Microscopic Calculations of Homogeneous and Inhomogeneous Neutron Matter

Stefano Gandolfi

Los Alamos National Laboratory (LANL)

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NUCLEI Nuclear Computational Low-Energy Initiative

www.computingnuclei.org

Overview

What is a system strongly correlated?

$$E_{FG} \sim V_{internal}$$

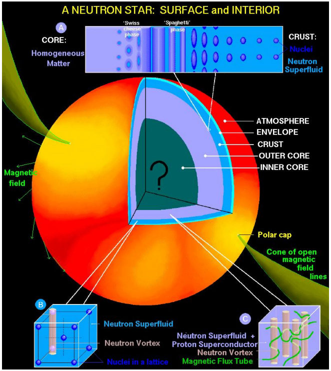
Examples:

- Nuclei
- Neutron stars
- Cold Atoms
- QCD

These systems require non-perturbative calculations to be studied

Neutron stars

Neutron star is a wonderful natural laboratory

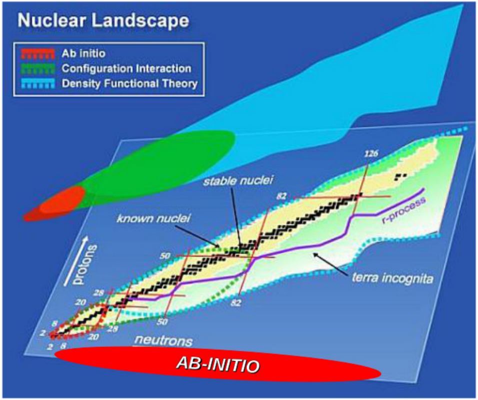


D. Page

- Atmosphere: atomic and plasma physics
- Crust: physics of superfluids (neutrons, vortex), solid state physics (nuclei)
- Inner crust: deformed nuclei, pasta phase
- Outer core: nuclear matter
- Inner core: hyperons? quark matter? π or K condensates?

There is job for very different fields, from condensed matter to string theory

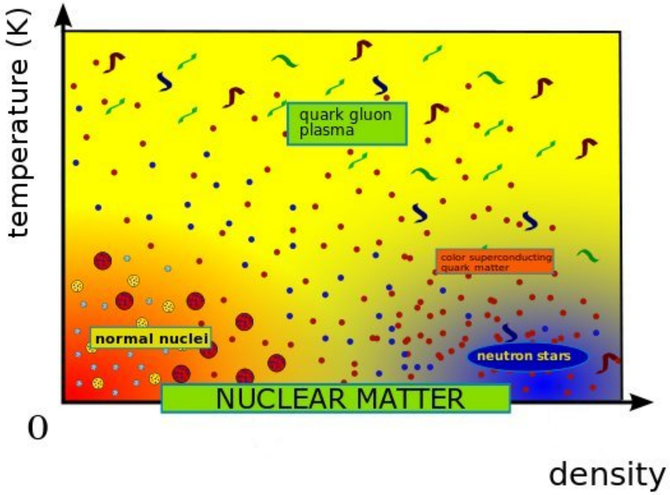
Nuclei



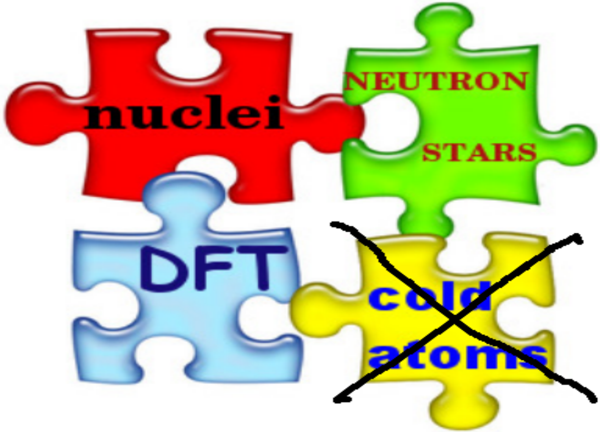
www.unedf.org

Large nuclei and inhomogeneous matter have to be studied using density functional theory. Note: if we know the nuclear DF, then we know the ground-state of any nuclear system.

