Light nuclei and neutron matter with chiral EFT Hamiltonians

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NUCLEI Nuclear Computational Low-Energy Initiative

www.computingnuclei.org

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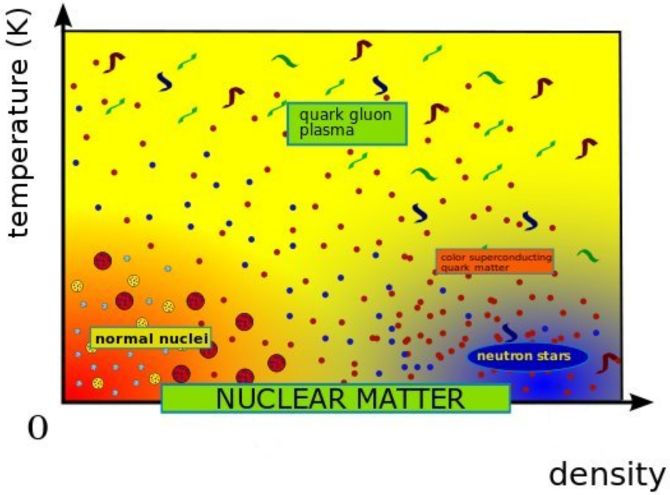
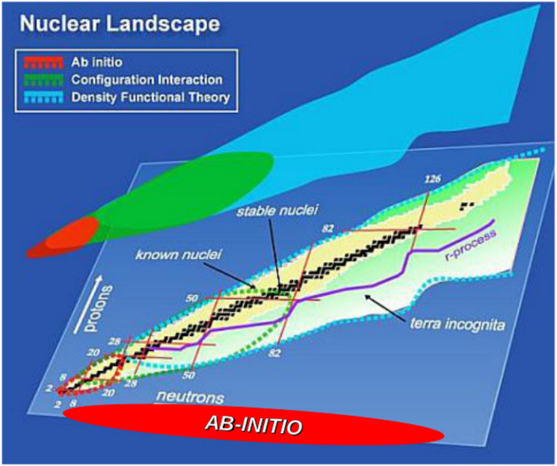
Homogeneous neutron matter



Nuclei



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Outline

- The Hamiltonian and Quantum Monte Carlo methods
- Nuclei and neutron matter with phenomenological Hamiltonians
- Chiral three-body forces, "technical" issues and open questions
- Results: A=3,4 binding energies, neutron-^{4}He scattering and neutron matter
- Conclusions

Nuclear Hamiltonian

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

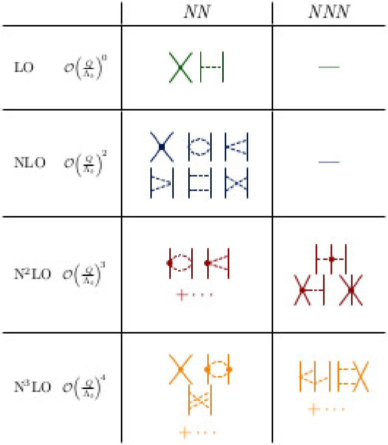
$$H = -\frac{\hbar^2}{2m}\sum_{i=1}^{A}\nabla_i^2 + \sum_{i<j} v_{ij} + \sum_{i<j<k} V_{ijk}$$

v_{ij} NN fitted on scattering data. Sum of operators:

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

- NN: Argonne AV8' and AV18. NNN: Urbana UIX and IL7.
- Local chiral forces up to N^2LO (Gezerlis, Tews, et al. PRL (2013), PRC (2014)).

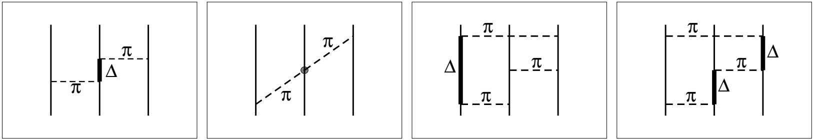
Chiral interactions permit to understand the evolution of theoretical uncertainties with the increasing of A.



- 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.

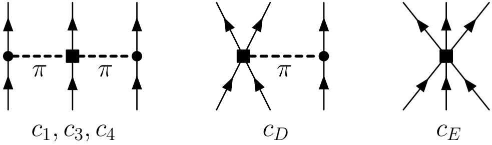
Slide by Joel Lynn, Scidac NUCLEI meeting 2014.

