The EOS of neutron matter, and the effect of Λ hyperons to neutron star structure

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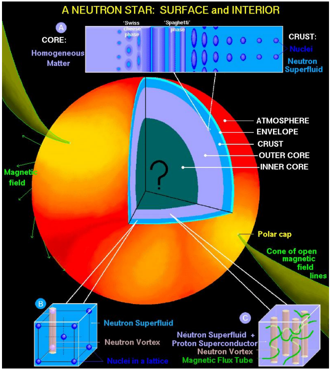
Neutron stars

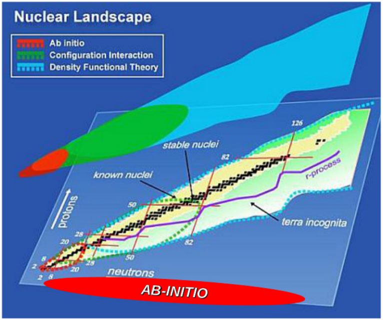
Neutron star is a wonderful natural laboratory

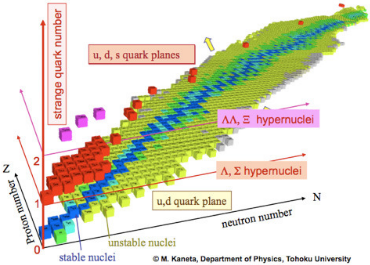


D. Page

- 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?

Nuclei and hypernuclei

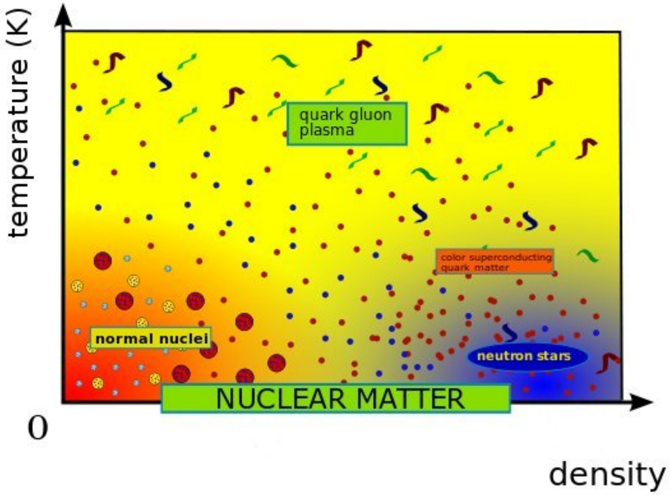




Few thousands of binding energies for normal nuclei are known.

Only few tens for hypernuclei.

Homogeneous neutron matter



Outline

- The model and the method
- Equation of state of neutron matter
- Symmetry energy
- Neutron star structure (I) - radius
- Λ-hypernuclei
- Λ-neutron matter
- Neutron star structure (II) - maximum mass
- Conclusions

Nuclear Hamiltonian

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

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

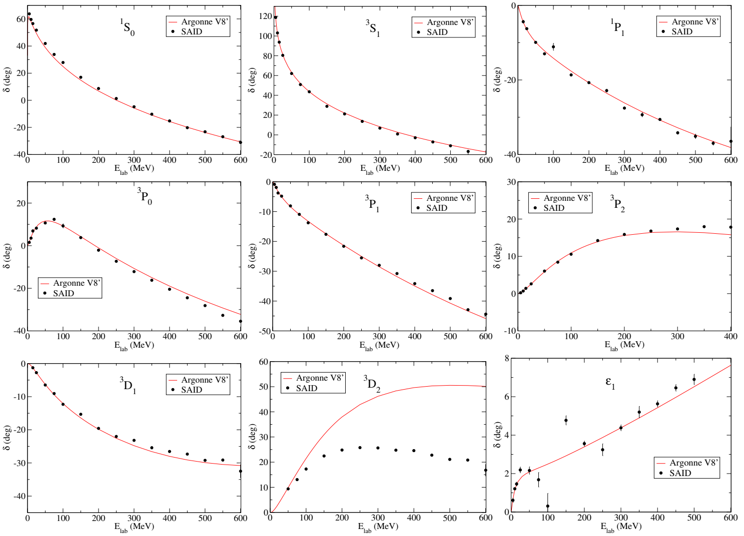
v_{ij} NN fitted on scattering data. Sum of operators:

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

Argonne AV8'.