Homogeneous neutron matter



Overview



The glue: Quantum Monte Carlo methods

Outline

- The model and the method
- **Homogeneous neutron matter**
  - Three-neutron force and the equation of state of neutron matter
  - Symmetry energy
  - Neutron star structure
- **Neutron stars observations**
- Conclusions:
  With microscopic calculations we study the relation between E_{sym} and the Mass-Radius diagram of neutron stars. The three-neutron force is the bridge!
- **Inhomogeneous neutron matter**
- Conclusions:
  Ab-initio calculation help to constrain nuclear density functionals

Nuclear Hamiltonian

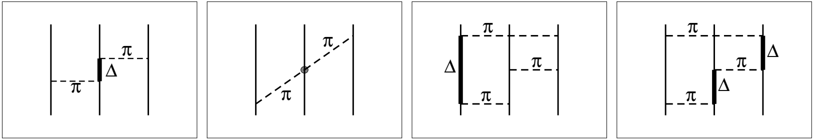
Model: non-relativistic nucleons interacting with an effective nucleon-nucleon force (NN) and three-nucleon interaction (TNI).

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

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

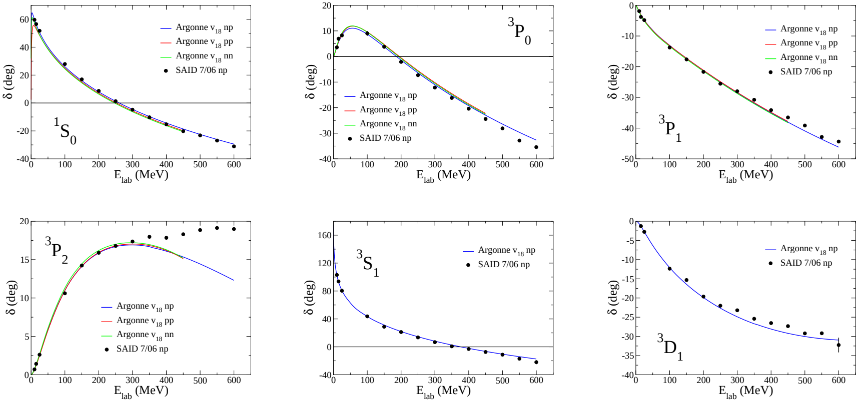
$$v_{ij} = \sum O_{ij}^{p=1,8} v^p(r_{ij})\,, \quad O_{ij}^p = (1, \vec{\sigma}_i \cdot \vec{\sigma}_j, S_{ij}, \vec{L}_{ij} \cdot \vec{S}_{ij}) \times (1, \vec{\tau}_i \cdot \vec{\tau}_j)$$

Urbana–Illinois V_{ijk} models processes like



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

Argonne NN interaction



Wiringa, Stoks, Schiavilla (1995)

Quantum Monte Carlo

We want to solve:

$$H\,\psi(\vec{r}_1\dots\vec{r}_N) = E\,\psi(\vec{r}_1\dots\vec{r}_N) \qquad \psi(R,t) = e^{-(H-E_T)t}\psi(R,0)$$

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

Propagation performed by

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

GFMC includes all spin-states of nucleons in the w.f., nuclei up to A=12
AFDMC samples spin states, pure neutron systems up to A$\sim$100

For a given (local) Hamiltonian, these methods solve 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 ψ_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:

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

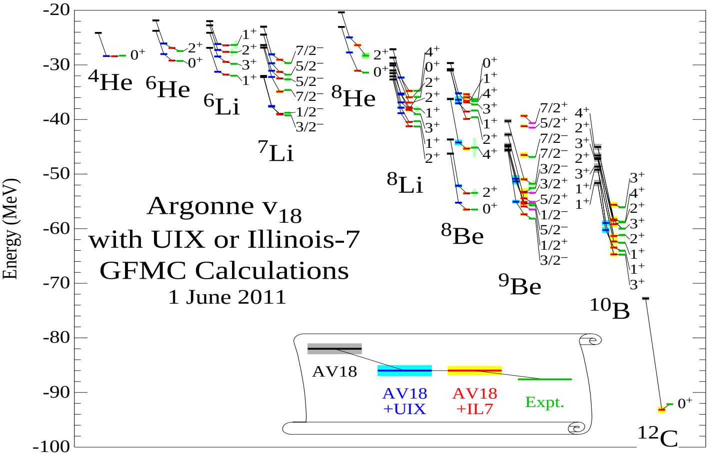
We must change the propagator by using the Hubbard-Stratonovich transformation:

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

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, but in some case there is some trick!