Urbana–Illinois V_{ijk} models processes like



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

Chiral forces at N^{2}LO:



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

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

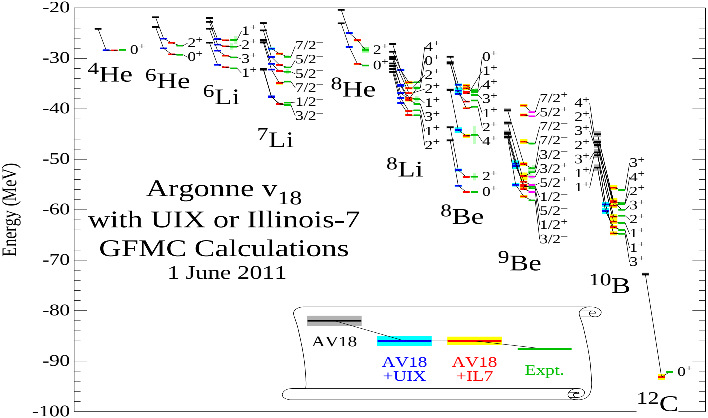
$$\psi(R,t) = \langle R|\psi(t)\rangle = \int dR'\,G(R,R',t)\psi(R',0)$$

- 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 %.

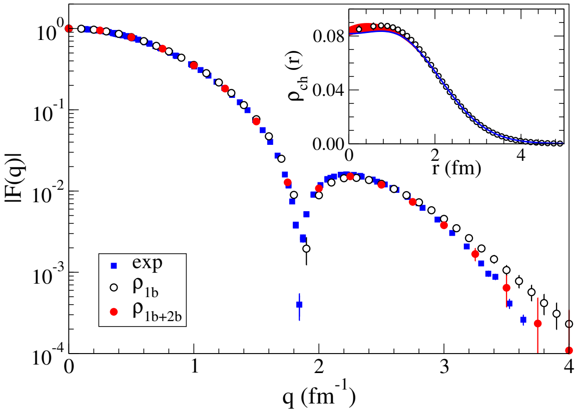
Light nuclei spectrum computed with GFMC



Carlson, Gandolfi, Pederiva, Pieper, Schiavilla, Schmidt, Wiringa, RMP (2015)

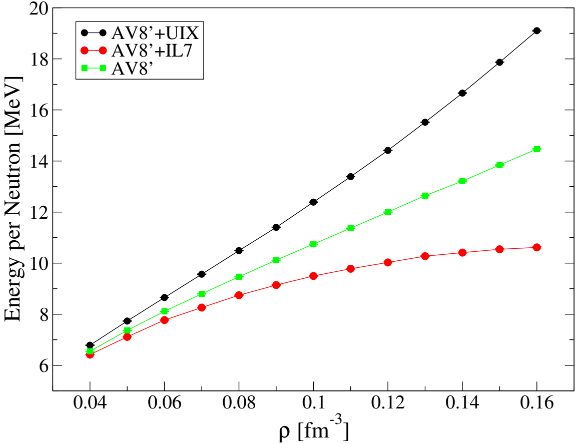
Also radii, densities, matrix elements, ...

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



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

Neutron matter and the deficiencies of three-body forces

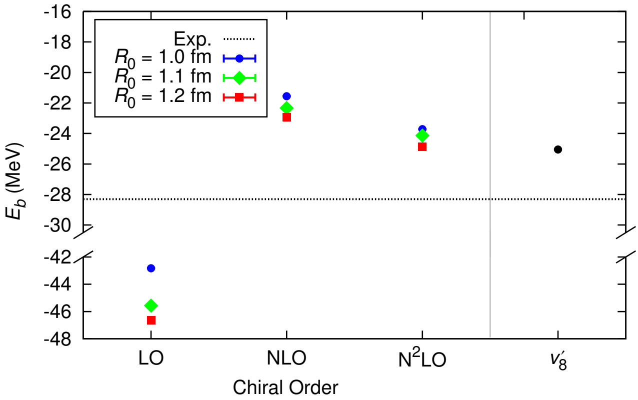


Maris, Vary, Gandolfi, Carlson, Pieper, PRC (2013)