Local chiral forces up to N^2LO has the similar spin/isospin operatorial structure of AV8' - Gezerlis, Tews, et al. PRL (2013), PRC (2014)

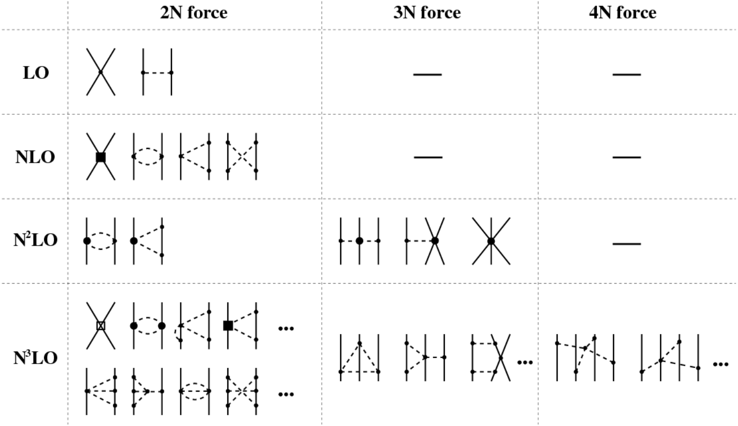
Phase shifts, AV8'



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

Nuclear Hamiltonian

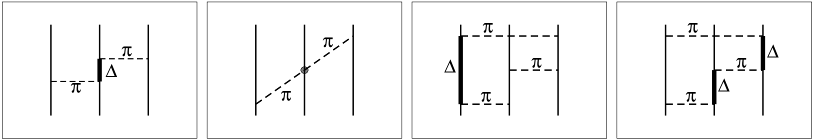
Chiral EFT interactions



Short range operators need to be regulated → cutoff dependency!

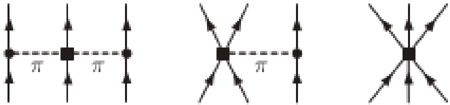
Three-body forces

Urbana–Illinois V_{ijk} models processes like



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

Chiral forces at N^2LO:



Nuclear Hamiltonians

Advantages:

- Argonne interactions fit phase shifts up to high energies: accurate up to high densities. 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: bad for high densities. How do they work at large momenta, (i.e. e and ν scattering)?

Important to consider both and compare predictions

Scattering data and neutron matter

The energy of scattering data included in the fit gives an idea of the validity of the interaction in dense 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 for dense matter well above ρ_0=0.16 fm^{-3}

Recent chiral forces fit $30 < E_{lab} < 200$ MeV.

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 $t \to \infty$.

