The Equation of State of Neutron Matter and Low-density Nuclear Matter

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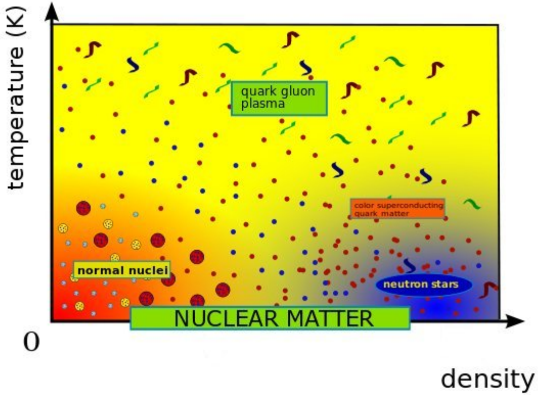
www.computingnuclei.org



- The model and the method
- Neutron matter and three-neutron force
- $E_{\rm sym}$ and neutron stars
- Nuclear matter at low densities
- Asymmetric matter, clustering
- Conclusions

Nuclear Hamiltonian

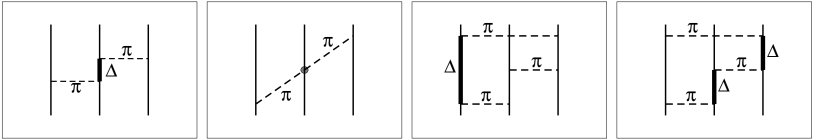
Model: non-relativistic nucleons interacting with an effective nucleon-nucleon force (NN) and three-nucleon interaction (TNI).

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

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

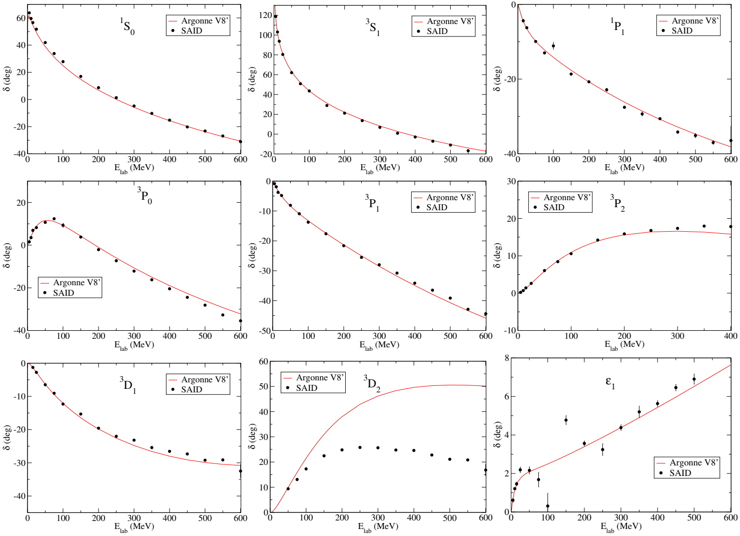
$$v_{ij} = \sum O_{ij}^{p=1,8} v^p(r_{ij})\,, \quad O_{ij}^p = (1, \vec{\sigma}_i \cdot \vec{\sigma}_j, S_{ij}, \vec{L}_{ij} \cdot \vec{S}_{ij}) \times (1, \vec{\tau}_i \cdot \vec{\tau}_j)$$

V_{ijk} models processes like



$+$ Phenomenological repulsive term.

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

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

that correspond to

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

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}

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 $t\to\infty$.

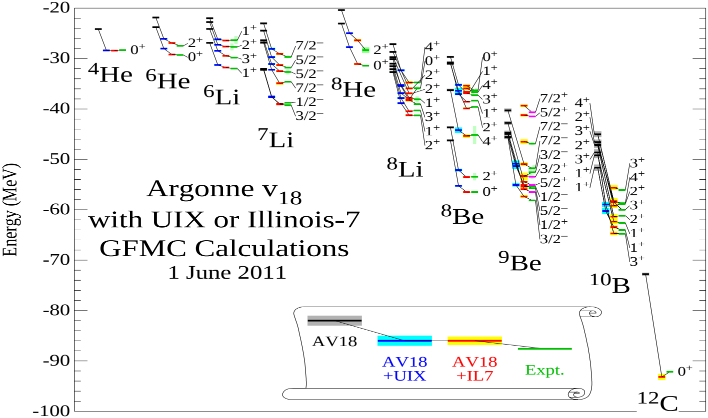
Propagation performed by

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

- $dR' \to dR_1\,dR_2\ldots,\ G(R,R',t)\to G(R_1,R_2,\delta t)\,G(R_2,R_3,\delta t)\ldots$
- 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 %.

