Low density nuclear matter

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NUCLEI Nuclear Computational Low-Energy Initiative

www.computingnuclei.org

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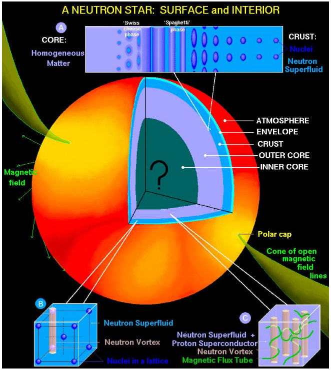
Neutron stars

Neutron star is a wonderful natural laboratory

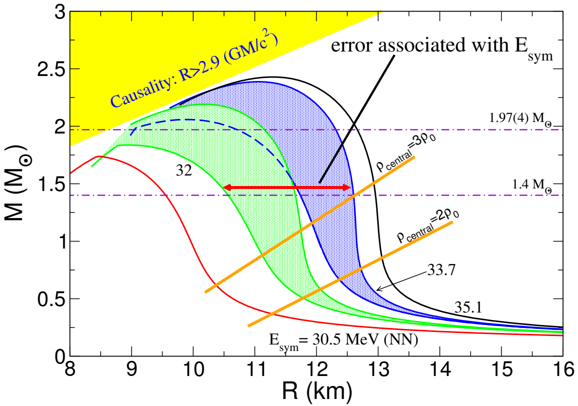


D. Page

- 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?

Outer core

EOS of neutron matter up to $\sim 2M_\odot$ determines radii of neutron stars:

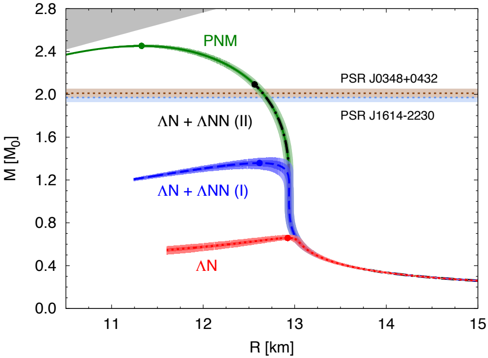


Gandolfi, Carlson, Reddy, PRC (2012).

Strong connection between symmetry energy and radii

Inner core

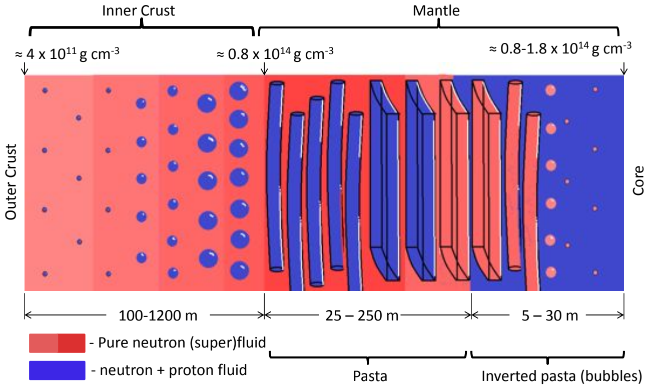
EOS at high density determines the maximum mass of neutron stars. Hyperons are expected to appear. Different Λ-nucleon interactions, giving similar results in hypernuclei, give very different EOS:



Lonardoni, Lovato, Pederiva, SG, PRL (2015).

More experimental data needed to better understand ΛN and ΛNN.

Crust of neutron stars very rich:



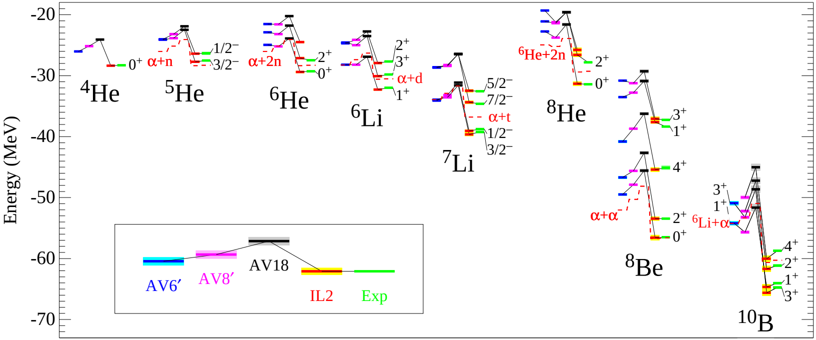
Newton, Gearheart, Hooker, Li (2012)

Can we study clustering in asymmetric nuclear using microscopic nuclear Hamiltonians?