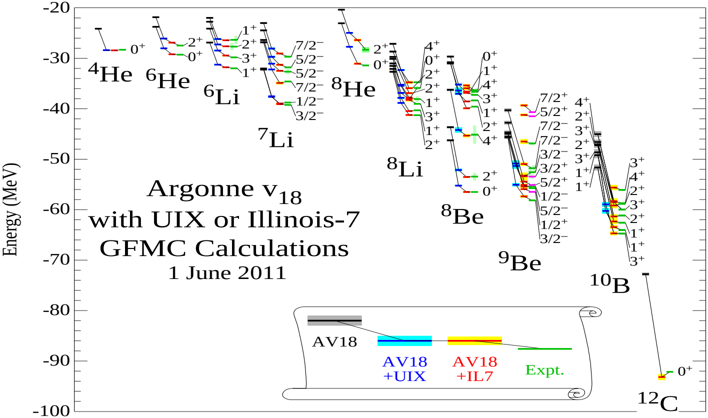
Propagation performed by

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

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

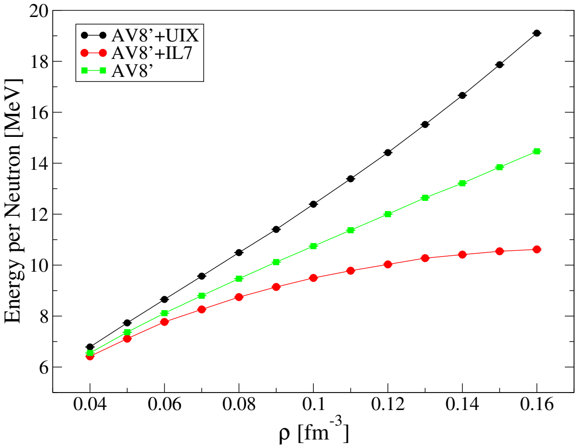
Ground–state obtained in a **non-perturbative way.** Systematic uncertainties within 1-2 %.

Light nuclei spectrum computed with GFMC



Many other observables (radii, densities, transitions, ...) also well described, Carlson, *et al*, RMP (2015)

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



Maris, *et al.*, PRC (2013)

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

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

Extended Data Table 2 | Key observables from chiral interactions. Predictions for ^{48}Ca (based on the interactions used in this work): binding energy BE, neutron separation energy S_n, three-point-mass difference Δ, electric-charge radius R_{ch}, and the weak-charge radius R_W. The last two columns show the symmetry energy of the nuclear equation of state and its slope L at saturation density. Energies are in MeV and radii in fm. Theoretical uncertainty estimates are about 1% for radii and energies.

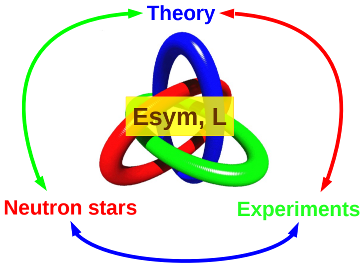
Interaction	BE	S_n	Δ	R_{ch}	R_W	S_v	L
$NNLO_{sat}$	404	9.5	2.69	3.48	3.65	26.9	40.8
1.8/2.0 (EM)	420	10.1	2.69	3.30	3.47	33.3	48.6
2.0/2.0 (EM)	396	9.3	2.66	3.34	3.52	31.4	46.7
2.2/2.0 (EM)	379	8.8	2.61	3.37	3.55	30.2	45.5
2.8/2.0 (EM)	351	8.0	2.41	3.44	3.62	28.5	43.8
2.0/2.0 (PWA)	346	7.8	2.82	3.55	3.72	27.4	44.0
Experiment	415.99	9.995	2.399	3.477			

Hagen, *et al.*, Nature Physics (2016)

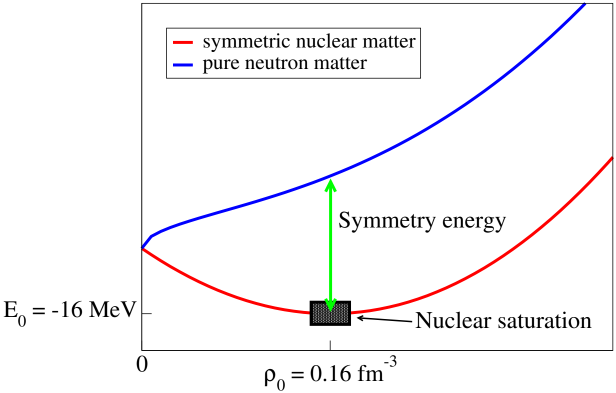
Similar trend: very low symmetry energies, soft EOS, probably leading too small radii in neutron stars.

Neutron matter equation of state

- Nucleon-nucleon interactions well constrained.
- 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.
- EOS of neutron matter gives the symmetry energy and its slope.
- Determines radii of neutron stars.



What is the Symmetry energy?