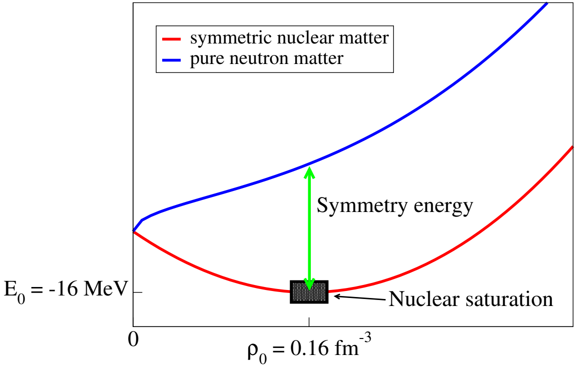
Light nuclei spectrum computed with GFMC



Carlson, *et al.*, arXiv:1412.3081, RMP in press.

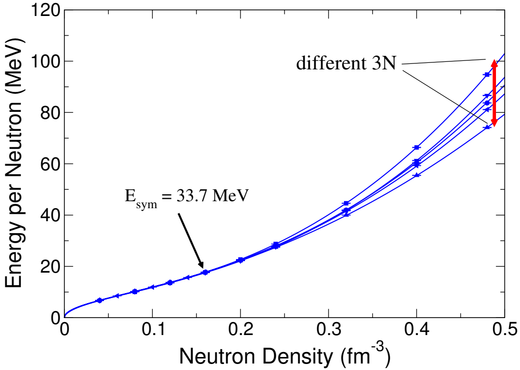
Neutron matter equation of state

- EOS of neutron matter gives the symmetry energy and its slope.
- Assume that NN is very good - fit scattering data with very high precision.
  Three-neutron force ($T = 3/2$) very weak in light nuclei, while $T = 1/2$ is the dominant part. No direct $T = 3/2$ experiments.



Neutron matter

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



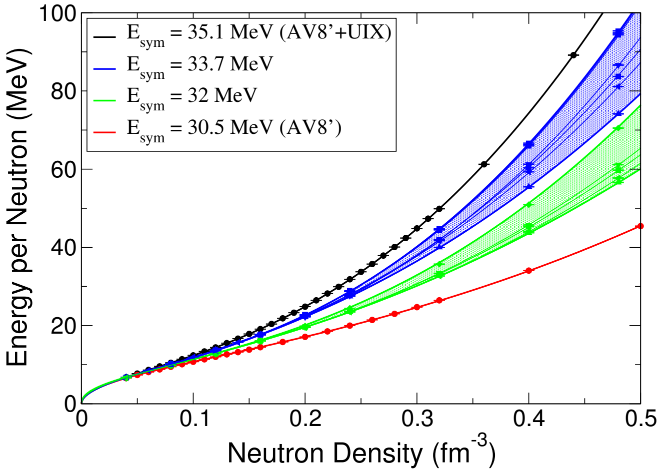
different 3N:

- $V_{2\pi} + \alpha V_R$
- $V_{2\pi} + \alpha V_R^{\mu}$ (several μ)
- $V_{2\pi} + \alpha \tilde{V}_R$
- $V_{3\pi} + \alpha V_R$

In this way we can understand the uncertainties to the model of 3N at large densities!

Neutron matter

Model uncertainty vs E_{sym} uncertainty:

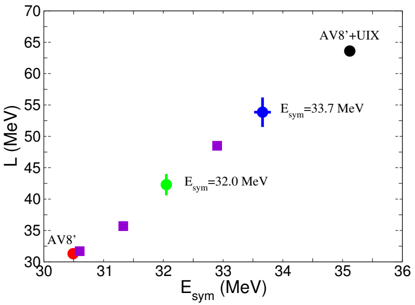


Gandolfi, Carlson, Reddy, PRC (2012)