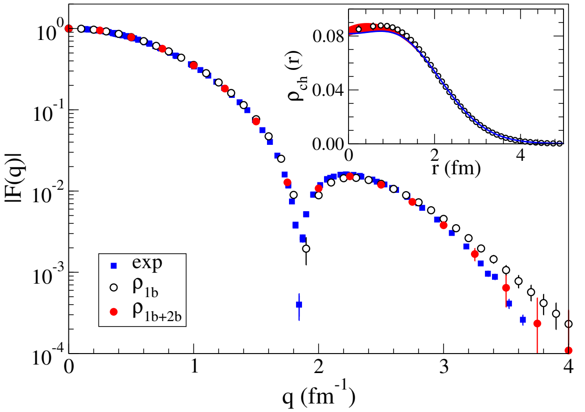
Light nuclei spectrum computed with GFMC



Carlson, Pieper, Wiringa, many papers

Charge form factor of ^{12}C

$$|F(q)| = \langle\psi|\rho_q|\psi\rangle \qquad \rho_q = \sum_i \rho_q(i) + \sum_{i<j} \rho_q(ij)$$



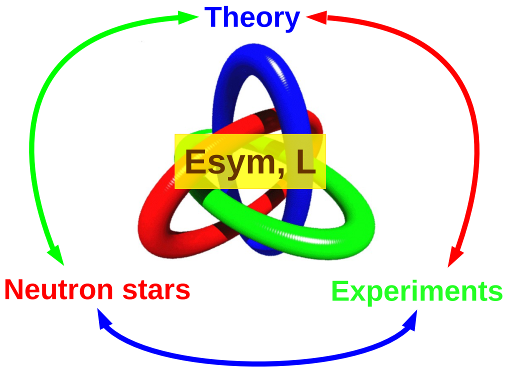
Lovato, Gandolfi, Butler, Carlson, Lusk, Pieper, Schiavilla PRL (2013)

Neutron matter

Why to study neutron matter?

- EOS of neutron matter gives the symmetry energy and its slope.
- EOS of neutron matter determines the structure of neutron stars.

Why to study symmetry energy?



Neutron matter

Assumptions:

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

  Note: at density ρ_0, $k_F \simeq 330$ MeV. Two neutrons have $\mathrm{E}_{CM} \simeq 120$ MeV, $\mathrm{E}_{LAB} \simeq 240$ MeV. $\rightarrow$ Argonne NN very accurate for densities up to $3\rho_0$.

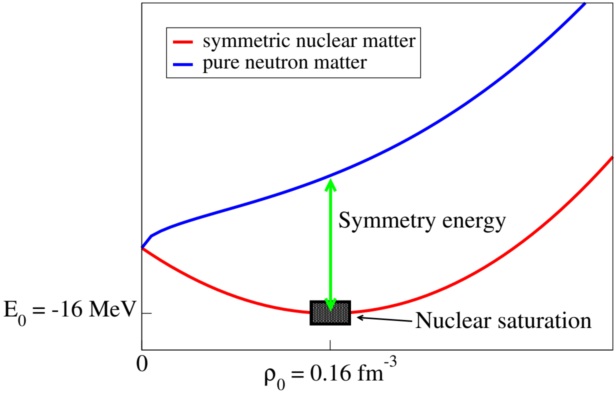
- The three-neutron force ($T = 3/2$) very weak in light nuclei, while $T = 1/2$ is the dominant part (but zero in neutron matter). **Difficult to study in light nuclei.**

Nuclear matter EOS:

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

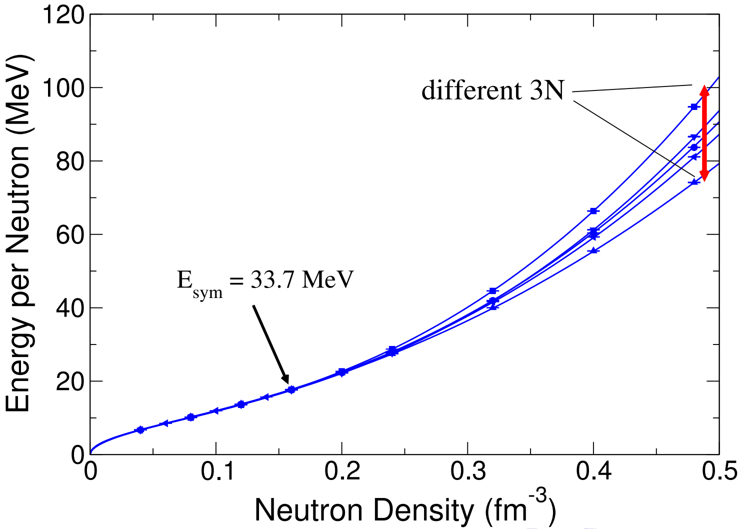
where

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



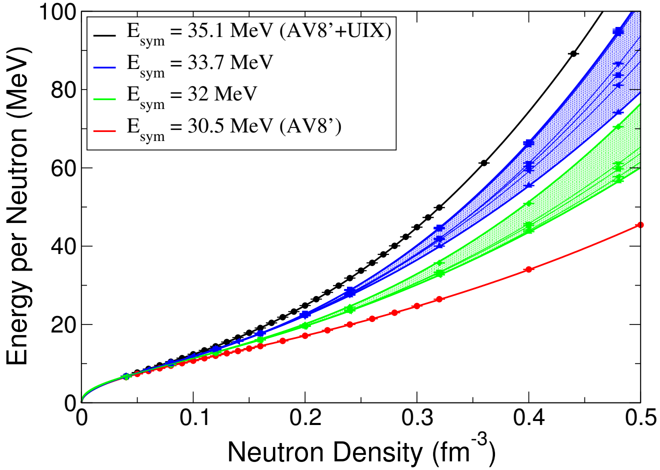
Neutron matter

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



Neutron matter and symmetry energy

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

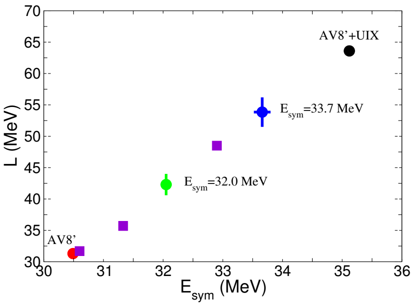


Gandolfi, Carlson, Reddy, PRC (2012).

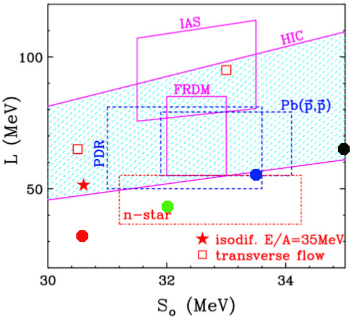
Neutron matter and symmetry energy

From the EOS, we can fit the symmetry energy around ρ_0 using

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



Gandolfi *et al.*, EPJ (2014)



Tsang *et al.*, PRC (2012)

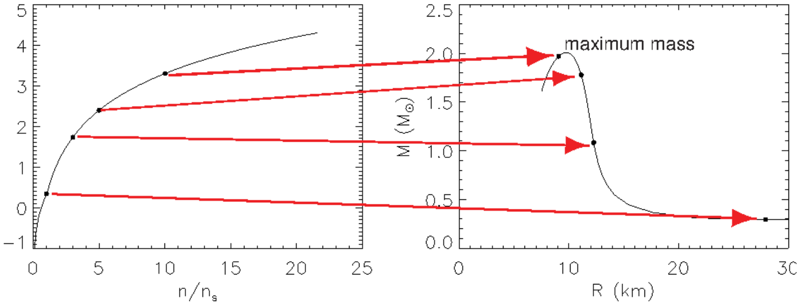
Very weak dependence to the model of 3N force for a given E_{sym}.
Role of NN? Four-body forces? Relativistic effects?