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

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

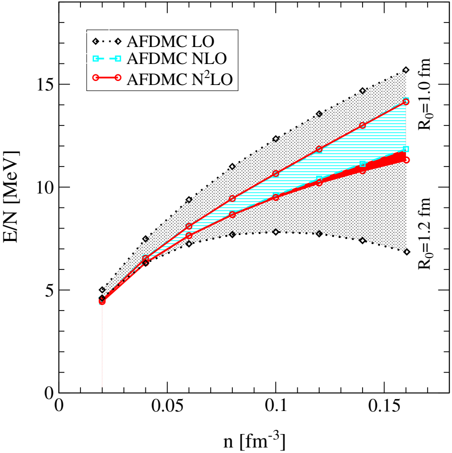
Binding energy of ^{4}He with only two-body interactions:



Lynn, Carlson, Epelbaum, Gandolfi, Gezerlis, Schwenk, PRL (2014).

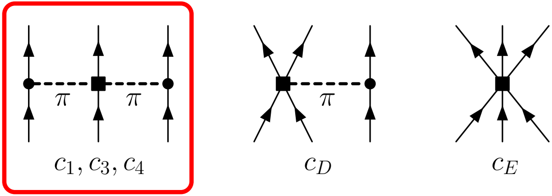
Neutron matter

Equation of state of neutron matter using NN chiral forces:



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

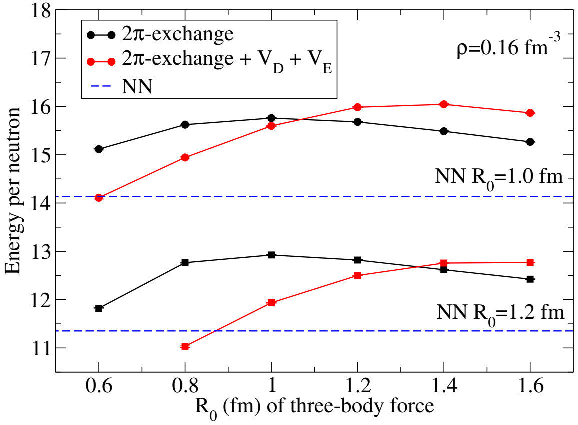
Chiral three-body forces, issue (I)



For a finite cutoff, there are "additional" V_D and V_E diagrams coming from Fourier transforming 2π exchange.

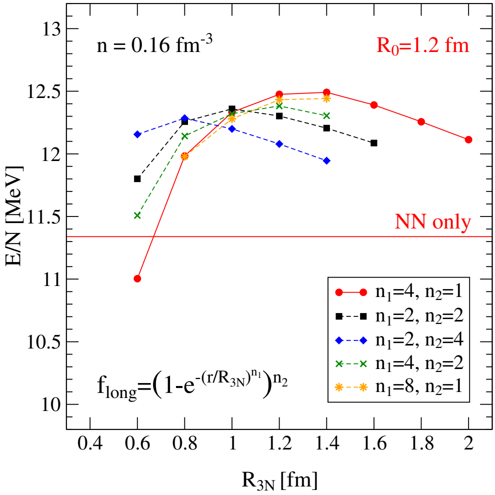
Usually they are effectively reabsorbed trough the fit of c_D and c_E, but often neglected in existing neutron matter calculations.

Contribution of the "additional" V_D and V_E terms, with $c_D = c_E = 0$.
AFDMC calculations.



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

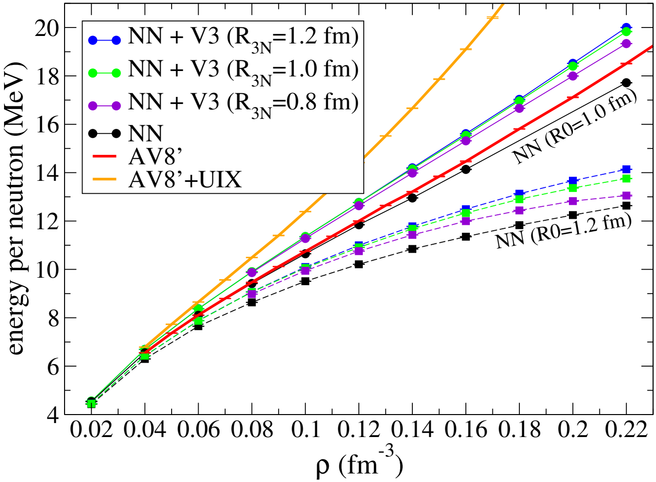
Exploring the form of the regulator and the cutoff:



