QMC calculations of the EOS of neutron matter from chiral interactions

Stefano Gandolfi

Los Alamos National Laboratory (LANL)

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and its implications for nuclear physics
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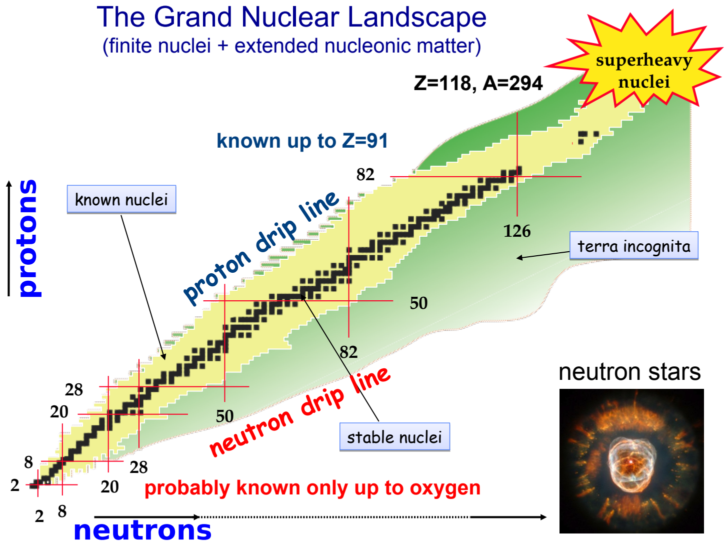
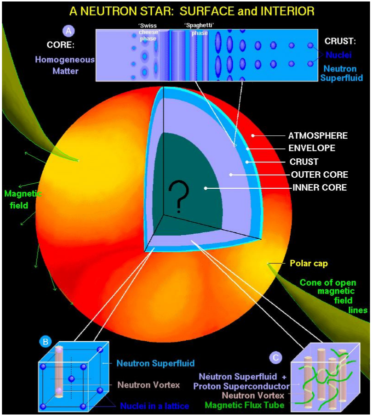
NUCLEI
Nuclear Computational Low-Energy Initiative
www.computingnuclei.org

The big picture



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: neutron/nuclear matter
- Inner core: hyperons? quark matter? π or K condensates?

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.

V_{ijk} typically constrained to reproduce light systems (A=3,4).

- "Phenomenological/traditional" interactions (Argonne/Illinois)
- Local chiral forces up to N^2LO (Gezerlis, et al. PRL 111, 032501 (2013), PRC 90, 054323 (2014), Lynn, et al. PRL 116, 062501 (2016)).

Quantum Monte Carlo

Propagation in imaginary time:

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

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

Propagation performed by

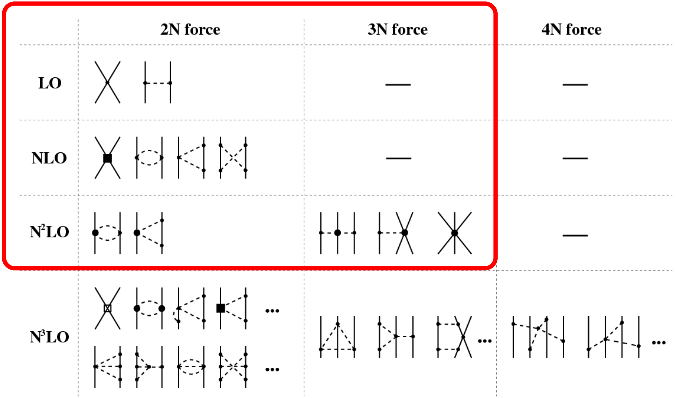
$$\psi(R,t) = \langle R|\psi(t)\rangle = \int dR'\,G(R,R',t)\psi(R',0)$$

- 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-path calculation possible in several cases (exact).