Neutron matter and neutron star structure

TOV equations:

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

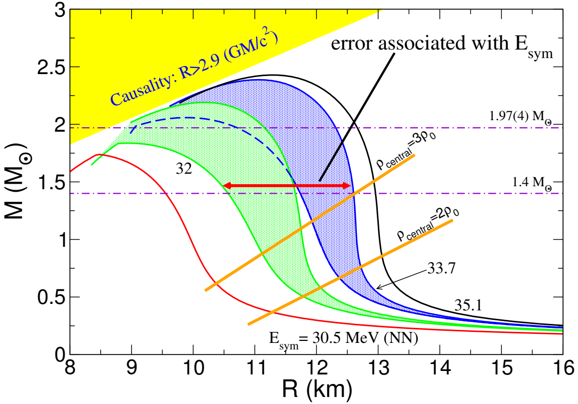
$$\frac{dm(r)}{dr} = 4\pi\epsilon r^2 \,,$$



J. Lattimer

Neutron star structure

EOS used to solve the TOV equations.

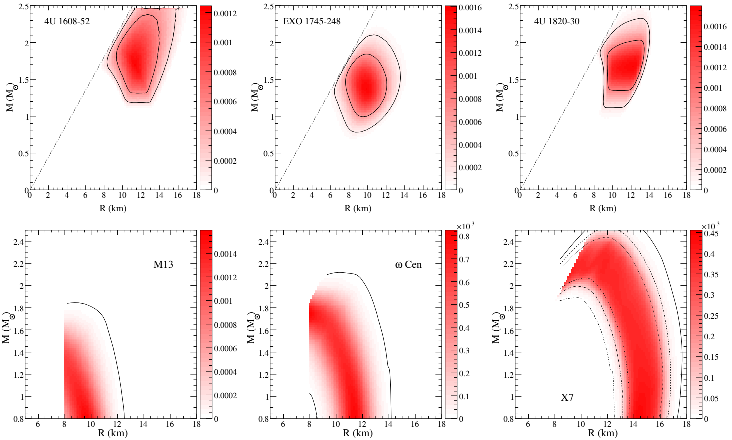


Gandolfi, Carlson, Reddy, PRC 032801, 85 (2012).

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

Neutron stars

Observations of the mass-radius relation are available:



Steiner, Lattimer, Brown, ApJ (2010)

We can use neutron star observations to 'measure' the EOS and constrain E_{sym} and L.

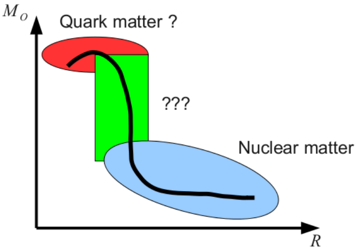
Neutron star matter

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

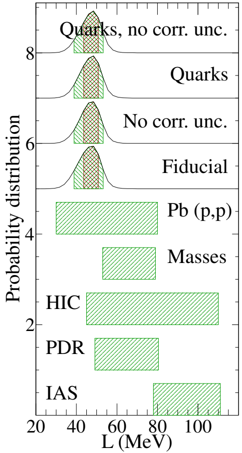


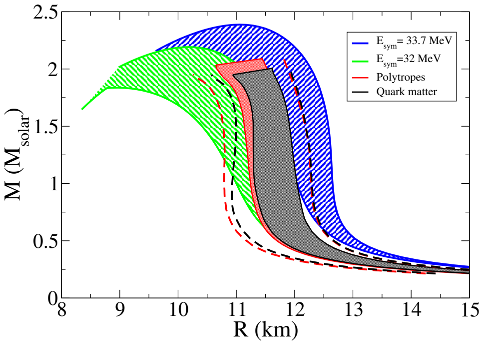
Corrections to include protons also included.

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

$$E_{sym} = a + b + 16\,, \quad L = 3(a\alpha + b\beta)$$

Neutron star observations





$32 < E_{sym} < 34$ MeV

$43 < L < 52$ MeV

Steiner, Gandolfi, PRL (2012).

Density Functional theory

For any system, if we have the functional $E[\rho]$, we can exactly solve the ground-state. In the real life it's almost impossible to have the exact one.