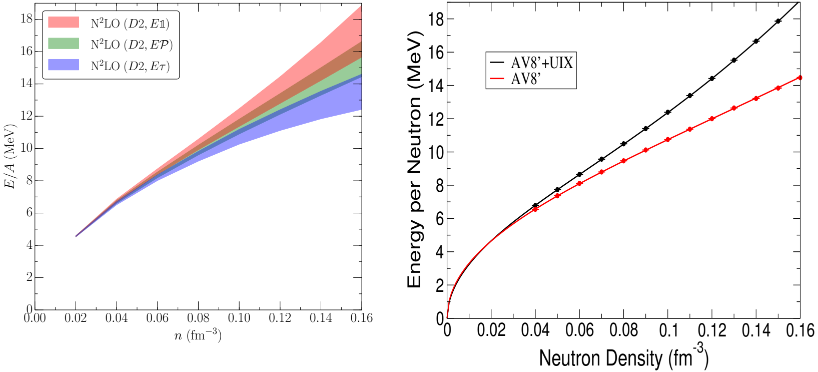


Assumption from experiments:

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

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

EOS of pure neutron matter: N2LO (R_0=1.0 fm) *vs* phenomenological AV8'(+UIX)

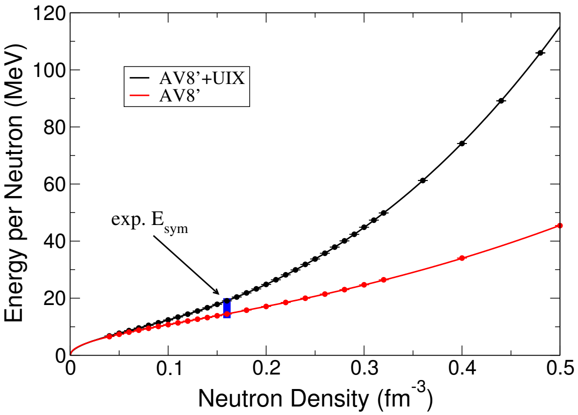


Lynn, *et al.*, PRL (2016).

Note: **the above** (but not all) chiral Hamiltonian able to describe A=3,4,5 nuclei and neutron matter "*reasonably*"

Neutron matter

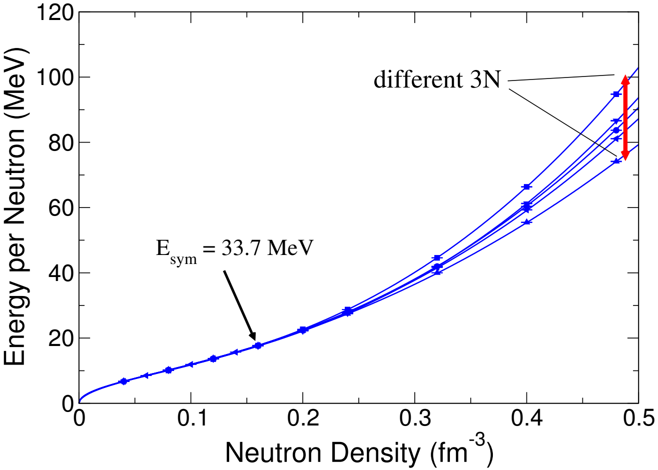
Equation of state of neutron matter using the AV8′+UIX Hamiltonian.



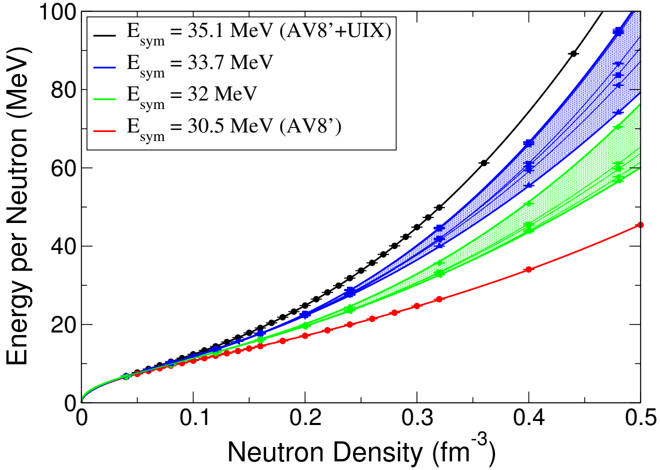
Incidentally these can be considered as "extremes" with respect to the measured E_{sym}.