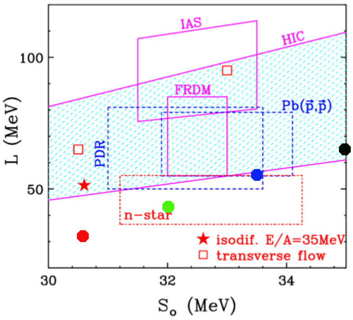
Neutron matter and symmetry energy

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

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



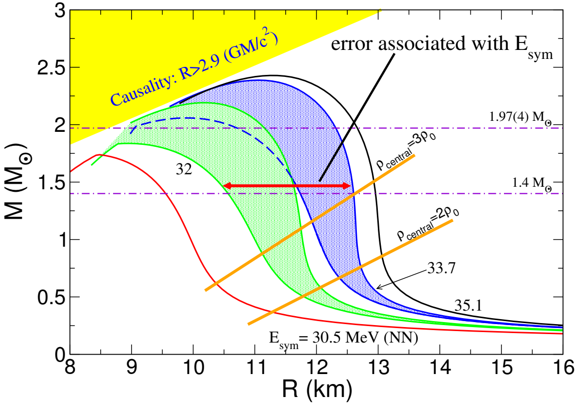
Gandolfi *et al.*, EPJ (2014)



Tsang *et al.*, PRC (2012)

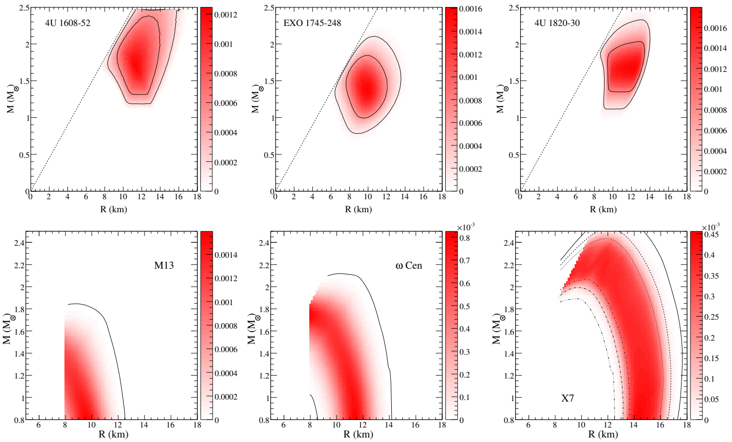
Very weak dependence to the model of 3N force for a given E_{sym}.
Knowing E_{sym} or L useful to constrain 3N! (within this model...)

EOS used to solve the TOV equations.



Gandolfi, Carlson, Reddy, PRC (2012).

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



Steiner, Lattimer, Brown, ApJ (2010)

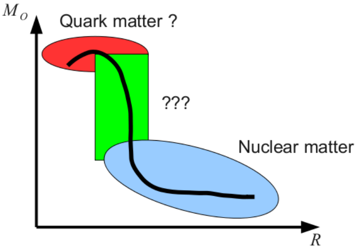
Neutron star observations can be used to 'measure' the EOS and constrain E_{sym} and L. (Systematic uncertainties still under debate...)

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,
contrast with the commonly used $E_{FG} + V$



and a high density model for $\rho > \rho_t$

i) two polytropes

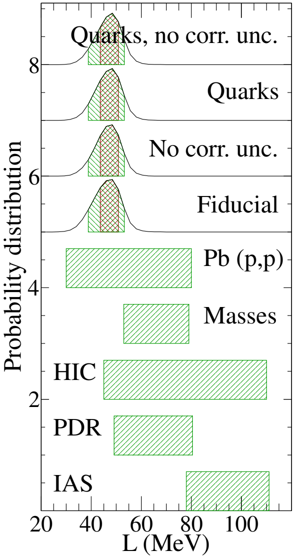
ii) polytrope+quark matter model

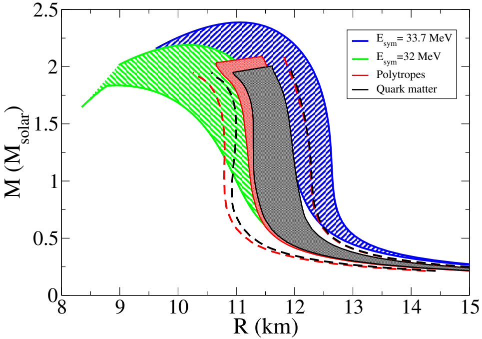
Neutron star radius sensitive to the EOS at nuclear densities!

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 matter really matters!