But we can make some guess

$$E[\rho] = E_{FG} + F[\rho_p, \rho_n] + G[\nabla\rho_p, \nabla\rho_n] + \ldots$$

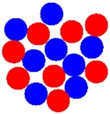
Various parameters, $\sim 14 - 18$, fitted to

- Nuclear matter EOS, mostly $F[\rho_p, \rho_n]$
- Neutron matter EOS, mostly $F[\rho_n]$
- Selected nuclei, mostly $G[\nabla\rho_p, \nabla\rho_n]$

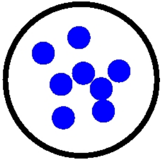
What about non-homogeneous neutron matter???

Inhomogeneous neutron matter – Neutron drops

What are, and why to study neutron drops?



NP self−bound



N confined

They model **inhomogeneous neutron matter**. Ab-initio→DFT

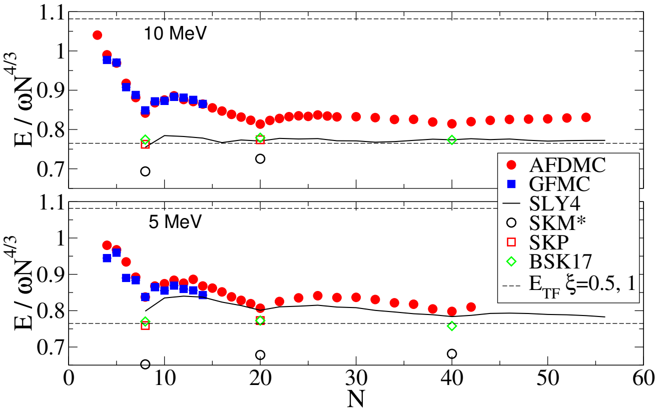
Neutrons are confined by an external potential:

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

V_{ext} tuned to change boundary conditions and densities.

Neutron drops, harmonic oscillator well

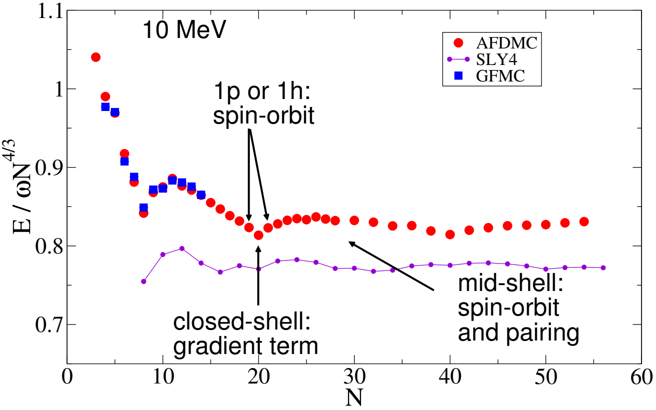
External well: harmonic oscillator with $\hbar\omega$=5, 10 MeV.



Skyrme systematically overbind neutron drops.

Neutron drops, harmonic oscillator well

Fixing Skyrme force:

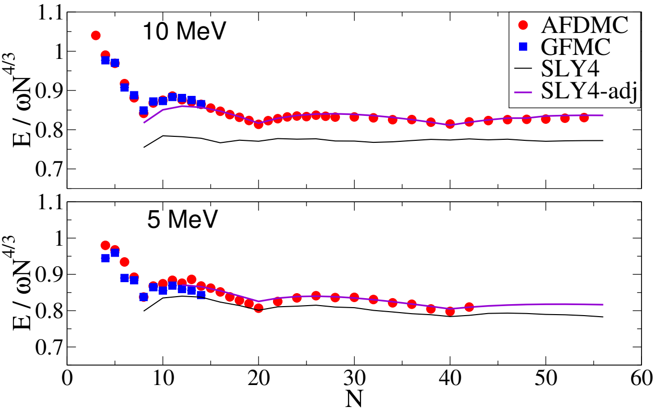


The correction is very similar in all the Skyrme forces we considered.

Neutron drops, adjusted Skyrme force

Note: bulk term of Skyrme fit neutron matter.