GFMC includes all spin-states of nucleons in the w.f., nuclei up to A=12
AFDMC samples spin states, bigger systems, less accurate than GFMC

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

Nuclear Hamiltonian



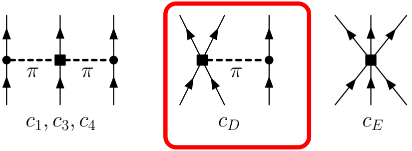
Expansion in powers of Q/Λ, Q$\sim$100 MeV, Λ $\sim$1 GeV.

Long-range physics given by pion-exchanges (no free parameters).

Short-range physics: contact interactions (LECs) to fit. Operators need to be regulated $\rightarrow$ cutoff dependency!

Order's expansion provides a way to quantify uncertainties!

Chiral three-body forces, issue (I)?



In the Fourier transformation of V_D two possible operator structures arise:

$$V_{D1} = \frac{g_A c_D m_\pi^2}{96\pi\Lambda_\chi F_\pi^4} \sum_{i<j<k} \sum_{\text{cyc}} \tau_i \cdot \tau_k \left[X_{ik}(r_{kj})\delta(r_{ij}) + X_{ik}(r_{ij})\delta(r_{kj}) - \frac{8\pi}{m_\pi^2}\sigma_i \cdot \sigma_k \delta(r_{ij})\delta(r_{kj}) \right]$$

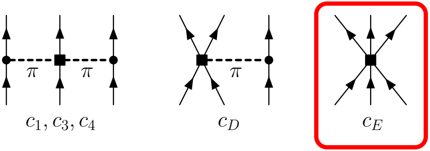
$$V_{D2} = \frac{g_A c_D m_\pi^2}{96\pi\Lambda_\chi F_\pi^4} \sum_{i<j<k} \sum_{\text{cyc}} \tau_i \cdot \tau_k \left[X_{ik}(r_{ik}) - \frac{4\pi}{m_\pi^2}\sigma_i \cdot \sigma_k \delta(r_{ik}) \right] \left[\delta(r_{ij}) + \delta(r_{kj}) \right]$$

$$X_{ij}(r) = T(r)S_{ij} + Y(r)\sigma_i \cdot \sigma_j$$

Navratil (2007), Tews et al PRC (2016), Lynn et al PRL (2016).

Equivalent only in the limit of an infinite cutoff. Implications in real life?

Chiral three-body forces, issue (II)?



Equivalent forms of operators entering in V_E (Fierz-rearrangement):

$$1, \quad \sigma_i \cdot \sigma_j, \quad \tau_i \cdot \tau_j, \quad \sigma_i \cdot \sigma_j \tau_i \cdot \tau_j, \quad \sigma_i \cdot \sigma_j \tau_i \cdot \tau_k, \quad [(\sigma_i \times \sigma_j) \cdot \sigma_k][(\tau_i \times \tau_j) \cdot \tau_k]$$

Epelbaum et al (2002). We investigated the following choices:

$$V_{E\tau} = \frac{c_E}{\Lambda_\chi F_\pi^4} \sum_{i<j<k} \sum_{\text{cyc}} \tau_i \cdot \tau_k \delta(r_{kj}) \delta(r_{ij})$$

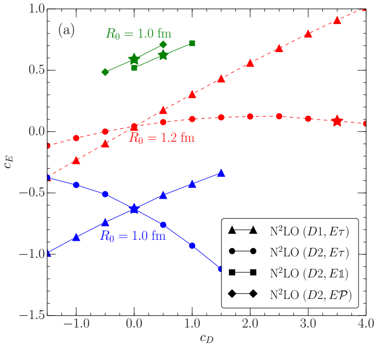
$$V_{E1} = \frac{c_E}{\Lambda_\chi F_\pi^4} \sum_{i<j<k} \sum_{\text{cyc}} \delta(r_{kj}) \delta(r_{ij})$$

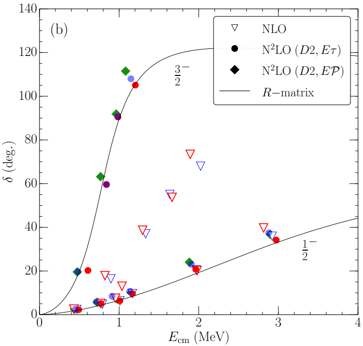
Qualitative differences expected, i.e. consider ^{4}He vs neutron matter!

