Quantum Monte Carlo calculations of neutron and nuclear matter

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NUCLEI Nuclear Computational Low-Energy Initiative

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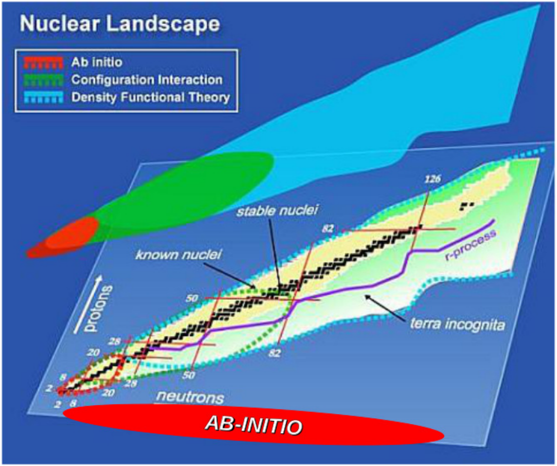
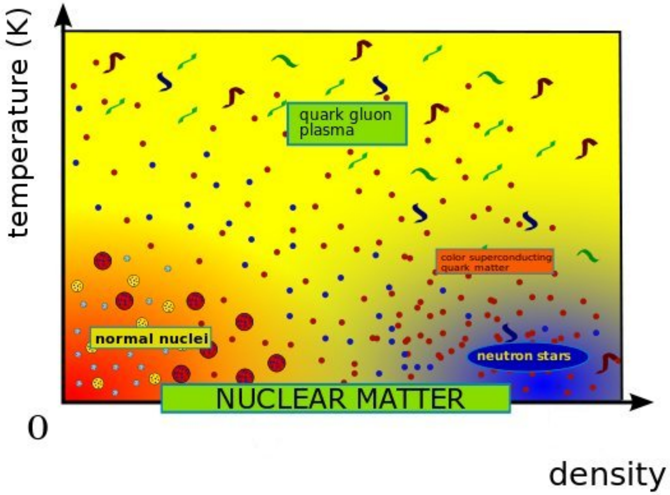
Nuclei



SciDAC UNEDF/NUCLEI

Homogeneous neutron matter



Outline

- The model and the method
- Neutron matter EOS, symmetry energy and neutron stars
- Nuclei and nuclear matter: role of the NN Hamiltonian
- 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 fitted on scattering data. Sum of operators:

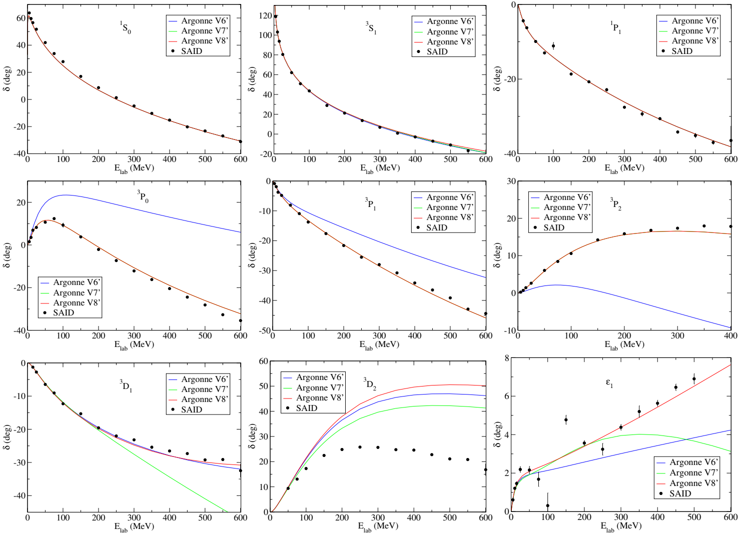
$$v_{ij} = \sum O_{ij}^{p=1,8} v^p(r_{ij}), \quad O_{ij}^p = (1, \vec{\sigma}_i \cdot \vec{\sigma}_j, S_{ij}, \vec{L}_{ij} \cdot \vec{S}_{ij}) \times (1, \vec{\tau}_i \cdot \vec{\tau}_j)$$

Argonne AV6' (no LS), AV7' (no LS-τ), AV8'.

Local chiral forces up to N^{2}LO has the same spin/isospin operatorial structure than AV7' - Gezerlis, Tews, et al. PRL (2013).