Neutron matter

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

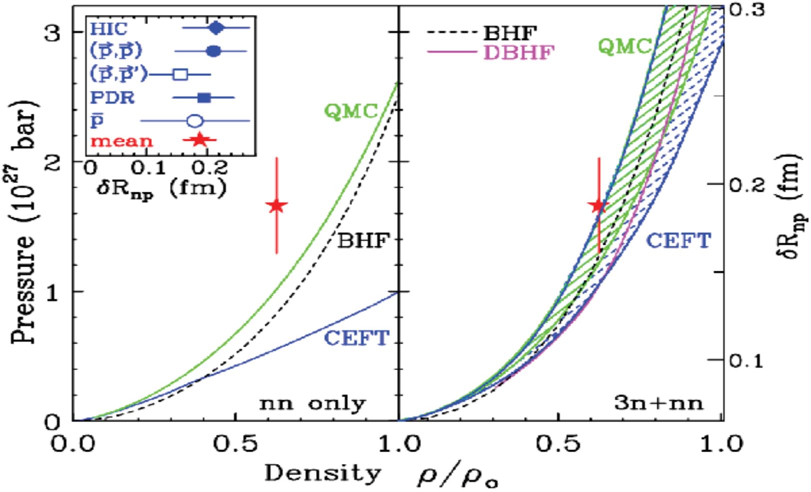


Equation of state of neutron matter using Argonne forces:



Gandolfi, Carlson, Reddy, PRC (2012)

Three-body force in neutron matter

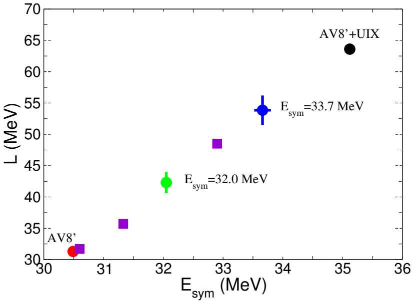


Tsang *et al.*, PRC (2012)

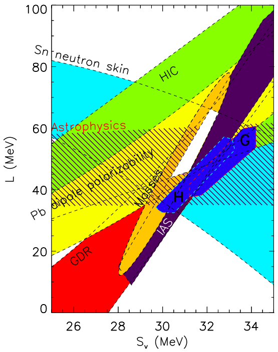
Neutron matter and symmetry energy

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

$$E_{sym}(\rho) = E_{sym} + \frac{L}{3}\frac{\rho - 0.16}{0.16} + \cdots \qquad \text{(often } \mathrm{E_{sym}} \text{ called } \mathrm{S_0})$$



Gandolfi *et al.*, EPJ (2014)



Lattimer, Steiner, EPJ (2014)

Very weak dependence to the model of 3N force for a given E_{sym}.

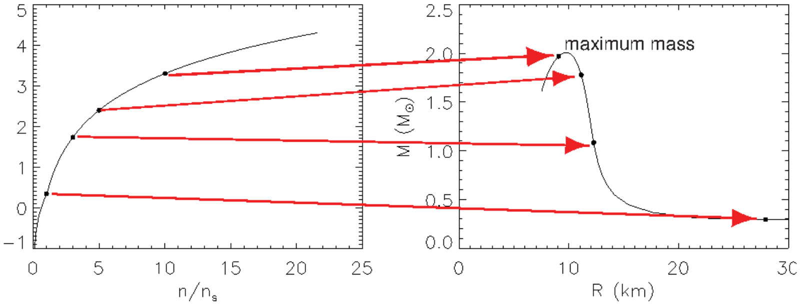
Chiral interactions give similar results.

Neutron matter and neutron star structure

TOV equations:

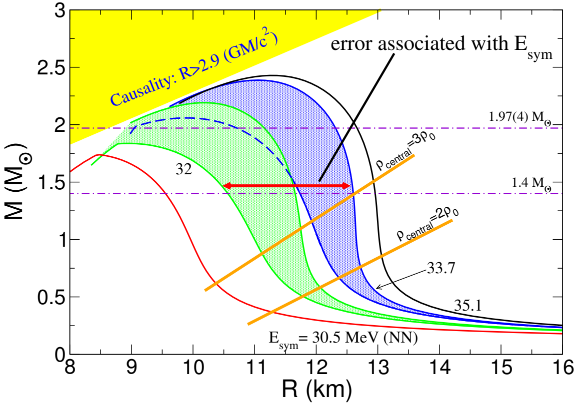
$$\frac{dP}{dr} = -\frac{G[m(r) + 4\pi r^3 P/c^2][\epsilon + P/c^2]}{r[r - 2Gm(r)/c^2]} \,,$$