Nuclear matter

NN interaction is the simpler AV6', no three-body forces included yet.

Qualitatively similar results in light nuclei as AV8' and AV18.

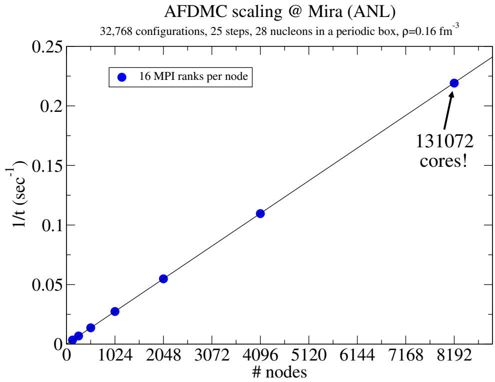


Wiringa, Pieper, PRL (2002).

Computational details

All the calculations are done using the Auxiliary Field Diffusion Monte Carlo (AFDMC),

$$\psi(t) = e^{-(H-E_T)t}\psi(0)$$

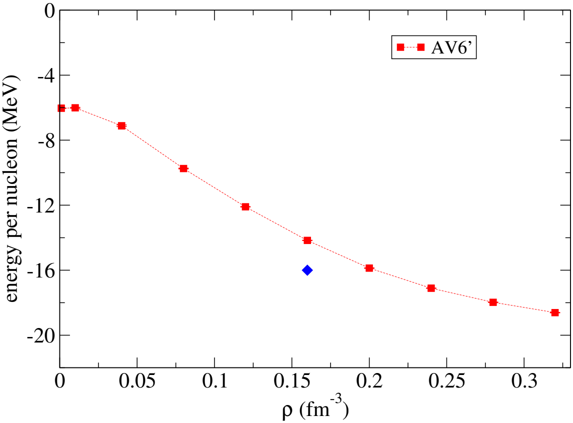


Many improvements done in the last year (accuracy and computational efficiency). Ask later for more details.

Nuclear matter

EOS of symmetric nuclear matter using Argonne AV6'.

Low density VERY PRELIMINARY!!!

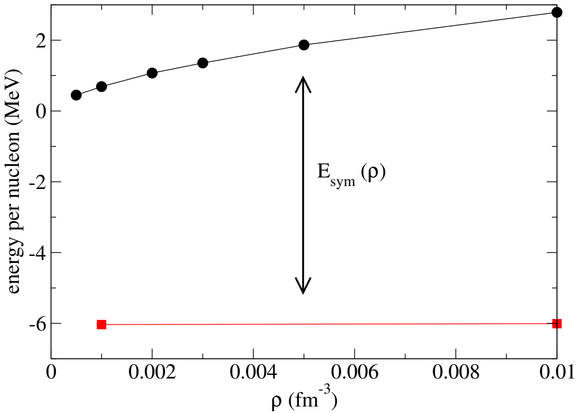


Gandolfi, Lovato, Carlson, Schmidt, PRC (2014)

Nuclear matter

VERY PRELIMINARY!!!

EOS of nuclear and neutron at low densities:



Note: important finite size effects in nuclear matter, no coulomb.

VERY PRELIMINARY!!!

By calculating the energy of 38 neutrons (closed shell) alone and with the addition of 2 protons, we estimate the energy of ^{4}He as:

$$E(^4He) = E(38n + 2p) - E(36n)$$

$E(36n)$ is obtained from the energy calculated for 38 neutrons.