Tews, Gandolfi, Gezerlis, Schwenk, PRC (2016)

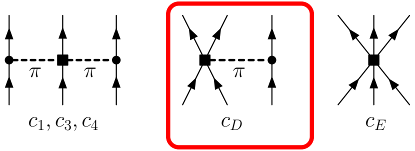
Neutron matter with chiral forces

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



Note: $c_D = c_E = 0$ (they will be non-zero in a few slides).

Chiral three-body forces, issue (II)



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

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

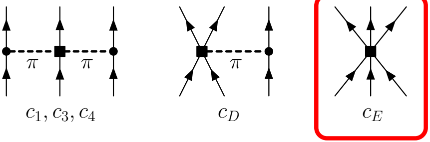
$$V_{D2} = \frac{g_A c_D m_\pi^2}{96\pi\Lambda_\chi F_\pi^4} \sum_{i<j<k} \sum_{\text{cyc}} \tau_i \cdot \tau_k \left[X_{ik}(r_{ik}) - \frac{4\pi}{m_\pi^2}\sigma_i \cdot \sigma_k \delta(r_{ik}) \right] \left[\delta(r_{ij}) + \delta(r_{kj}) \right]$$

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

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 (III)



Equivalent forms of operators entering in V_E (or combinations of them):

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

Epelbaum et al (2002). We investigated three choices:

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

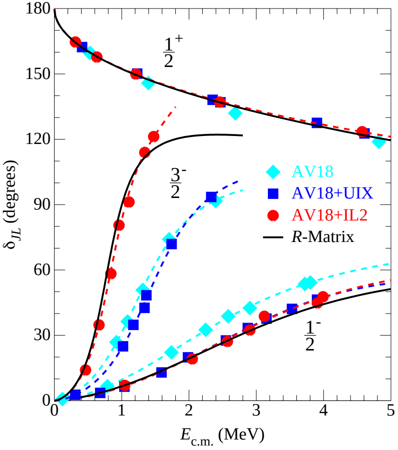
$$V_{E1} = \frac{c_E}{\Lambda_\chi F_\pi^4} \sum_{i<j<k} \sum_{\text{cyc}} \delta(r_{kj})\delta(r_{ij})$$

$$V_{E\mathcal{P}} = \frac{c_E}{\Lambda_\chi F_\pi^4} \sum_{i<j<k} \sum_{\text{cyc}} \mathcal{P}_{S,T=1/2}\, \delta(r_{kj})\delta(r_{ij})$$

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

Chiral three-body forces

Coefficients c_D and c_E fit to reproduce the binding energy of ^{4}He and neutron-^{4}He scattering. $\rightarrow$ more information on T=3/2 part of three-body interaction.

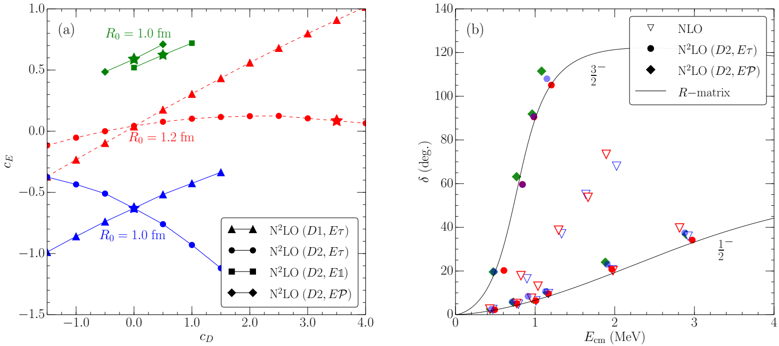


GFMC neutron-^{4}He results using Argonne Hamiltonians.

Nollett, Pieper, Wiringa, Carlson, Hale, PRL (2007).