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



J. Lattimer

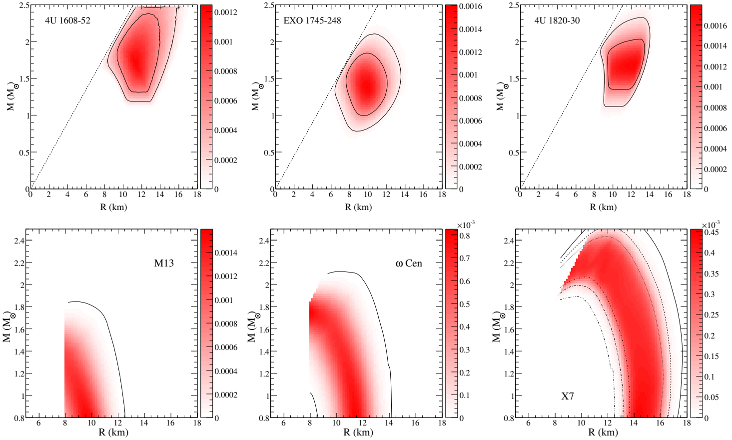
EOS used to solve the TOV equations.



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:

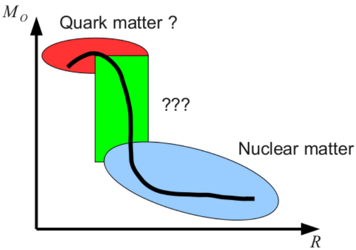
$$\text{crust}+\text{E}_{\text{NSM}} = \text{a}\left(\frac{\rho}{\rho_0}\right)^{\alpha} + \text{b}\left(\frac{\rho}{\rho_0}\right)^{\beta}, \rho < \rho_{\text{t}}$$

(form suggested by QMC simulations),

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

i) two polytropes

ii) polytrope+quark matter model

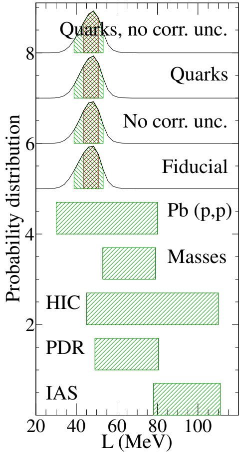


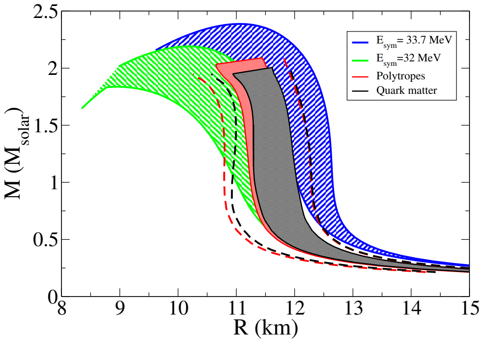
Neutron star radius sensitive to the EOS at nuclear densities!

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!





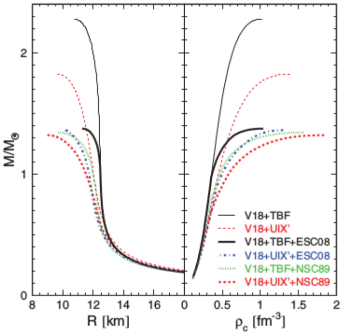
$32 < E_{sym} < 34\, MeV, \; 43 < L < 52\, MeV$

Steiner, Gandolfi, PRL (2012).

High density neutron matter

If chemical potential large enough ($\rho \sim 2-3\rho_0$), nucleons produce Λ, Σ, ...

Non-relativistic BHF calculations suggest that available hyperon-nucleon Hamiltonians support an EOS with $M > 2M_\odot$:



Schulze and Rijken PRC (2011).

Vidana, Logoteta, Providencia, Polls, Bombaci EPL (2011).

Note: (Some) other relativistic model support $2M_\odot$ neutron stars.

