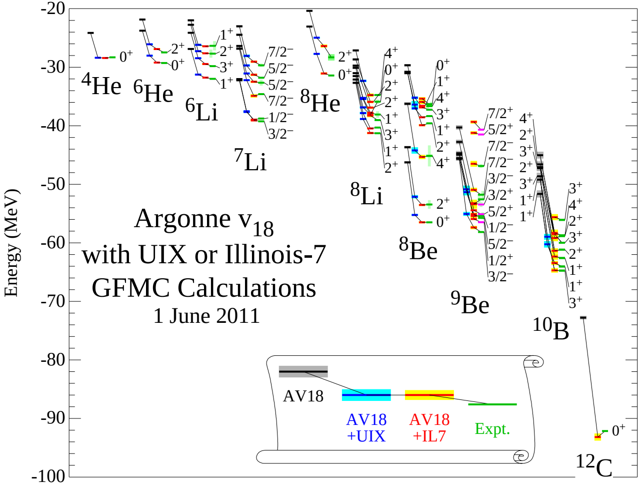
$$\psi = \mathcal{A}\left[\xi_{s_1}\begin{pmatrix} a_1 \\ b_1 \end{pmatrix}\xi_{s_2}\begin{pmatrix} a_2 \\ b_2 \end{pmatrix}\xi_{s_3}\begin{pmatrix} a_3 \\ b_3 \end{pmatrix}\right]$$

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.
Using AFDMC we can accurately compute the energy of large systems (up to $A \approx 100$). Other operators are difficult.

Nuclei



Results by Steve Pieper

Neutron drops

To confine neutrons we add an external potential:

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

V_{ext} is a Wood-Saxon or Harmonic well:

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

$$V_{HO} = \frac{1}{2}m\omega^2 r^2 \qquad (1)$$

$\Longrightarrow$ different geometries and densities.

Neutron drops: Harmonic oscillator well

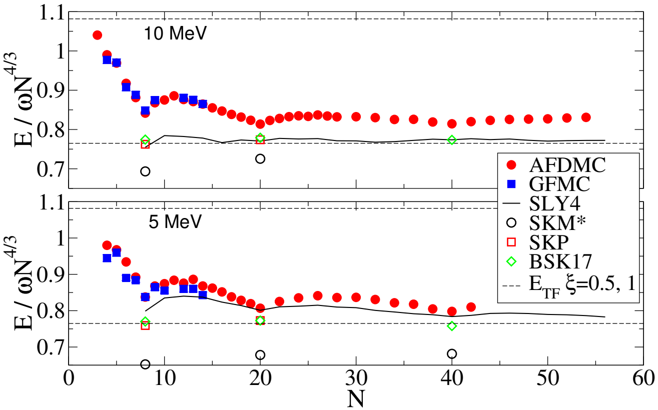
Comparison of GFMC and AFDMC energies.
Hamiltonian: AV8' + UIX + Harmonic oscillator well

N	J^π	$\hbar\omega = 5 MeV$ GFMC	$\hbar\omega = 5 MeV$ AFDMC	$\hbar\omega = 10 MeV$ GFMC	$\hbar\omega = 10 MeV$ AFDMC
8	0^+	67.00(1)	67.13(6)	135.80(4)	134.7(1)
9	$1/2^+$	80.90(4)	81.25(8)	163.7(1)	163.5(1)
9	$5/2^+$	81.20(3)	81.95(8)	163.2(1)	162.5(1)
10	0^+	92.1(1)	94.6(1)	188.1(6)	188.5(1)
12	0^+	118.1(1)	121.1(1)	242.0(6)	240.8(1)
13	$5/2^+$	131.5(1)	135.7(2)	267.6(6)	266.3(2)
13	$1/2^+$	130.8(1)	134.1(2)	268.0(5)	267.2(2)
14	0^+	142.2(2)	146.7(2)	291.9(2)	291.7(2)

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

Neutron drops, harmonic oscillator well

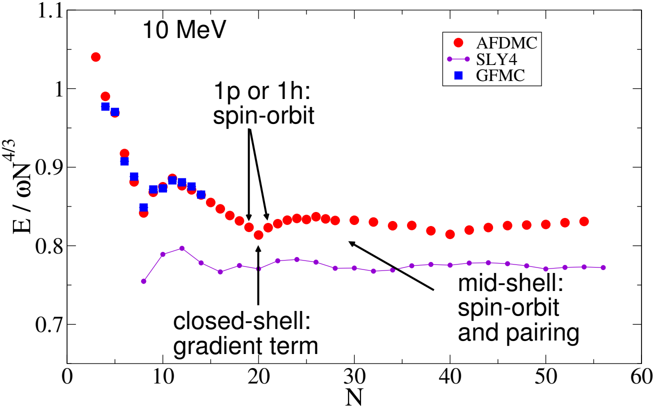
External well: harmonic oscillator with $\hbar\omega$=5, 10 MeV.