ρ (fm^{-3})	$E(^4He)$ (MeV)
0.0005	-18.2(5)
0.001	-17.7(5)
0.002	-18.4(5)
0.005	-24.3(5)
0.01	-34.1(5)

Energy of 4 nucleons in same boxes is -27.2(1) MeV.

Effect of pairing? Different proton fractions?

Pair correlation functions

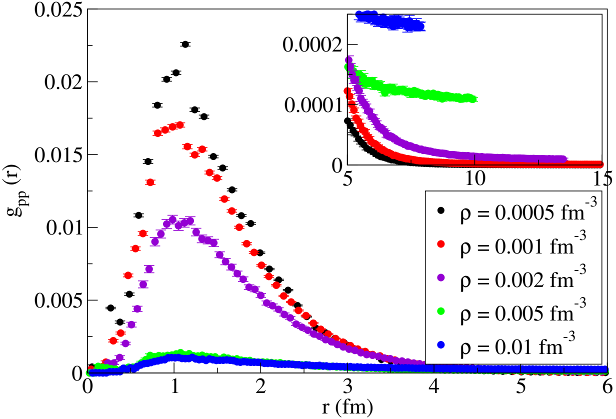
Pair correlation functions are defined as:

$$g_{\hat{O}}(r) = \frac{1}{4\pi r^2} \langle \Psi | \sum_{i<j} \hat{O}_{ij} \delta(r - r_{ij}) | \Psi \rangle$$

For $\hat{O} = 1$ they tell the probability to find two particles at distance r.
Even more useful if $\hat{O}$=np, nn, pp.

Pair correlation functions

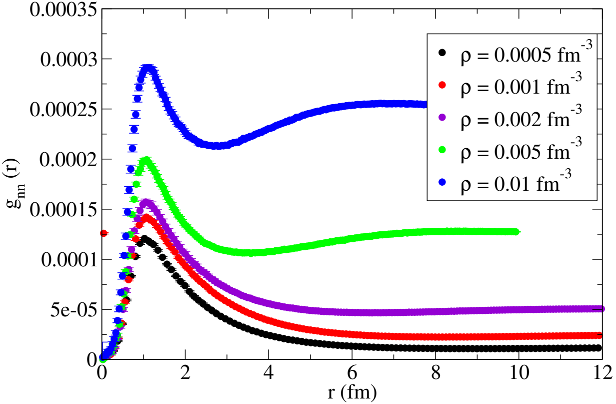
VERY PRELIMINARY!!! Proton-proton, for different densities:



The cluster seems to form at densities below 0.005 fm^{-3}.

Pair correlation functions

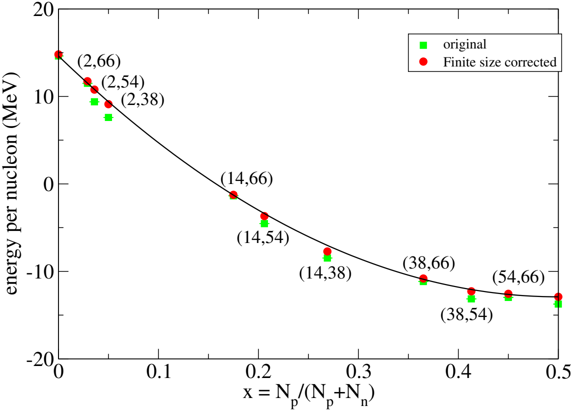
VERY PRELIMINARY!!! Neutron-neutron, for different densities:



Similar behavior, main peak increases at lower densities.

Nuclear matter

Asymmetric nuclear matter, ρ=0.16 fm^{-3}:



Gandolfi, Lovato, Carlson, Schmidt, PRC (2014).

Quadratic dependence to isospin-asymmetry looks fine.

Summary

Study of low-density nuclear matter is in progress.

Open questions:

- Why binding energy of ^{4}He with neutrons higher than 4 nucleons?
- Role of pairing/BCS correlations?
- Different proton fractions? (so far 38 neutrons and 2 protons)
- Possible to compare with other calculations?