Often called *Hyperon puzzle*

Λ-systems, outline

Λ-hypernuclei and hypermatter

$$H = H_N + \frac{\hbar^2}{2m_\Lambda}\sum_{i=1}^{A}\nabla_i^2 + \sum_{i<j} v_{ij}^{\Lambda N} + \sum_{i<j<k} V_{ijk}^{\Lambda NN}$$

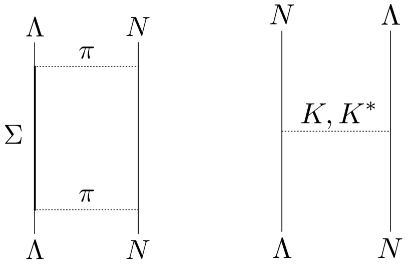
Λ-binding energy calculated as the difference between the system with and without Λ.

Λ-nucleon interaction

The Λ-nucleon interaction is constructed similarly to the Argonne potentials (Usmani). $\Lambda - \Sigma$ mixing not included

Argonne NN: $v_{ij} = \sum_p v_p(r_{ij}) O^p_{ij}\,,\, O_{ij} = (1, \sigma_i \cdot \sigma_j, S_{ij}, \vec{L}_{ij} \cdot \vec{S}_{ij}) \times (1, \tau_i \cdot \tau_j)$

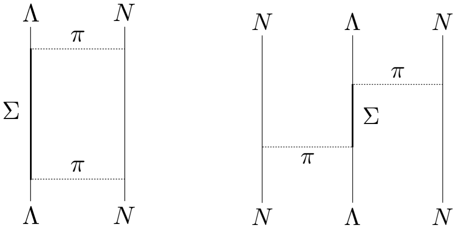
Usmani ΛN: $v_{ij} = \sum_p v_p(r_{ij}) O^p_{ij}\,,\, O_{\lambda j} = (1, \sigma_\lambda \cdot \sigma_j) \times (1, \tau^z_j)$



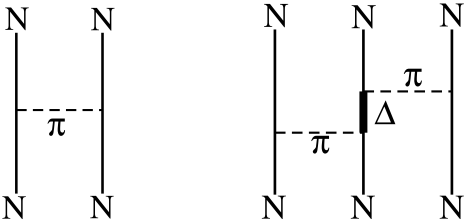
Unfortunately... ∼4500 NN data, ∼30 of ΛN data.

Let's *pretend* that ΛN is just fine...

ΛNN has the same range of ΛN

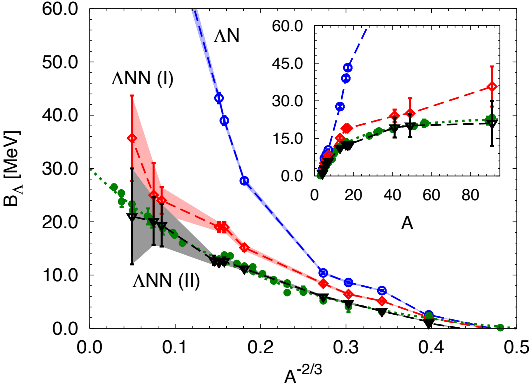


Differently from NN and NNN interactions:



Λ hypernuclei

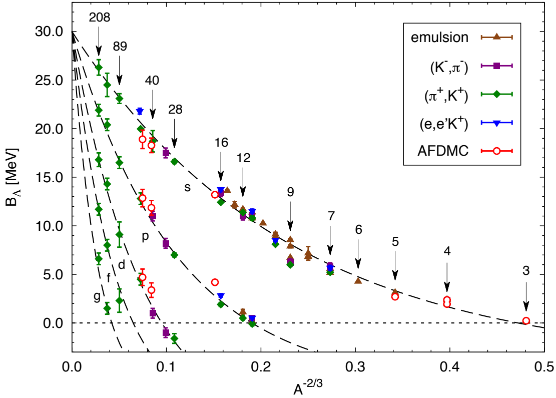
$v^{\Lambda N}$ and $V^{\Lambda NN}$(I) are phenomenological (Usmani).
$V^{\Lambda NN}$ (II) is a new form where the parameters have been readjusted.



Lonardoni, Gandolfi, Pederiva, PRC (2013) and PRC (2014).