Skyrme systematically overbind neutron drops.

Neutron drops, harmonic oscillator well

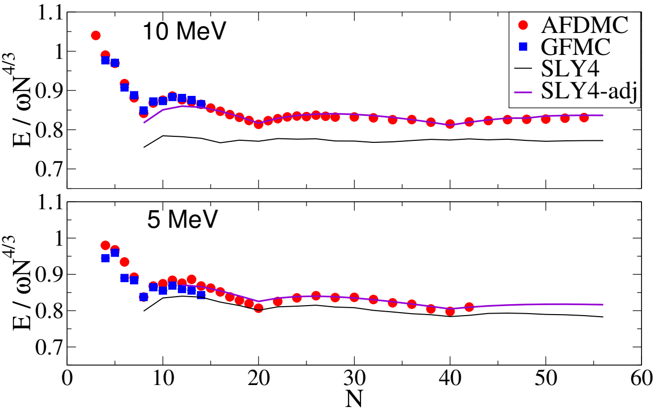
Fixing Skyrme force:



Neutron drops, adjusted Skyrme force

Note: bulk term of Skyrme fit neutron matter.

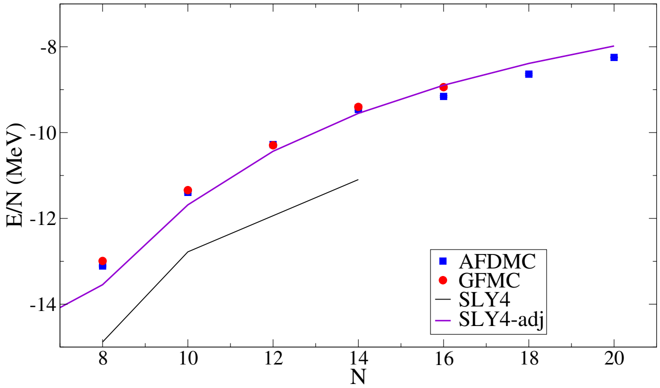
We add the **missing repulsion** by adjusting the gradient term $G_d[\nabla\rho_n]^2$, the pairing and spin-orbit terms.



Gandolfi, Carlson, Pieper, PRL 106, 012501 (2011).