What's next:

- Inclusion of three-body forces in the propagator (perturbative calculation already possible using Urbaba IX).
- Improve the wave function to deal with spin-orbit terms (AV8' and local chiral potentials)
- Calculate properties of matter and nuclei, energies, radii, transitions, ...

Extra slides

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:

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

NN interaction - Argonne AV8' and AV6'.

Variational wave function

$$E_0 \leq E = \frac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle} = \frac{\int dr_1 \dots dr_N \, \psi^*(r_1 \dots r_N) H \psi^*(r_1 \dots r_N)}{\int dr_1 \dots dr_N \, \psi^*(r_1 \dots r_N) \psi^*(r_1 \dots r_N)}$$

$\rightarrow$ Monte Carlo integration. Variational wave function:

$$|\Psi_T\rangle = \left[\prod_{i<j} f_c(r_{ij})\right] \left[\prod_{i<j<k} f_c(r_{ijk})\right] \left[1 + \sum_{i<j,p} \prod_k u_{ijk} f_p(r_{ij}) O^p_{ij}\right] |\Phi\rangle$$

where O^p are spin/isospin operators, f_c, u_{ijk} and f_p are obtained by minimizing the energy. About 30 parameters to optimize.

$|\Phi\rangle$ is a mean-field component, usually HF. Sum of many Slater determinants needed for open-shell configurations.

BCS correlations can be included using a Pfaffian.

Quantum Monte Carlo

Projection in imaginary-time t:

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

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

Propagation performed by

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

- $dR' \to dR_1\, dR_2\ldots,\ G(R,R',t)\to G(R_1,R_2,\delta t)\,G(R_2,R_3,\delta t)\ldots$
- Importance sampling: $G(R,R',\delta t)\to G(R,R',\delta t)\,\Psi_I(R')/\Psi_I(R)$
- Constrained-path approximation to control the sign problem. Unconstrained calculation possible in several cases (exact).

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

The Sign problem in one slide

Evolution in imaginary-time:

$$\psi_I(R')\Psi(R',t+dt) = \int dR\, G(R,R',dt)\frac{\psi_I(R')}{\psi_I(R)}\psi_I(R)\Psi(R,t)$$

note: $\Psi(R,t)$ must be positive to be "Monte Carlo" meaningful.

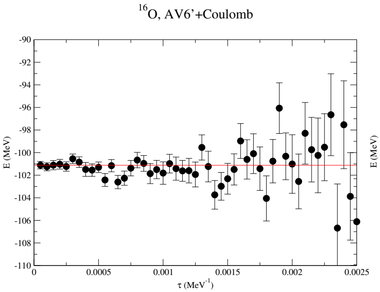
Fixed-node approximation: solve the problem in a restricted space where $\Psi > 0$ (Bosonic problem) $\Rightarrow$ upperbound.

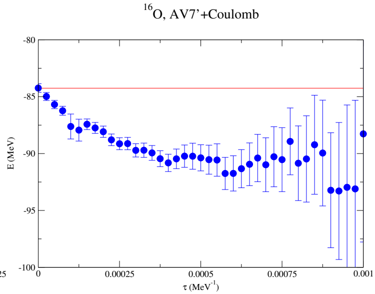
If Ψ is complex:

$$|\psi_I(R')||\Psi(R',t+dt)| = \int dR\, G(R,R',dt)\left|\frac{\psi_I(R')}{\psi_I(R)}\right||\psi_I(R)||\Psi(R,t)|$$

Constrained-path approximation: project the wave-function to the real axis. Multiply the weight term by $\cos\Delta\theta$ (phase of $\frac{\Psi(R')}{\Psi(R)}$), $Re\{\Psi\} > 0$ $\Rightarrow$ not necessarily an upperbound.