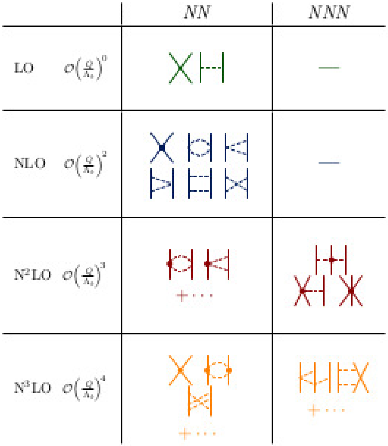
Nuclear Hamiltonian

Phase shifts, Argonne AV6', AV7' and AV8'



Nuclear Hamiltonian

Chiral interactions permit to understand the evolution of theoretical uncertainties with the increasing of A.

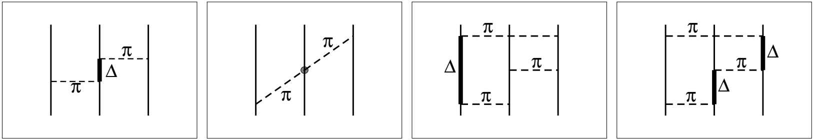


- Chiral EFT is an expansion in powers of Q/Λ_b.
  $Q \sim m_\pi \sim 100$ MeV;
  $\Lambda_b \sim 800$ MeV.
- Long-range physics: given explicitly (no parameters to fit) by pion-exchanges.
- Short-range physics: parametrized through contact interactions with low-energy constants (LECs) fit to low-energy data.
- Many-body forces enter systematically and are related via the same LECs.

Slide by Joel Lynn, Scidac NUCLEI meeting 2014.

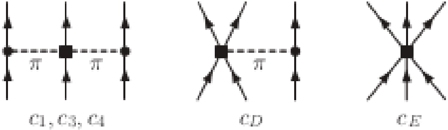
Three-body forces

Urbana–Illinois V_{ijk} models processes like



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

Chiral forces at N^{2}LO:



Nuclear Hamiltonians

Advantages:

- Argonne interactions fit phase shifts up to high energies. At $\rho = \rho_0$, $k_F \simeq 330$ MeV. Two neutrons have $E_{CM} \simeq 120$ MeV, $E_{LAB} \simeq 240$ MeV. $\rightarrow$ accurate up to (at least) 2-3ρ_0. Provide a very good description of several observables in light nuclei.
- Interactions derived from chiral EFT can be systematically improved. Changing the cutoff probes the physics and energy scales entering into observables. They are generally softer, and make most of the calculations easier to converge.

Disadvantages:

- Phenomenological interactions are phenomenological, not clear how to improve their quality. Systematic uncertainties hard to quantify.
- Chiral interactions describe low-energy (momentum) physics. How do they work at large momenta, (i.e. e and ν scattering)?

Important to consider both and compare predictions

Quantum Monte Carlo

The goal is to solve the many-body Schrödinger equation:

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

Ground-state extracted in the limit of $t\to\infty$.

Propagation performed by

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

- Importance sampling: $G(R,R',t)\to G(R,R',t)\,\Psi_I(R')/\Psi_I(R)$
- Constrained-path approximation to control the sign problem.
- Trial wave function includes spin/isospin dependent two- and three-body correlations.

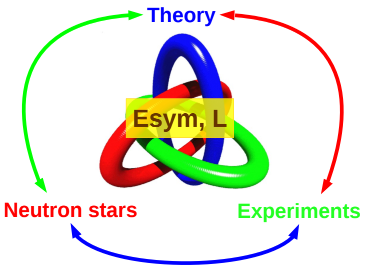
GFMC includes all spin-states of nucleons in the w.f., nuclei up to A=12
AFDMC samples spin states, A∼100, limitations to the form of H

Ground–state obtained in a **non-perturbative way.** Systematic uncertainties within 1-2 %.

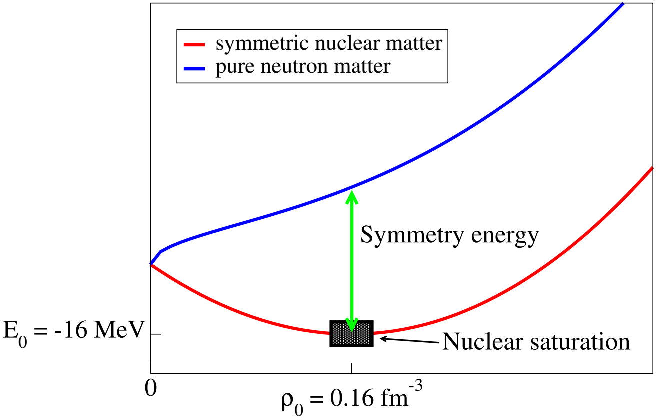
Neutron matter equation of state

Why do we care of neutron matter?