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

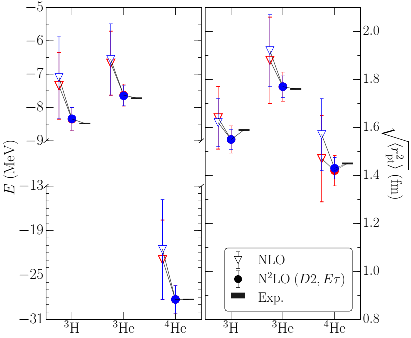
Cutoff R_0 taken consistently with the two-body interaction.



No fit to both observables can be obtained for $R_0 = 1.2$ fm and V_{D1}

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

A=3, 4 nuclei at N2LO



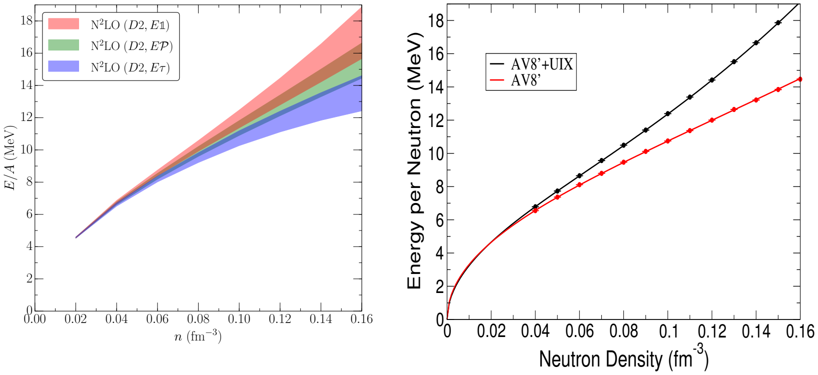
Error quantification: define $Q = \max\left(\frac{p}{\Lambda_b}, \frac{m_\pi}{\Lambda_b}\right)$ and calculate:

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

Epelbaum, Krebs, Meissner (2014).

Neutron matter at N2LO

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



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

Summary

- Ab-initio QMC methods useful to study nuclear systems in a coherent framework using phenomenological and local chiral forces.
- Spectrum of nuclei and other properties well reproduced with Argonne Hamiltonians, but problems in describing neutron matter.
- Many ambiguities regarding the choice of three-body operators. Effect in heavier nuclei and nuclear matter?
  Provocation: Same issue for NN???
- (some) local chiral interaction describe A=3,4,5 and neutron matter.

Acknowledgments:

- Joe Carlson (LANL)
- Ingo Tews (INT)
- Joel Lynn, Achim Schwenk (Darmstadt)
- Alex Gezerlis (Guelph)
- Kevin Schmidt (ASU)
- Evgeny Epelbaum (Bochum)

Extra slides

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}

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 $t\rightarrow\infty$.

Propagation performed by

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

- Importance sampling: $G(R,R',t)\rightarrow G(R,R',t)\,\Psi_I(R')/\Psi_I(R)$
- 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.

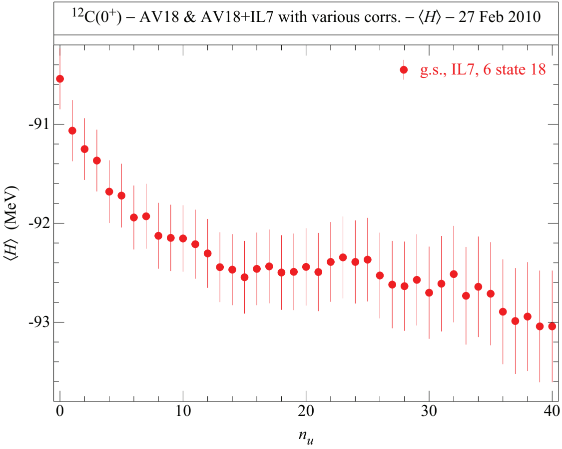
If Ψ is complex:

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

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.