After some equilibration within constrained-path, release the constraint:

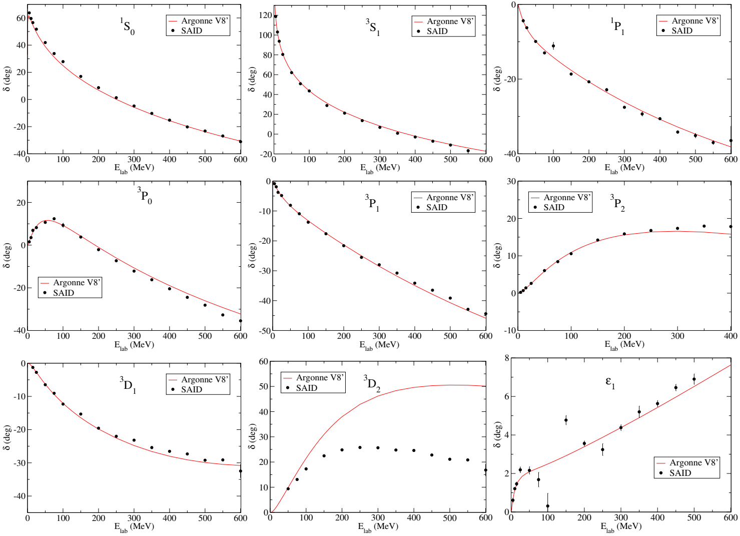




The difference between CP and UP results is mainly due to the presence of LS terms in the Hamiltonian. Same for heavier systems.

Work in progress to improve Ψ and to "fully" include three-body forces.

Phase shifts, AV8'



Difference AV8′-AV18 less than 0.2 MeV per nucleon up to A=12.

Scattering data and neutron matter

Two neutrons have

$$k \approx \sqrt{E_{lab}\, m/2}\,, \qquad \to k_F$$

that correspond to

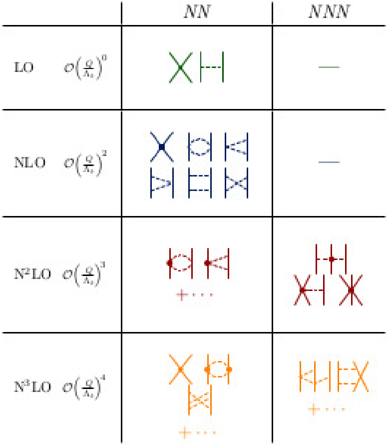
$$k_F \to \rho \approx (E_{lab}\, m/2)^{3/2}/2\pi^2\,.$$

E_{lab}=150 MeV corresponds to about 0.12 fm^{-3}.

E_{lab}=350 MeV to 0.44 fm^{-3}.

Argonne potentials useful to study dense matter above ρ_0=0.16 fm^{-3}

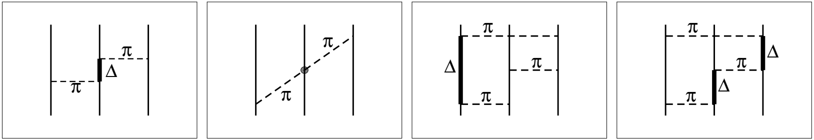
Chiral interactions permit to understand the evolution of theoretical uncertainties with the increasing of A.



- 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.

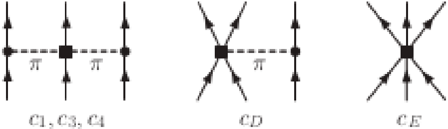
Slide by Joel Lynn, Scidac NUCLEI meeting 2014.

Urbana–Illinois V_{ijk} models processes like

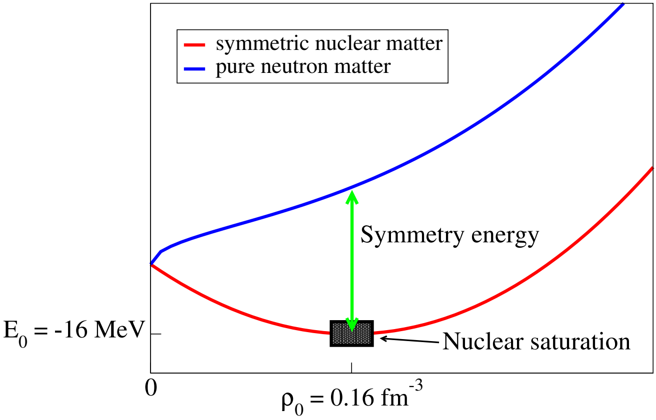


$+$ short-range correlations (spin/isospin independent).