^{4}He binding energy and p-wave n-^{4}He scattering

Regulator: $\delta(r) = \frac{1}{\pi\Gamma(3/4)R_0^3}\exp(-(r/R_0)^4)$

Cutoff R_0 taken consistently with the two-body interaction.

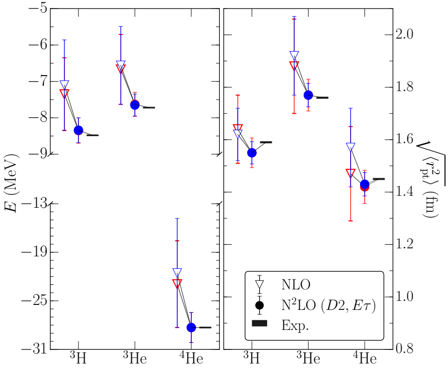




No fit can be obtained for $R_0 = 1.2$ fm and V_{D1} - Issue (I)

Lynn, Tews, Carlson, Gandolfi, Gezerlis, Schmidt, Schwenk PRL (2016).

A=3, 4 nuclei at N2LO



Lynn, Tews, et al. PRL 116, 062501 (2016).

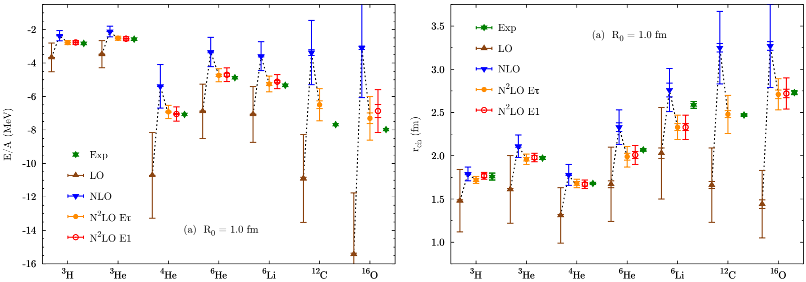
Error quantification: define $Q = \max\left(\frac{p}{\Lambda_b}, \; \frac{m_\pi}{\Lambda_b}\right)$ and calculate:

$$\Delta(N2LO) = \max\left(Q^4|\hat{O}_{LO}|, \; Q^2|\hat{O}_{LO} - \hat{O}_{NLO}|, \; Q|\hat{O}_{NLO} - \hat{O}_{N2LO}\right)$$

Epelbaum, Krebs, Meissner (2014).

AFDMC calculations

Energies and charge radii, cutoff 1.0 fm:



Lonardoni, et al., arXiv:1709.09143, arXiv:1802.08932.

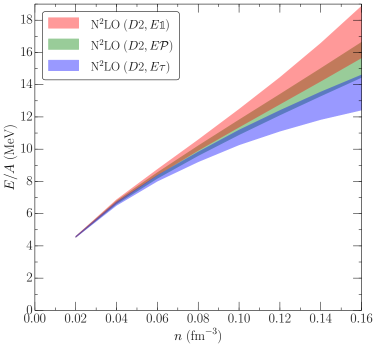
Qualitative good description of both energies and radii.

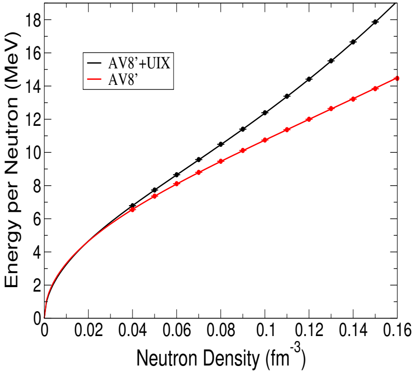
Good convergence (although uncertainties still large if LO included).

Different V_E operators give similar results.

Neutron matter at N2LO

EOS of pure neutron matter at N2LO, R_0=1.0 fm
Error quantification estimated as previously.