- EOS of neutron matter useful to study the symmetry energy and its slope at saturation.
- Main input for neutron stars.
- The three-neutron force ($T = 3/2$) very weak in light nuclei. The dominant $T = 1/2$ is zero in neutron matter.
  No direct $T = 3/2$ experimental probe available!



What is the Symmetry energy?



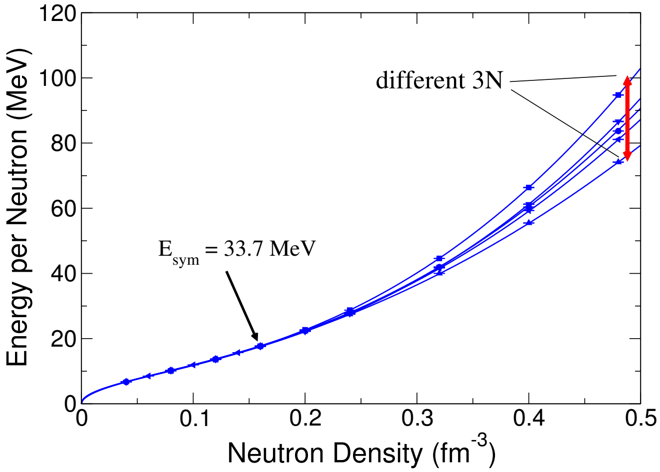
Assumption from experiments:

$$E_{SNM}(\rho_0) = -16 MeV \,, \quad \rho_0 = 0.16 fm^{-3} \,, \quad E_{sym} = E_{PNM}(\rho_0) + 16$$

At ρ_0 we access E_{sym} by studying PNM.

Neutron matter

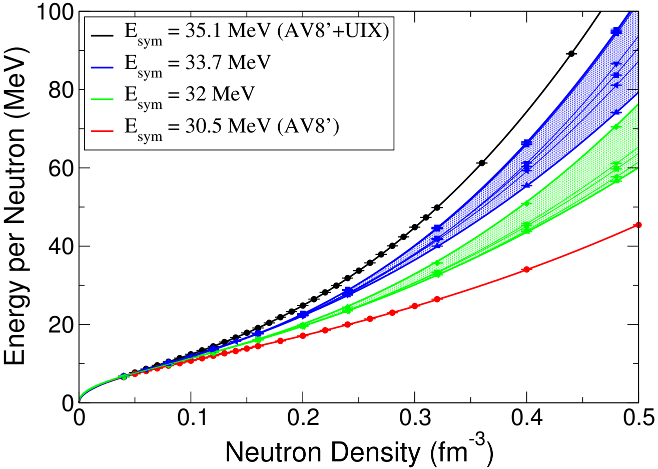
We consider different forms of three-neutron interaction by only requiring a particular value of E_{sym} at saturation.



Gandolfi, *et al.*, EPJA (2014).

Neutron matter

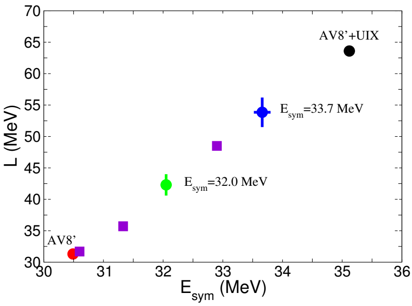
Equation of state of neutron matter using Argonne forces:



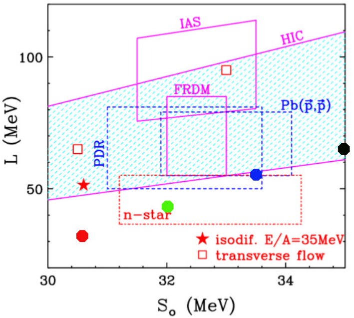
Gandolfi, Carlson, Reddy, PRC (2012)

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)

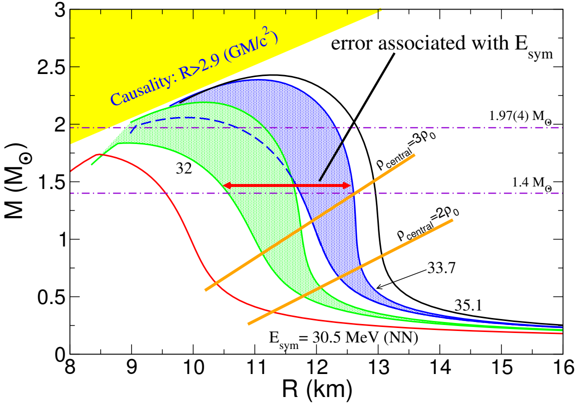


Tsang *et al.*, PRC (2012)

Very weak dependence to the model of 3N force for a given E_{sym}.
Chiral Hamiltonians give compatible results.