Chiral forces at N^{2}LO:



What is the Symmetry energy?



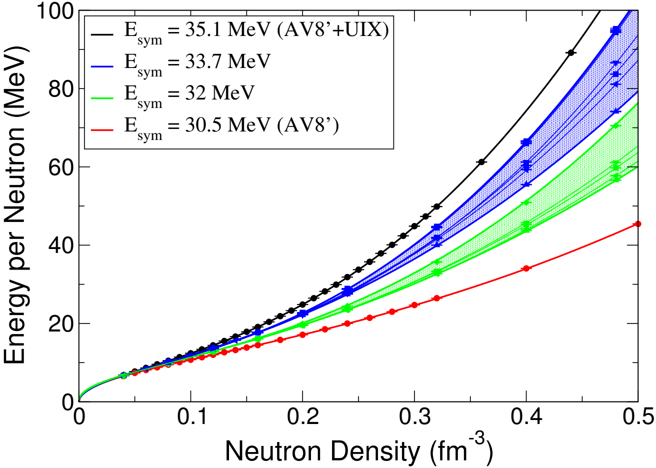
Assumption from experiments:

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

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

Neutron matter

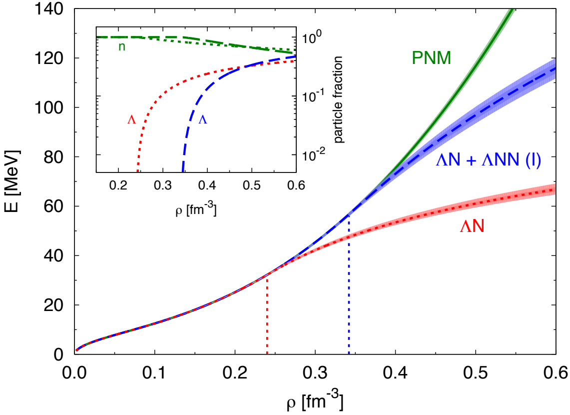
Equation of state of neutron matter using Argonne forces:



Gandolfi, Carlson, Reddy, PRC (2012)

Λ-neutron matter

EOS obtained by solving for $\mu_\Lambda(\rho, x) = \mu_n(\rho, x)$

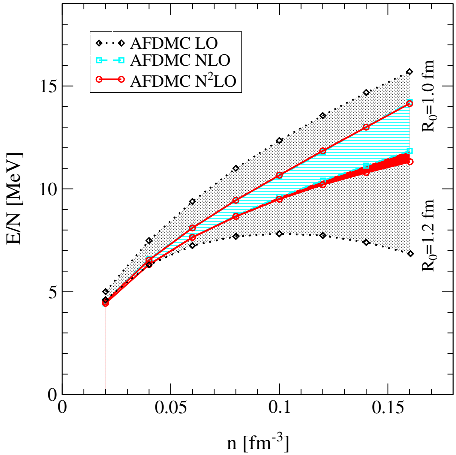


Lonardoni, Lovato, Pederiva, SG, arXiv:1407.4448.

No hyperons up to $\rho = 0.5$ fm^{-3} using ΛNN (II)!!!