Unconstrained-path

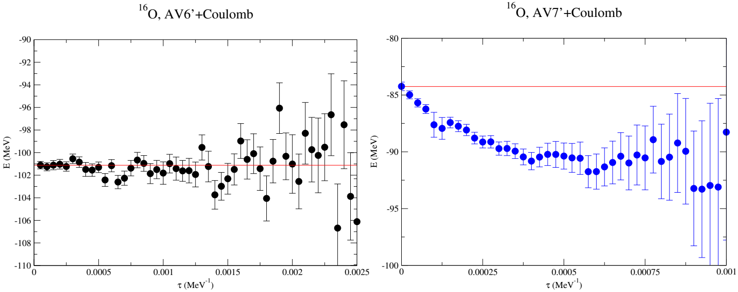
GFMC unconstrained-path propagation:



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.

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

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

Propagation performed by

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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:

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

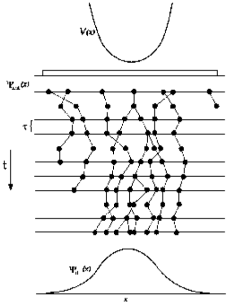
Algorithm for each time-step:

- 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:

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

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^2LO can be exactly included in the case of neutrons.

For example:

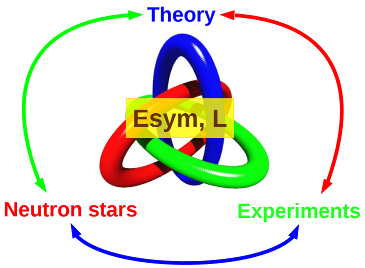
$$O_{2\pi} = \sum_{cyc}\left[\{X_{ij},X_{jk}\}\{\tau_i\cdot\tau_j,\tau_j\cdot\tau_k\}+\frac{1}{4}[X_{ij},X_{jk}][\tau_i\cdot\tau_j,\tau_j\cdot\tau_k]\right]$$
$$= 2\sum_{cyc}\{X_{ij},X_{jk}\}=\sigma_i\sigma_k f(r_i,r_j,r_k)$$

The above form can be included in the AFDMC propagator.

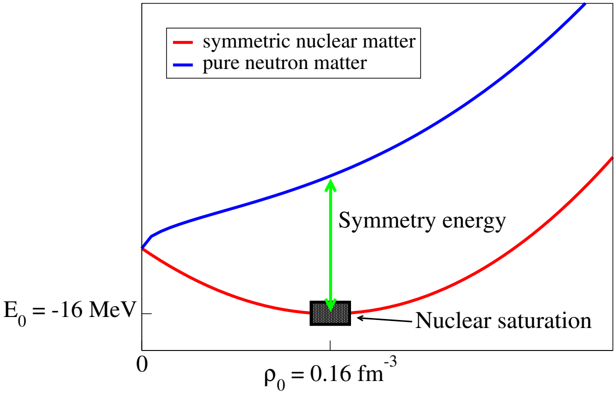
Neutron matter equation of state

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?



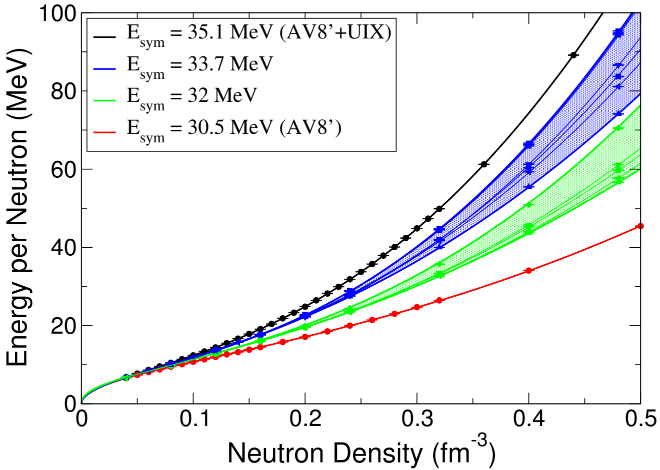
Assumption from experiments:

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

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

Neutron matter

Model uncertainty vs E_{sym} uncertainty:

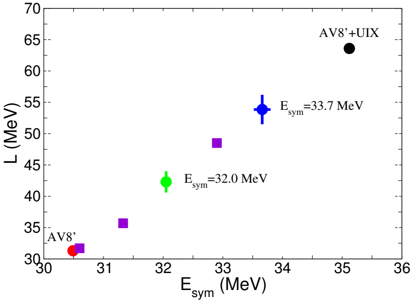


Gandolfi, Carlson, Reddy, PRC (2012)