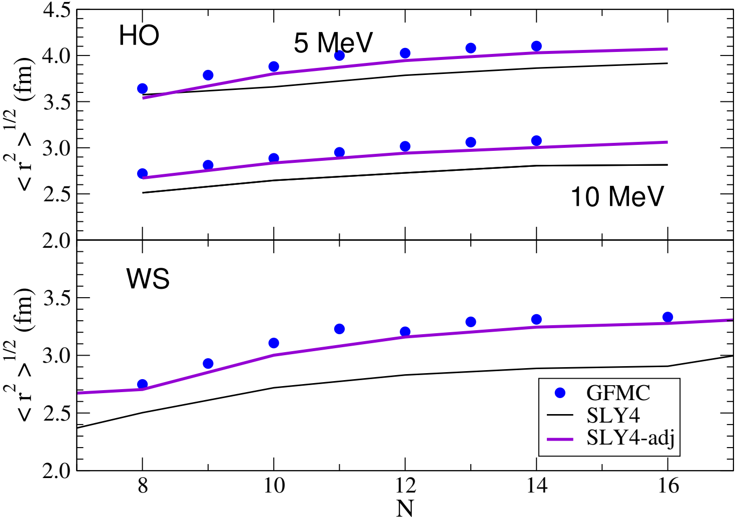
Neutron drops, adjusted Skyrme force

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



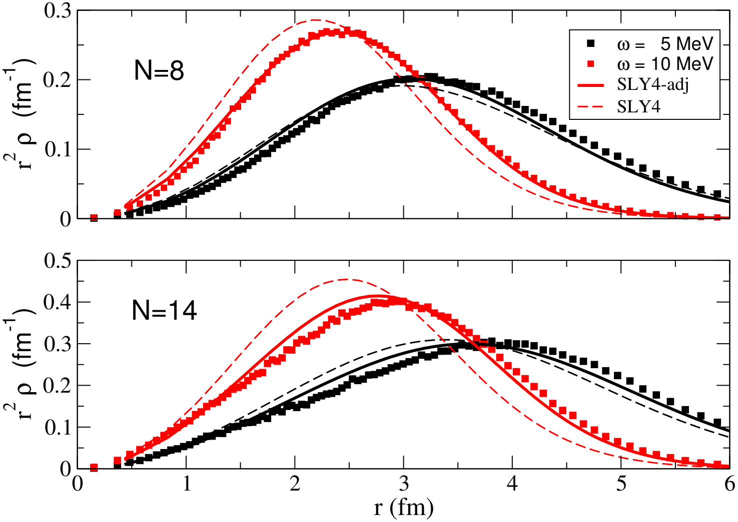
Neutron drops: radii

Correction to radii using the adjusted-SLY4.



Neutron drops: radial density

Neutron radial density:



The correction of G_d is also very important here.

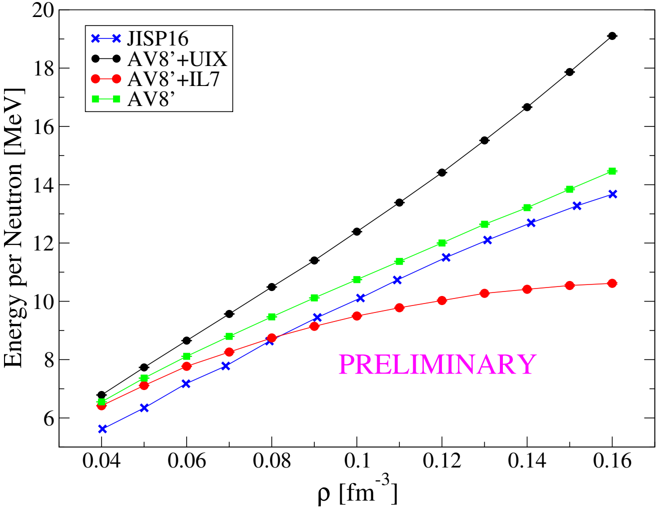
Gradient term

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

Neutron matter EOS:

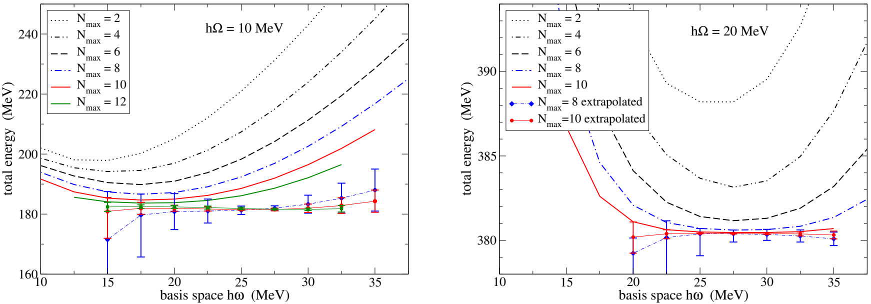


Thanks to Scott Bogner & Andrey Shirokov for JISP16 neutron matter calculation.

No Core Full Configuration

NCFC is used to study neutron drops with the JIPS16 Hamiltonian.

Convergence of 10 neutrons:

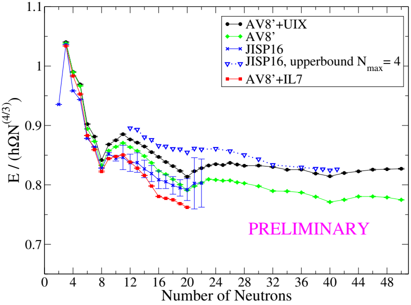


Carlson, Gandolfi, Pieper, Vary, Maris, work in progress

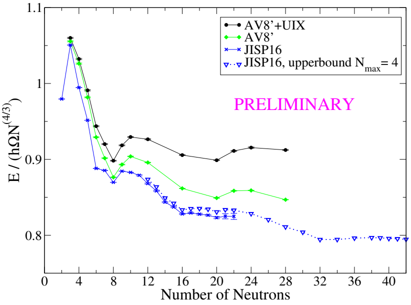
Neutron drops: a comparison

Ground state energy:

$\hbar\omega = 10$ MeV



$\hbar\omega = 20$ MeV

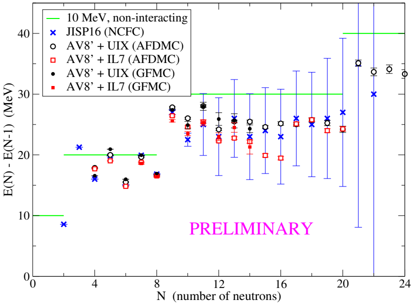


Carlson, Gandolfi, Pieper, Vary, Maris, work in progress

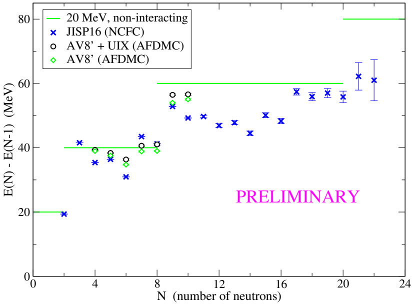
Neutron drops: a comparison

Single energy differences $E(N) - E(N-1)$

$\hbar\omega = 10$ MeV



$\hbar\omega = 20$ MeV



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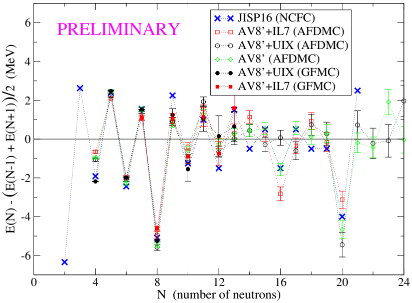
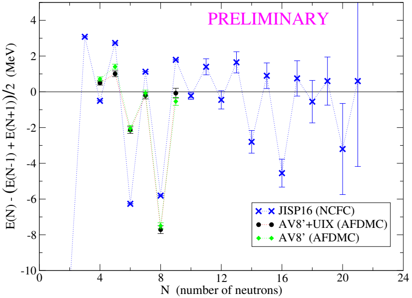
Neutron drops: a comparison

Double energy differences $E(N) - \frac{1}{2}(E(N-1) + E(N+1))$

$\hbar\omega = 10$ MeV



$\hbar\omega = 20$ MeV

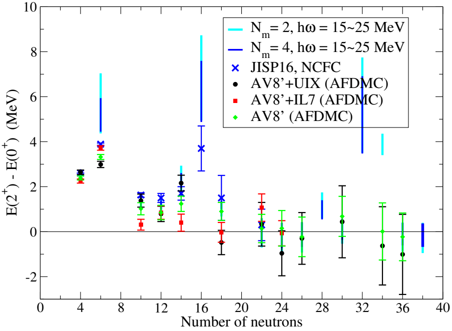


Carlson, Gandolfi, Pieper, Vary, Maris, work in progress

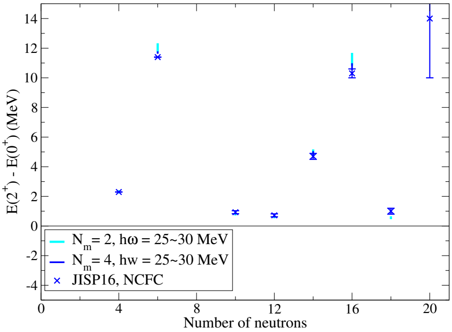
Neutron drops: $0^+ - 2^+$ splitting

$0^+ - 2^+$ splitting

$\hbar\omega = 10$ MeV



$\hbar\omega = 10$ MeV



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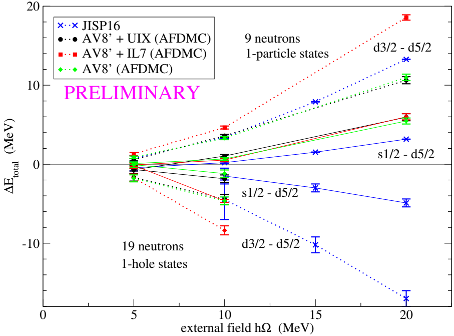
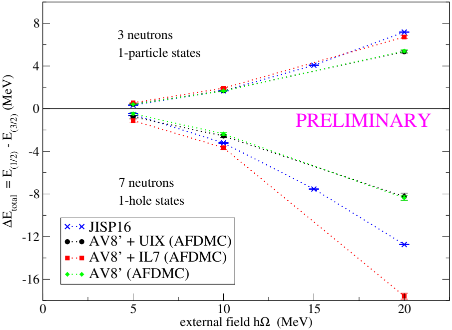
Neutron drops: spin-orbit splitting

Spin-orbit splitting





Carlson, Gandolfi, Pieper, Vary, Maris, work in progress

Conclusions

Conclusions

- We show how to adjust Skyrme forces to deal with large isospin-asymmetry.
- We presented a comparison using different Hamiltonians with and without three-body forces.
- Excited states more in agreement.
- All the results can be used to make Skyrme forces working better.

Thanks

Thanks for the attention