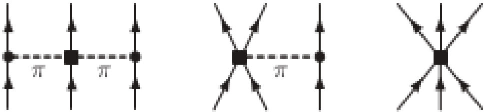
Neutron matter

Equation of state of neutron matter using NN chiral forces:



Gezerlis, Tews, *et al.*, PRL (2013), PRC (2014)

Chiral three-body forces



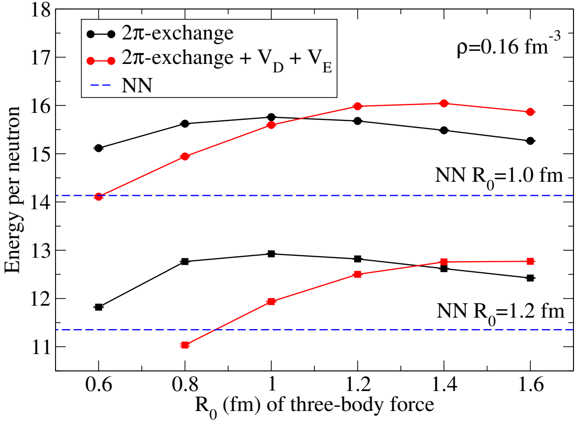
For a finite cutoff, there are "additional" V_D and V_E diagrams that contribute in pure neutron matter.

They have been often neglected in existing neutron matter calculations!

All the above terms have been written in coordinate space, and included into AFDMC.

Neutron matter with chiral forces

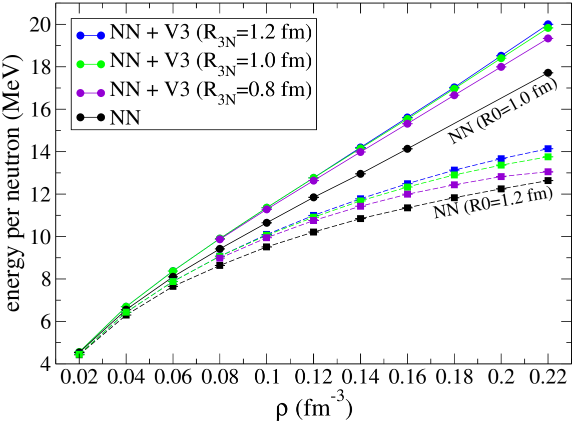
Preliminary! Contribution of "additional" V_D and V_E terms:



Note: Contribution of FM (2π exchange) about 0.9 MeV with AV8'

Preliminary!

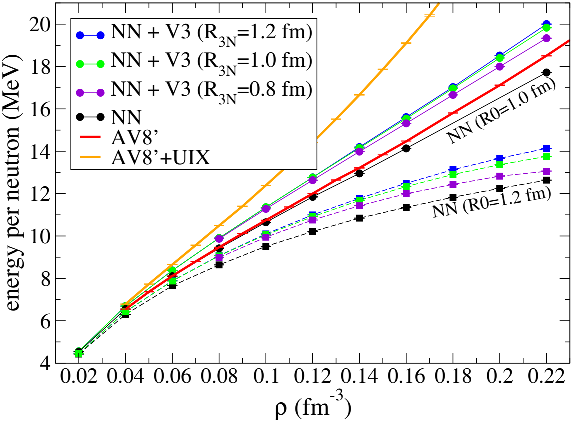
Equation of state of neutron matter at N^{2}LO.



Note: the "real" V_D and V_E terms are not included yet.

Preliminary!

Equation of state of neutron matter, a comparison.



Quantum Monte Carlo

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

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. Unconstrained calculation possible in several cases (exact).

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

Overview

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) potential gives the weight of the configuration:

$$e^{-V(R)\Delta\tau}\psi(R) = w\psi(R)$$

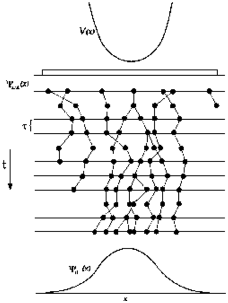
Algorithm for each time-step:

- 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!

Branching

The configuration weight w is efficiently sampled using the branching technique:



Configurations are replicated or destroyed with probability

$$int[w + \xi] \quad (1)$$

Note: the re-balancing is the bottleneck limiting the parallel efficiency.

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 simulate larger systems (up to $A \approx 100$). Operators (except the energy) are very hard to be computed, but in some case there is some trick!