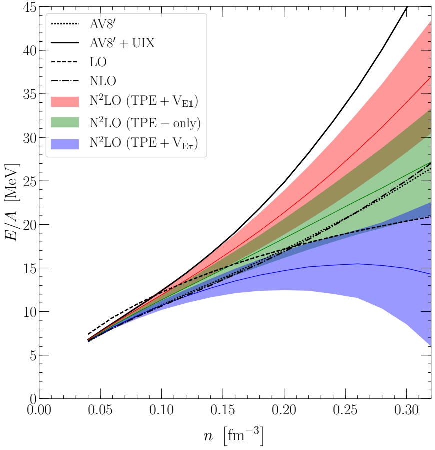




Lynn, Tews, et al. PRL 116, 062501 (2016).
Results qualitatively consistent.
Significant dependence to the choice of V_E - Issue (II)

Neutron matter at N2LO

EOS of pure neutron matter at N2LO, R_0=1.0 fm.



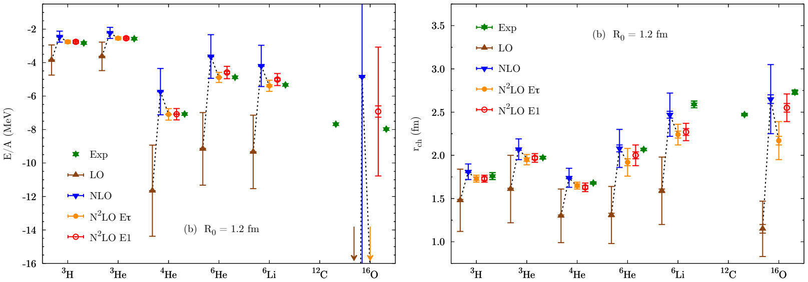
Tews, Carlson, Gandolfi, Reddy, arXiv:1801.01923

Large uncertainties above 0.16 fm^{-3}.

Blue EOS certainly too soft.

See Ingo Tews talk for consequences in neutron stars

Energies and charge radii, cutoff 1.2 fm:



Lonardoni, et al., arXiv:1709.09143, arXiv:1802.08932.

Qualitative good description up to A=6.

Different V_E operators give very different results for ^{16}O.

Useful for neutron matter???

Energy contribution

Expectation value of the N^2LO energy contributions ^{16}O:

Potential	$E_{\rm kin} + v_{ij}$	V_{ijk}	$V^{2\pi,P}$	$V^{2\pi,S}$	V_D	V_E
2b, 1.0	−134(2)					
$E\tau$, 1.0	−130(2)	−44(1)	−55(1)	0.85(1)	0	8.50(4)
$E1$, 1.0	−131(2)	−41(1)	−54(1)	0.72(1)	−4.03(5)	15.7(1)
2b, 1.2	−151(3)					
$E\tau$, 1.2	−156(7)	−202(3)	−101(2)	−0.72(9)	−94(2)	−5.43(3)
$E1$, 1.2	−152(2)	−26(1)	−34(1)	0.94(1)	4.53(8)	1.90(1)

LECs c_D and c_E for different cutoffs and parametrizations of the three-body force (other strengths are the same):

V_{ijk}	R_0 (fm)	c_D	c_E
$E\tau$	1.0	0.0	−0.63
$E1$	1.0	0.5	0.62
$E\tau$	1.2	3.5	0.09
$E1$	1.2	−0.75	0.025

Summary

- Equation of state of neutron matter calculated from microscopic Hamiltonians.
- Quantum Monte Carlo calculations for larger nuclei is now possible (at least up to A=16, work in progress...)
- Chiral EFT provides a way to constrain nuclear interactions and estimate systematic uncertainties

But...

- Effect of the cutoff important to explore
- Effect of using different ("equivalent") operators important to explore

Predictive power???