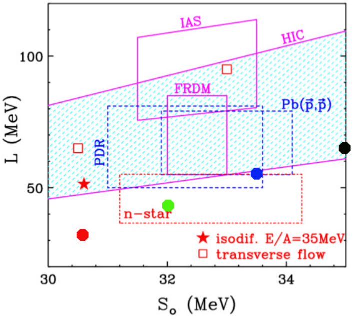
Neutron matter and symmetry energy

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)

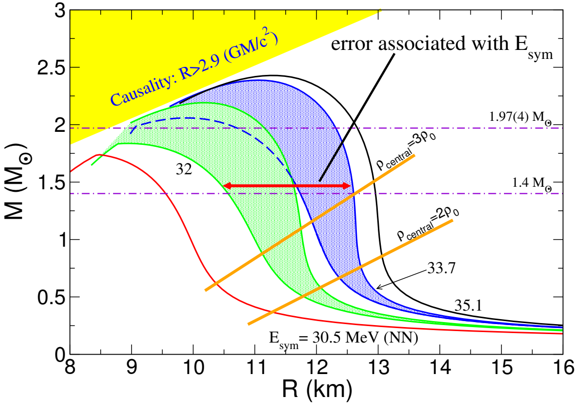


Tsang *et al.*, PRC (2012)

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

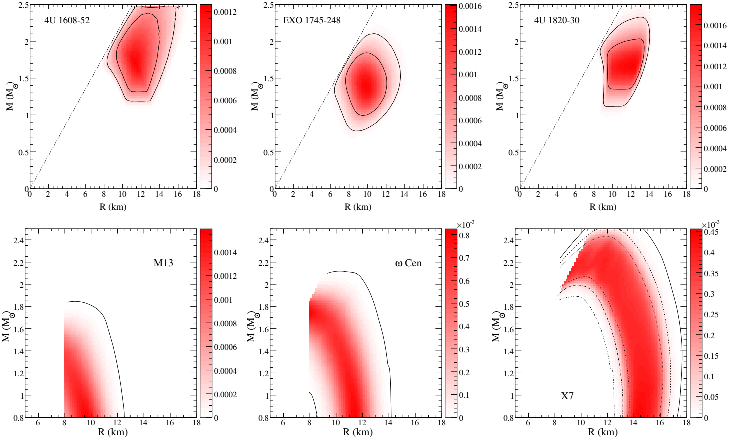
EOS used to solve the TOV equations.



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:

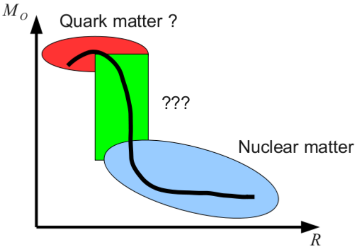
$$E_{NSM} = a\left(\frac{\rho}{\rho_0}\right)^{\alpha} + b\left(\frac{\rho}{\rho_0}\right)^{\beta}, \quad \rho < \rho_t$$

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

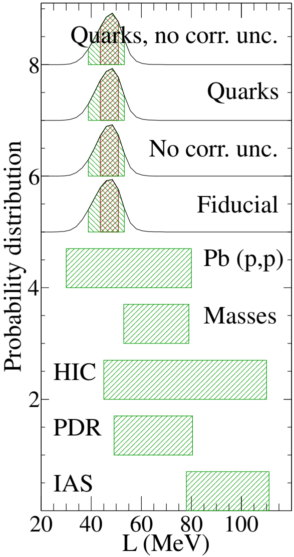


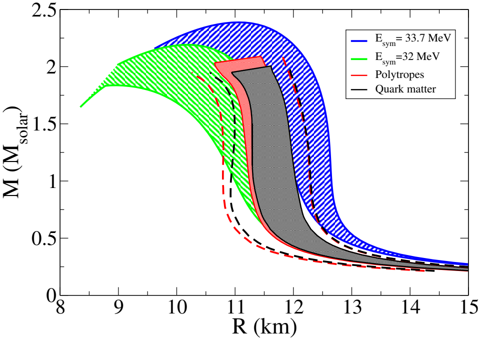
Neutron star radius sensitive to the EOS at nuclear densities!

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).