Neutron star structure

EOS used to solve the TOV equations.

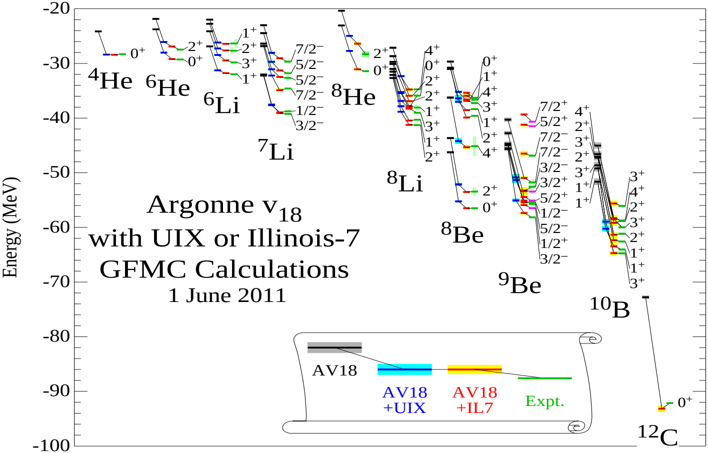


Gandolfi, Carlson, Reddy, PRC (2012).

Strong interplay between E_{sym} and neutron star radii.

more details Thur. at 11.15, session DL

Light nuclei spectrum computed with GFMC

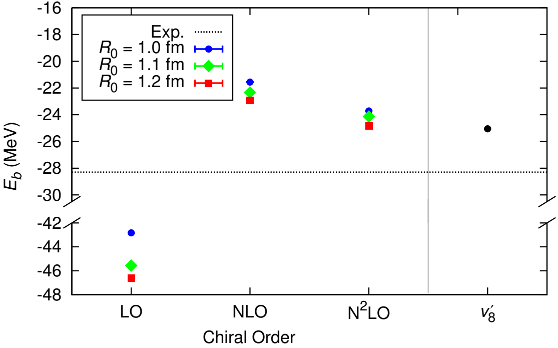


Carlson, Pieper, Wiringa, many papers

Also radii, densities, matrix elements, ...

^{4}He energy with chiral two-body interactions.

It's important to explore:
the role of i) the chiral expansion and ii) the cutoff.



Lynn, Carlson, Epelbaum, Gandolfi, Gezerlis, Schwenk, arXiv:1406.2787.

Three-body terms not yet included. AFDMC gives results within 1%

See Joel lynn talk Wed. at 10.00 pm, session CK

Nuclei

	AV6'	AV7'	exp
^{4}He	-27.09(3)	-25.7(2)	-28.295
^{16}O	-115.6(3)	-90.6(4)	-127.619
^{40}Ca	-322(2)	-209(1)	-342.051

Gandolfi, Lovato, Carlson, Schmidt, arXiv:1406.3388

About 10 to 40% of binding energy missing.

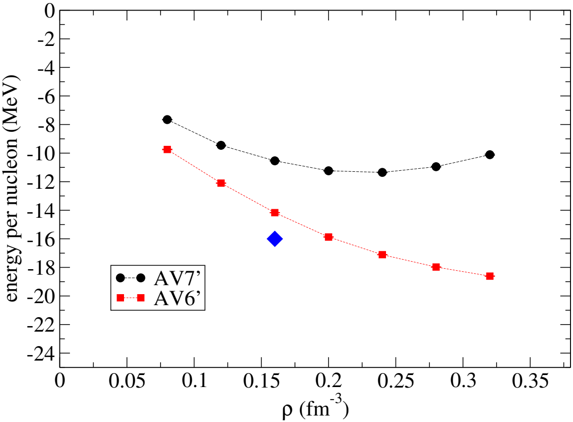
Preliminary: ^{16}O binding energy with chiral potentials:

	R_0=1.2 fm	R_0=1.0 fm
LO	-1210.1(3)	-269.9(4)
NLO	-87.4(2)	-35.9(7)
N^2LO	-116.1(2)	-91.1(3)

Different orders do not even overlap for both ^{4}He and ^{16}O.