$32 < E_{sym} < 34\ MeV$

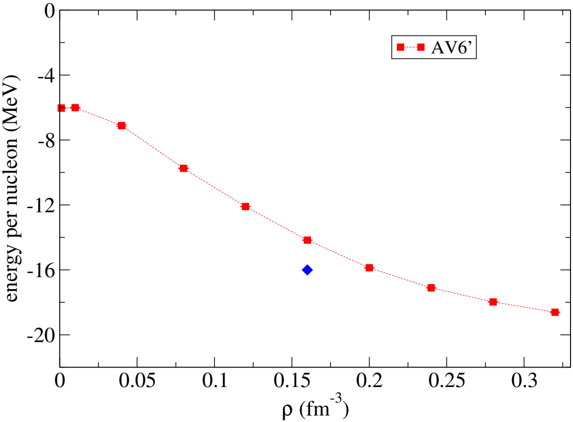
$43 < L < 52\ MeV$

Steiner, Gandolfi, PRL (2012).

Nuclear matter

EOS of symmetric nuclear matter using Argonne AV6' (no three-body).

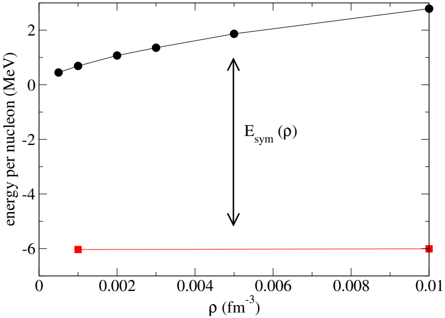
Low density VERY PRELIMINARY!!!

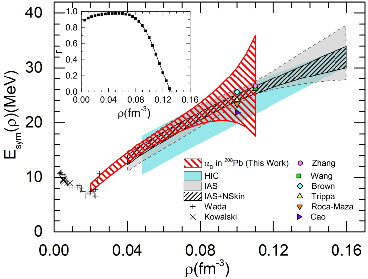


Gandolfi, Lovato, Carlson, Schmidt, PRC (2014)

VERY PRELIMINARY!!!

Symmetry energy at low densities (28 nucleons):

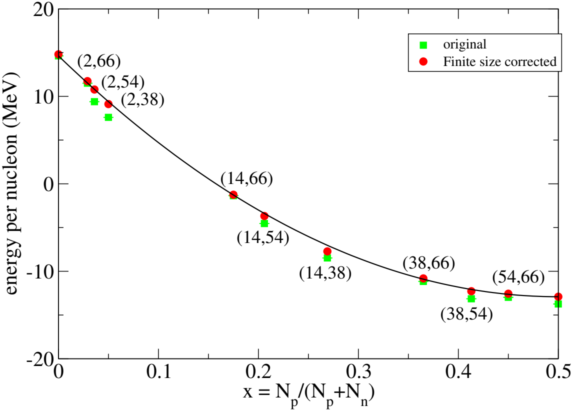




Zhang, Chen, arXiv:1504.01077

Nuclear matter

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



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

Quadratic dependence to isospin-asymmetry is fine. BCS/pairing? V3?

Low density nuclear matter

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:

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

where $E(36n)$ is obtained from the energy per particle 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.

Pair correlation functions

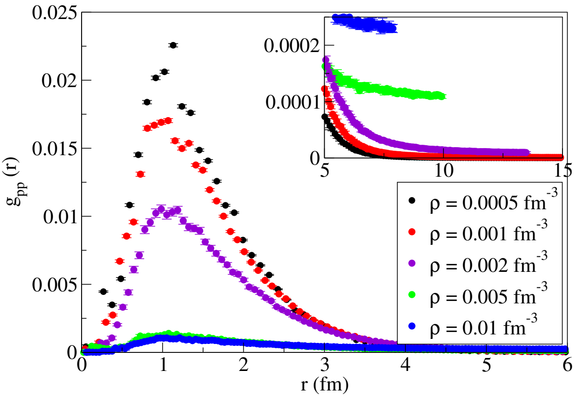
These are defined as:

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

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

VERY PRELIMINARY!!!

Proton-proton, for different densities:

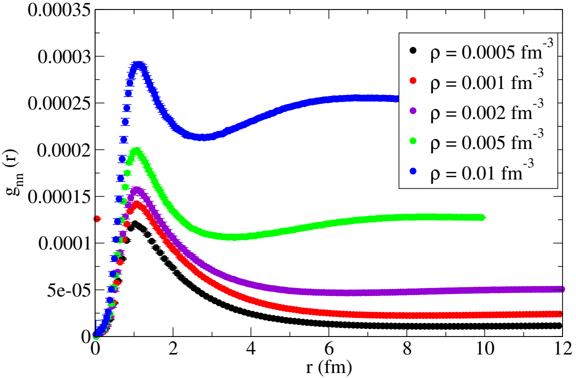


The cluster seems to form at densities below 0.005 fm^{-3}.