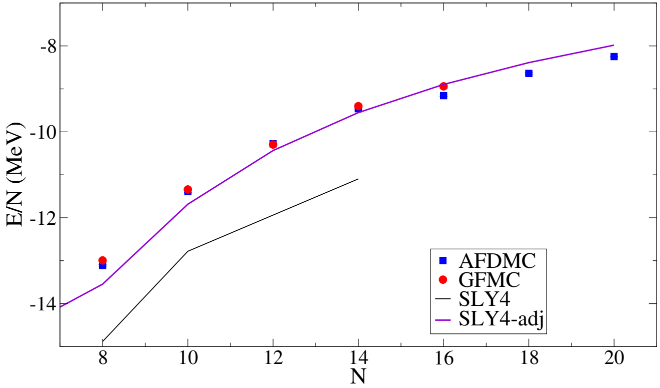
We add the **missing repulsion** by adjusting the gradient term $G_d[\nabla\rho_n]^2$, the pairing and spin-orbit terms.



Gandolfi, Carlson, Pieper PRL (2011).

Neutron drops, adjusted Skyrme force

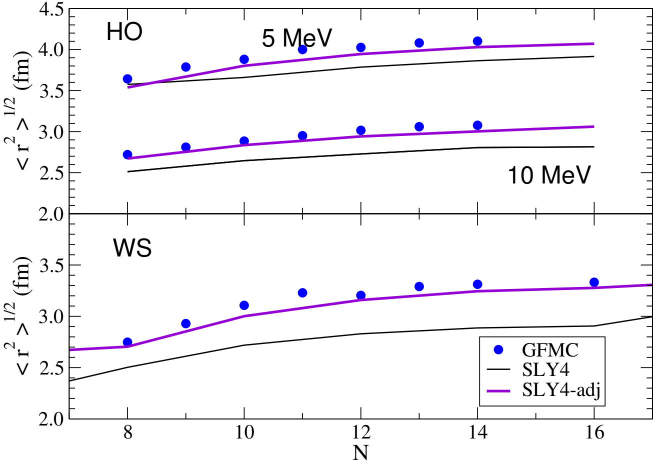
Neutrons in the Wood-Saxon well are also better reproduced by the adjusted SLY4.



Gandolfi, Carlson, Pieper PRL (2011).

Neutron drops: radii

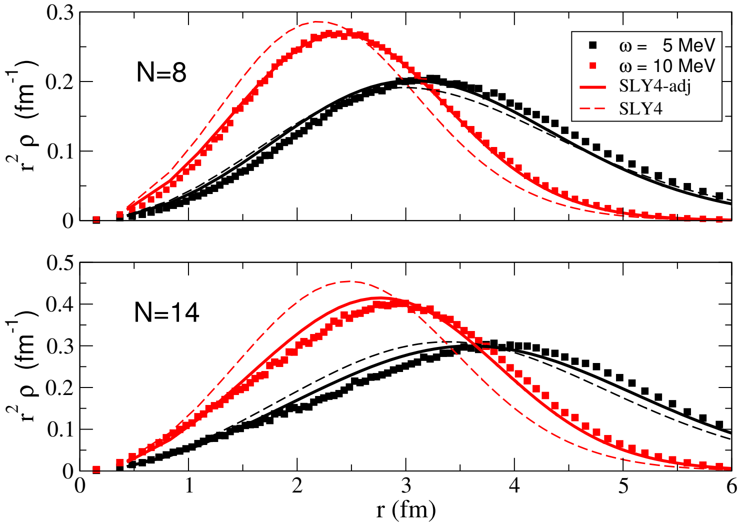
Correction to radii using the adjusted-SLY4.



Gandolfi, Carlson, Pieper (2011).

Neutron drops: radial density

Neutron radial density:



Gandolfi, Carlson, Pieper (2011).

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

QMC methods useful to study nuclear systems in a coherent framework:

- Light nuclei spectra and form factors well in agreement with experimental data. Calculation of neutron matter EOS now possible with the same accuracy.
- Three-neutron force is the bridge between E_{sym} and neutron star structure.
- Neutron star observations becoming competitive with experiments.
- Properties of confined neutrons useful to test iso-vector terms of nuclear energy density functionals

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Thank you!