Propagator

We first rewrite the potential as:

$$
\begin{aligned}
V &= \sum_{i<j} [v_\sigma(r_{ij})\vec{\sigma}_i \cdot \vec{\sigma}_j + v_t(r_{ij})(3\vec{\sigma}_i \cdot \hat{r}_{ij}\vec{\sigma}_j \cdot \hat{r}_{ij} - \vec{\sigma}_i \cdot \vec{\sigma}_j)] = \\
&= \sum_{i,j} \sigma_{i\alpha} A_{i\alpha;j\beta} \sigma_{j\beta} = \frac{1}{2}\sum_{n=1}^{3N} O_n^2 \lambda_n
\end{aligned}
$$

where the new operators are

$$
O_n = \sum_{j\beta} \sigma_{j\beta} \psi_{n,j\beta}
$$

Now we can use the HS transformation to do the propagation:

$$
e^{-\Delta\tau \frac{1}{2}\sum_n \lambda O_n^2}\psi = \prod_n \frac{1}{\sqrt{2\pi}} \int dx e^{-\frac{x^2}{2} + \sqrt{-\lambda\Delta\tau} x O_n}\psi
$$

Computational cost $\approx (3N)^3$.

Three-body forces

Three-body forces, Urbana, Illinois, and local chiral N^{2}LO can be exactly included in the case of neutrons.

For example:

$$
\begin{aligned}
O_{2\pi} &= \sum_{cyc}\left[\{X_{ij},X_{jk}\}\{\tau_i\cdot\tau_j,\tau_j\cdot\tau_k\}+\frac{1}{4}[X_{ij},X_{jk}][\tau_i\cdot\tau_j,\tau_j\cdot\tau_k]\right] \\
&= 2\sum_{cyc}\{X_{ij},X_{jk}\}=\sigma_i\sigma_k f(r_i,r_j,r_k)
\end{aligned}
$$

The above form can be included in the AFDMC propagator.

What about three-body forces?

The full inclusion of three-body forces for nuclei/nuclear matter in AFDMC is not possible. Ideas:

- Reduce $V_3 \to V_2(\rho)$ in the AFDMC propagator, and calculate perturbatively:

$$\delta_3 = \frac{\langle\psi|V_3 - V_2(\rho)|\psi\rangle}{\langle\psi|\psi\rangle}$$

- "Partially" include three-body terms in the propagator: some of them can be treated exactly. Example, Fujita-Miyazawa:

$$\begin{aligned} O_{2\pi} &= \sum_{cyc}\left[\{X_{ij}, X_{jk}\}\{\tau_i\cdot\tau_j, \tau_j\cdot\tau_k\} + \frac{1}{4}[X_{ij}, X_{jk}][\tau_i\cdot\tau_j, \tau_j\cdot\tau_k]\right] \\ \Rightarrow O_{2\pi}^{eff} &= \alpha\sum_{cyc}\left[\{X_{ij}, X_{jk}\}\{\tau_i\cdot\tau_j, \tau_j\cdot\tau_k\}\right] \end{aligned}$$

and calculate the difference perturbatively.

Efficiency

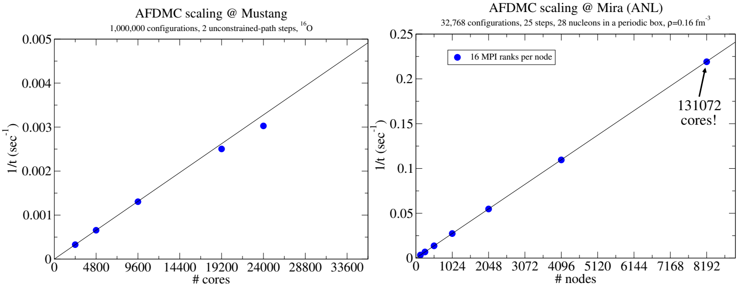


Figure : Efficiency of the AFDMC code. On Mustang we tested the unconstrained-path AFDMC for the ^{16}O (left panel), and the constrained-path version using fewer configurations on Mira for 28 nucleons in a box (right panel).