Pair correlation functions

VERY PRELIMINARY!!!

Neutron-neutron, for different densities:



Similar behavior, main peak increases at lower densities.

Summary

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

- Three-neutron force is the bridge between E_{sym} and neutron star structure.
- Neutron star observations becoming competitive with experiments (but systematic uncertainties still to be understood).
- Study of low-density nuclear matter is in progress.
  - Why binding energy of ^{4}He with neutrons higher than 4 nucleons?
  - Role of pairing/BCS correlations?
  - Role of three-body interactions?
  - Different proton fractions? (so far 38 neutrons and 2 protons)

THANK YOU!

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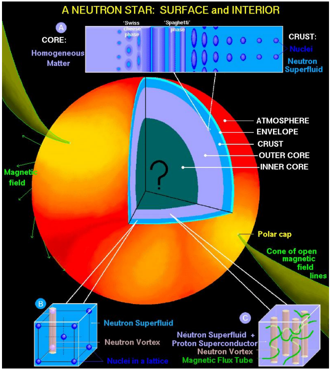
Extra slides

Neutron stars

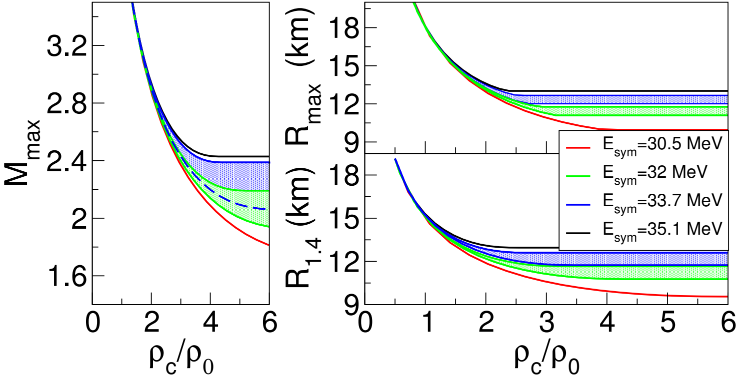
Neutron star is a wonderful natural laboratory



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?

Maximally stiff EOS with $c_s = 1$ above ρ_c.



Gandolfi, Carlson, Reddy, PRC (2012)

With strong chnges to the EOS, larger radii and masses are not excluded.

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:

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

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.

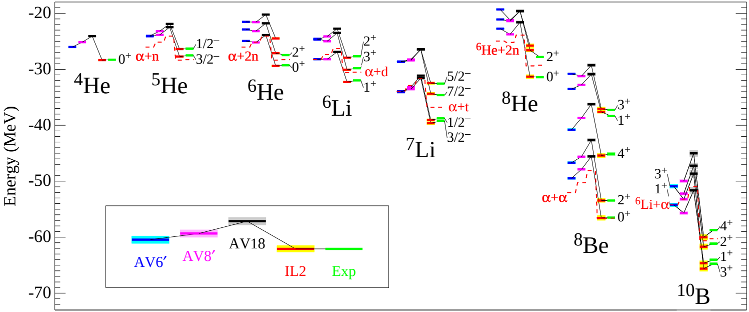
$|\Phi\rangle$ is a mean-field component, usually HF. Sum of many Slater determinants needed for open-shell configurations.

BCS correlations can be included using a Pfaffian.

Nuclear matter

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

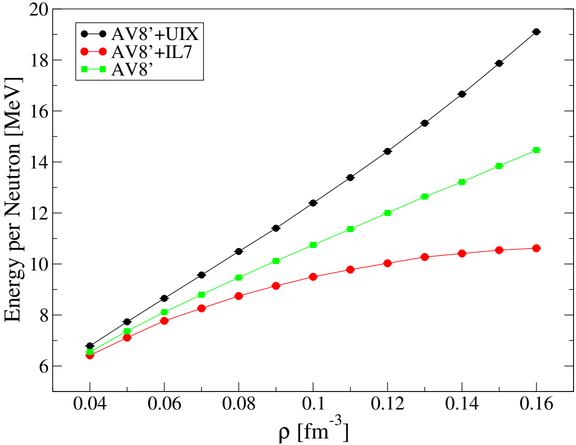
Not too different results in light nuclei than AV8' and AV18.



Wiringa, Pieper, PRL (2002).