Acknowledgments:

- J. Carlson (LANL), D. Lonardoni (LANL and FRIB)
- I. Tews, S. Reddy (INT)
- J. Lynn, A. Schwenk (Darmstadt)
- K.E. Schmidt (ASU)

Extra slides

Scattering data and neutron matter

Two neutrons have

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

that correspond to

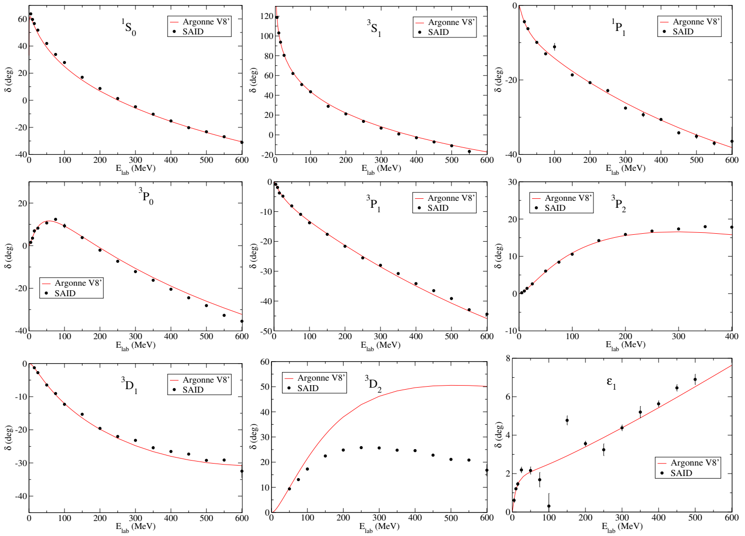
$$k_F \to \rho \approx (E_{lab}\, m/2)^{3/2}/2\pi^2\,.$$

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}

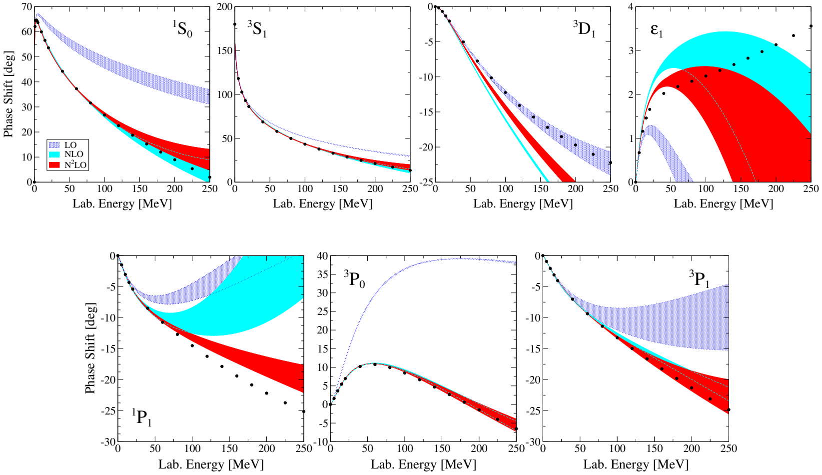
Phase shifts, AV8'



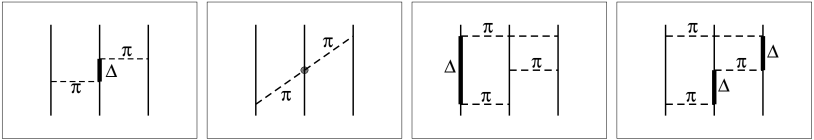
Difference AV8′-AV18 less than 0.2 MeV per nucleon up to A=12.

Nuclear Hamiltonian

Phase shifts, LO, NLO and N^2LO with R_0=1.0 and 1.2 fm:

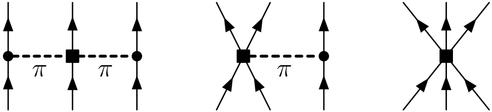


Urbana–Illinois V_{ijk} models processes like



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

Chiral forces at N^{2}LO:



Advantages:

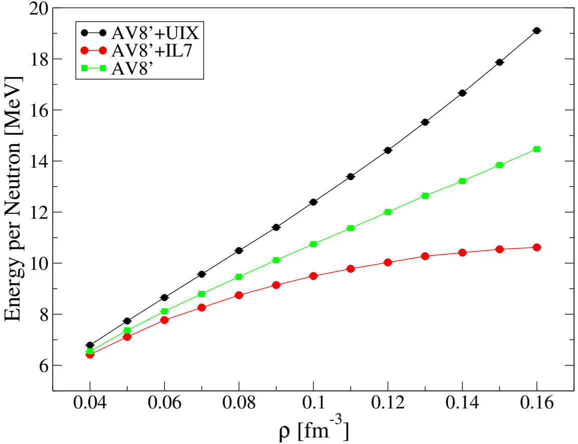
- Argonne interactions fit phase shifts up to high energies. At $\rho = \rho_0$, $k_F \simeq 330$ MeV. Two neutrons have $E_{CM} \simeq 120$ MeV, $E_{LAB} \simeq 240$ MeV. → accurate up to (at least) 2-3ρ_0. Provide a very good description of several observables in light nuclei.
- Interactions derived 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

Neutron matter and the *crisis* of three-body forces



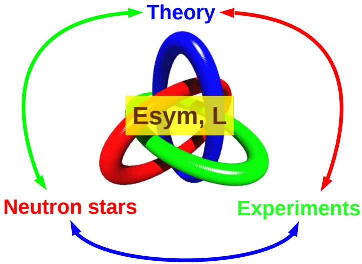
Maris, Vary, Gandolfi, Carlson, Pieper, PRC (2013)

Note: AV8'+UIX and AV8' are stiff enough to support observed neutron stars. AV8'+IL7 too soft. → How to reconcile with nuclei???

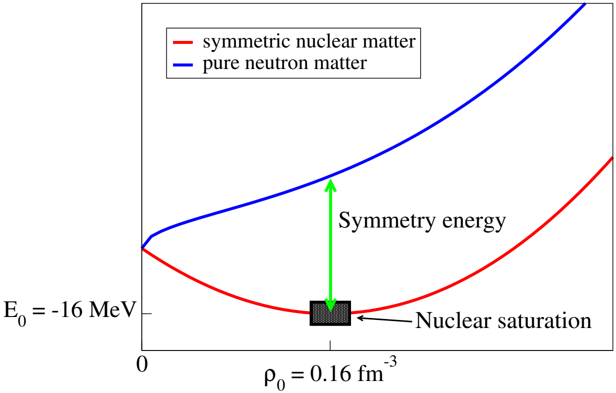
Neutron matter equation of state

Neutron matter is an "exotic" system. Why do we care?

- EOS of neutron matter gives the symmetry energy and its slope.
- The 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 available.
- Determines radii of neutron stars.



What is the Symmetry energy?

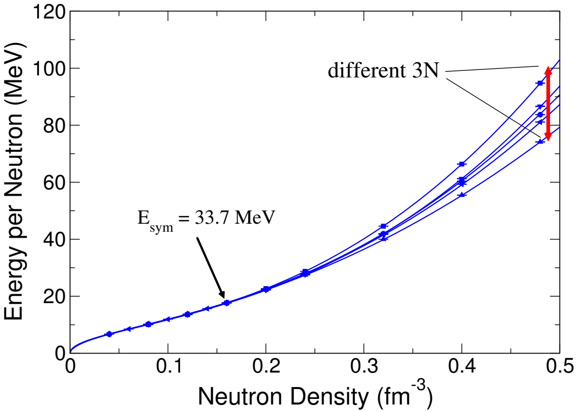


Assumption from experiments:

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

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

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

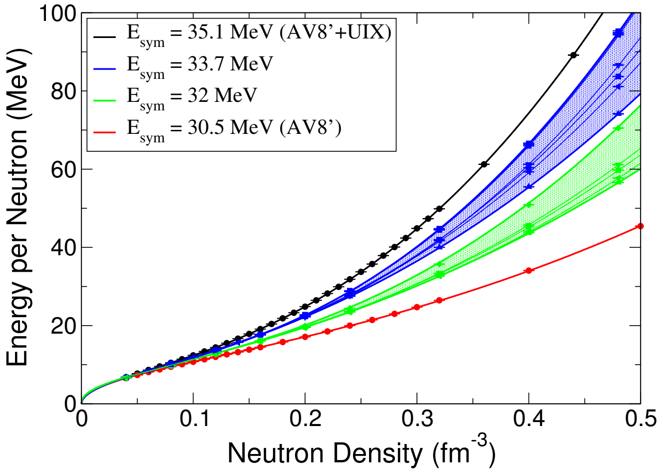


different 3N:

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

Neutron matter

Model uncertainty vs E_{sym} uncertainty:

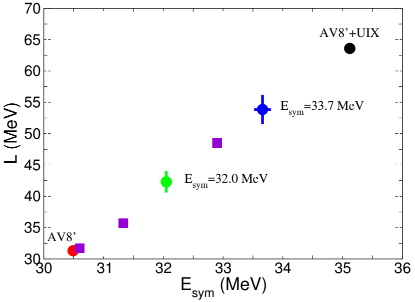


Gandolfi, Carlson, Reddy, PRC (2012)

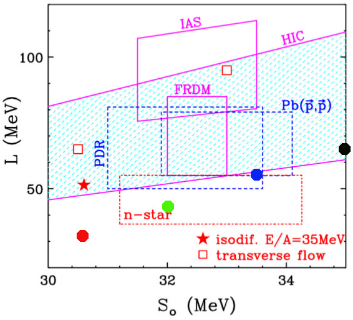
Neutron matter and symmetry energy

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)



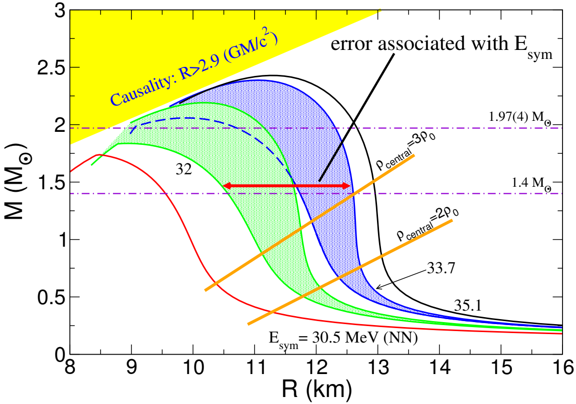
Tsang *et al.*, PRC (2012)

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...)

Neutron star structure

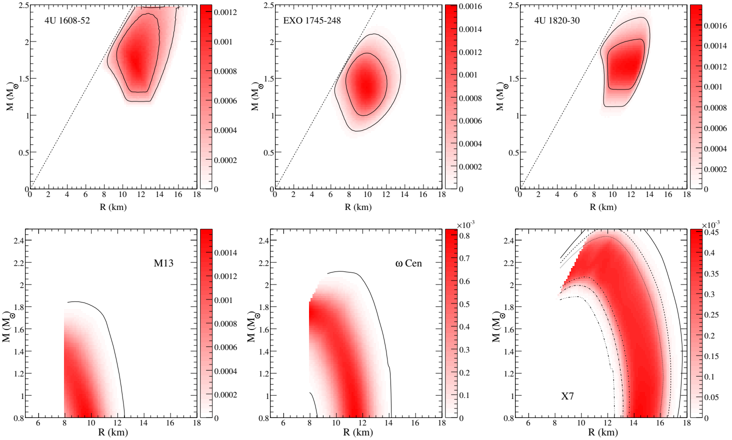
EOS used to solve the TOV equations.



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}!