Nuclear matter

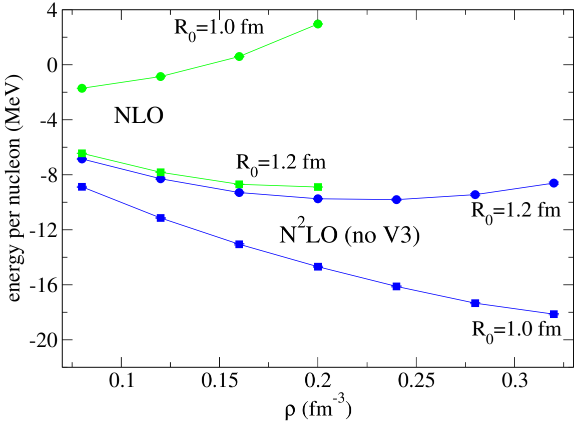
EOS of symmetric nuclear matter using Argonne AV6' and AV7':



Gandolfi, Lovato, Carlson, Schmidt, arXiv:1406.3388

Preliminary results!

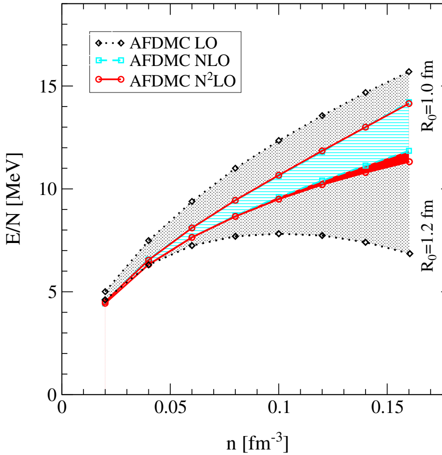
EOS of symmetric nuclear matter with chiral forces:



Same qualitative behavior of nuclei.

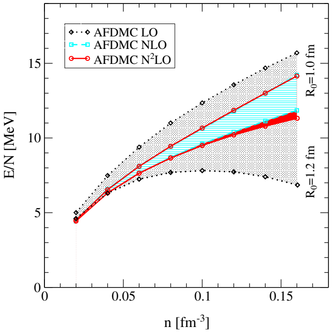
Neutron matter

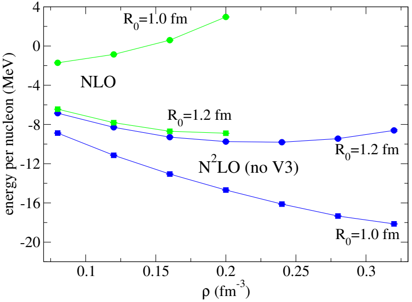
Equation of state of neutron matter using NN chiral forces:



Gezerlis, Tews, Epelbaum, SG, Hebeler, Nogga, Schwenk, PRL (2013), and arXiv:1406.0454 (2014)

Nuclear/neutron matter



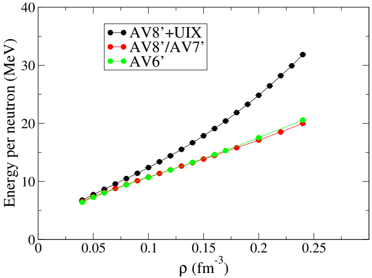


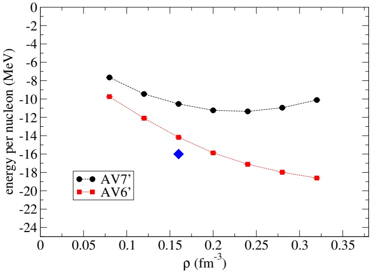
Nuclear matter is more correlated than neutron matter.

Open questions:

Perturbative vs non-perturbative?
Importance of phase shifts?
Importance of the (not included yet) V3?

Nuclear/neutron matter





Same behavior with Argonne forces.

Summary

AFDMC/GFMC methods useful to study nuclear systems in a coherent framework: same Hamiltonians and same many-body machinery

- Three-neutron force is the (strong) bridge between E_{sym} and neutron star structure.
- Chiral potentials show some convergence in light nuclei (but three-body terms not included yet). Error bars given by varying the cutoff grow quickly with the size of the system.
- Nuclear and neutron matter have very different behavior with both Argonne and chiral forces. Further investigation needed. Due to the phase shifts?

Acknowledgments

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- K. Schmidt (ASU)
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