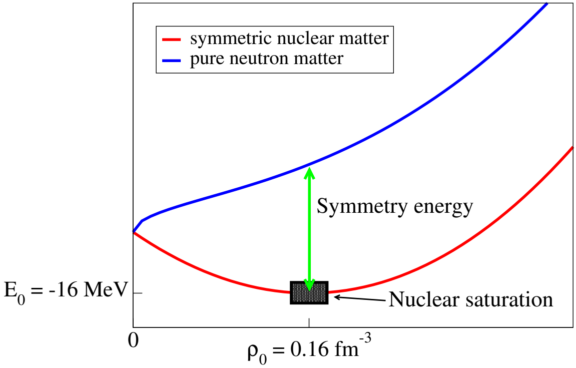
Good enough for qualitative studies.

Neutron matter and the "puzzle" of the three-body force



Note: AV8'+UIX and (almost) AV8' are stiff enough to support observed neutron stars. → How to reconcile with nuclei???

What is the Symmetry energy?



Assumption from experiments:

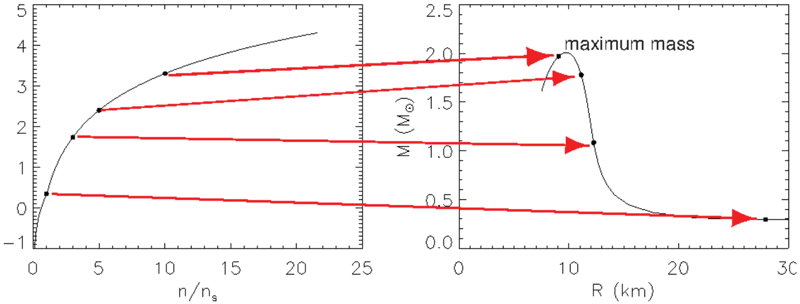
$$E_{SNM}(\rho_0) = -16 MeV \,, \quad \rho_0 = 0.16 fm^{-3} \,, \quad E_{sym} = E_{PNM}(\rho_0) + 16$$

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

TOV equations:

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

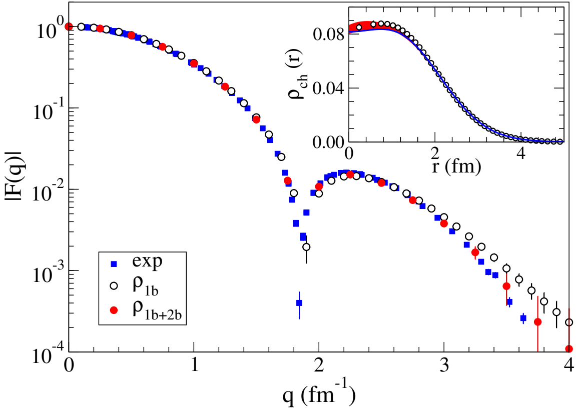
$$\frac{dm(r)}{dr} = 4\pi\epsilon r^2,$$



J. Lattimer

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)

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

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:

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

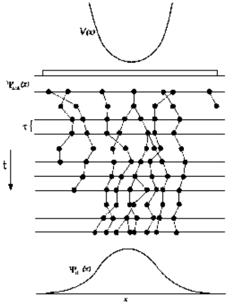
Algorithm for each time-step:

- 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

$$int[w + \xi] \tag{1}$$

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:

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

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 $\approx (3N)^3$.

AFDMC variational wave function

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

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

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

BCS correlations can be included using a Pfaffian.

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.

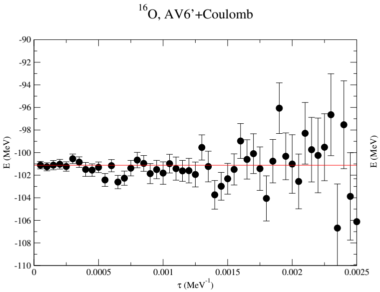
Fixed-node approximation: solve the problem in a restricted space where $\Psi > 0$ (Bosonic problem) $\Rightarrow$ upperbound.

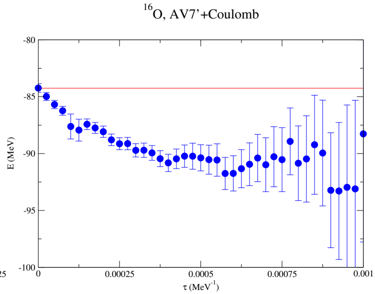
If Ψ is complex:

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

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.

Three-body forces

Three-body forces, Urbana, Illinois, and local chiral N^2LO 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 $V_3 \rightarrow V_2(\rho)$ 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:

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

and calculate the difference perturbatively.