Neutron stars



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:

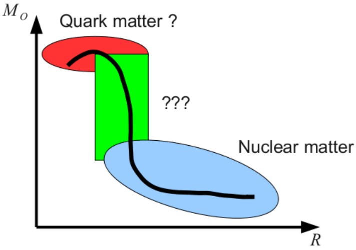
$$E_{NSM} = a\left(\frac{\rho}{\rho_0}\right)^{\alpha} + b\left(\frac{\rho}{\rho_0}\right)^{\beta}, \quad \rho < \rho_t$$

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

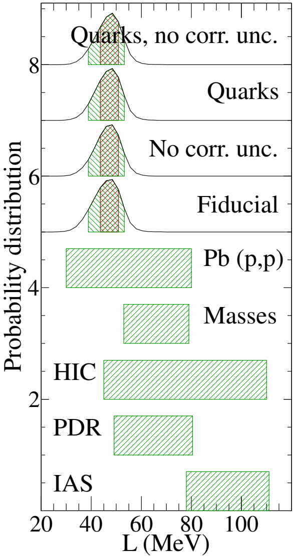


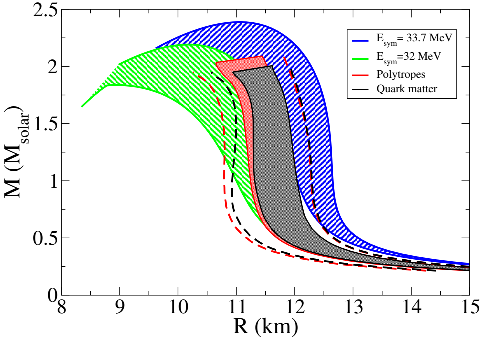
Neutron star radius sensitive to the EOS at nuclear densities!

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).

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

Propagation in imaginary time:

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

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-path calculation possible in several cases (exact).

GFMC includes all spin-states of nucleons in the w.f., nuclei up to A=12
AFDMC samples spin states, bigger systems, less accurate than GFMC

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.

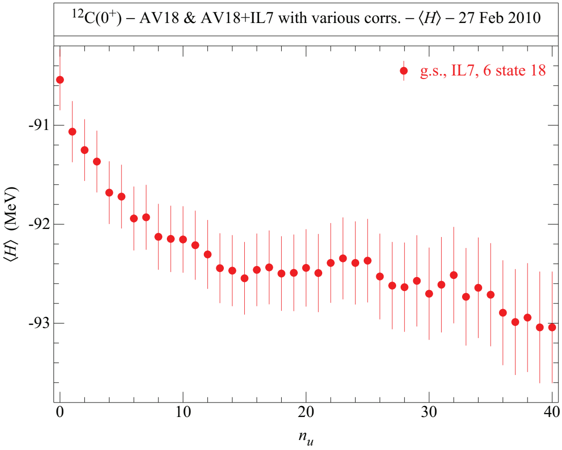
Fixed-node approximation: solve the problem in a restricted space where $\Psi > 0$ (Bosonic problem) $\Rightarrow$ upperbound.

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. Extra weight given by $\cos\Delta\theta$ (phase of $\frac{\Psi(R')}{\Psi(R)}$), $Re\{\Psi\} > 0 \Rightarrow$ not necessarily an upperbound.

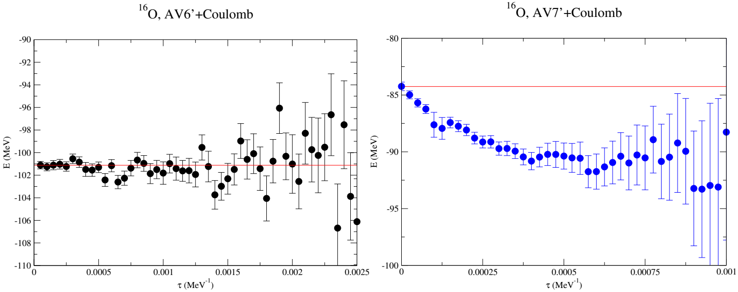
GFMC unconstrained-path propagation:



Changing the trial wave function gives same results.

Unconstrained-path

AFDMC unconstrained-path propagation:



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 to improve the constrained-path.

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:

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

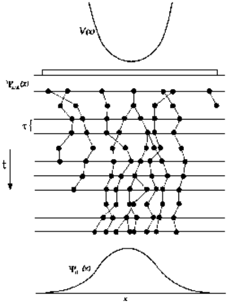
Algorithm for each time-step:

- 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

$$int[w + \xi]$$

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 $\approx (3N)^3$.

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.