ΛNN crucial for saturation! (as expected...)

Λ in different states:



Pederiva, Catalano, Lonardoni, Lovato, Gandolfi, arXiv:1506.04042

Hyper-neutron matter

Neutrons and Λ particles:

$$\rho = \rho_n + \rho_\Lambda \,, \qquad\qquad x = \frac{\rho_\Lambda}{\rho}$$

$$E_{\rm HNM}(\rho,x) = \Big[E_{\rm PNM}((1-x)\rho)+m_n\Big](1-x)+\Big[E_{\rm P\Lambda M}(x\rho)+m_\Lambda\Big]x+f(\rho,x)$$

where $E_{P\Lambda M}$ is the non-interacting energy (no $v_{\Lambda\Lambda}$ interaction),

$$E_{PNM}(\rho) = a\left(\frac{\rho}{\rho_0}\right)^\alpha + b\left(\frac{\rho}{\rho_0}\right)^\beta$$

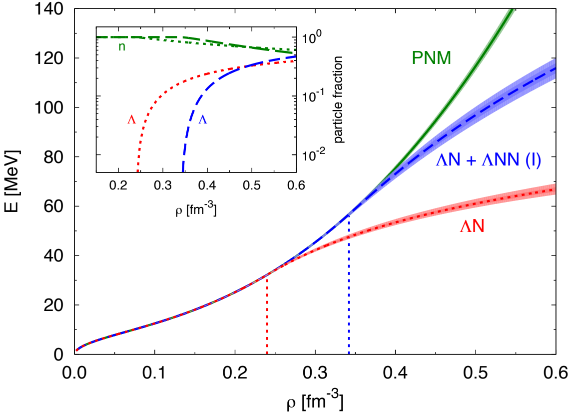
and

$$f(\rho,x) = c_1\frac{x(1-x)\rho}{\rho_0} + c_2\frac{x(1-x)^2\rho^2}{\rho_0^2}$$

All the parameters are fit to Quantum Monte Carlo results.

Λ-neutron matter

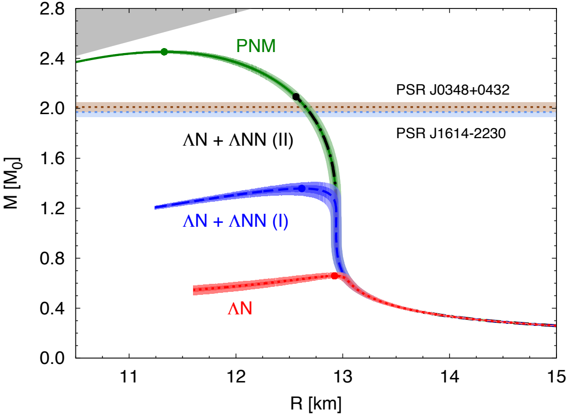
EOS obtained by solving for $\mu_\Lambda(\rho, x) = \mu_n(\rho, x)$



Lonardoni, Lovato, Gandolfi, Pederiva, PRL (2015)

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

Λ-neutron matter



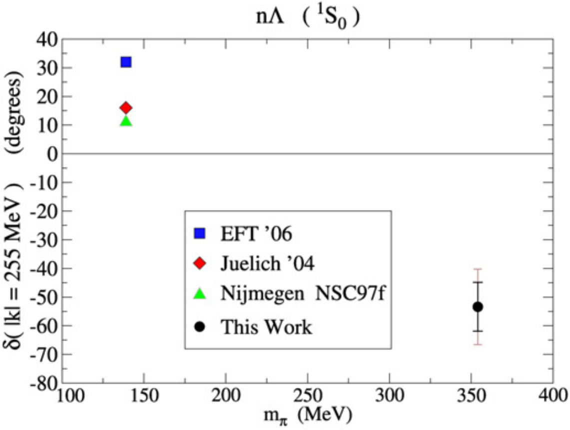
Lonardoni, Lovato, Gandolfi, Pederiva, PRL (2015)

Drastic role played by ΛNN. Calculations can be compatible with neutron star observations.

Note: no $v_{\Lambda\Lambda}$, no protons, and no other hyperons included yet...

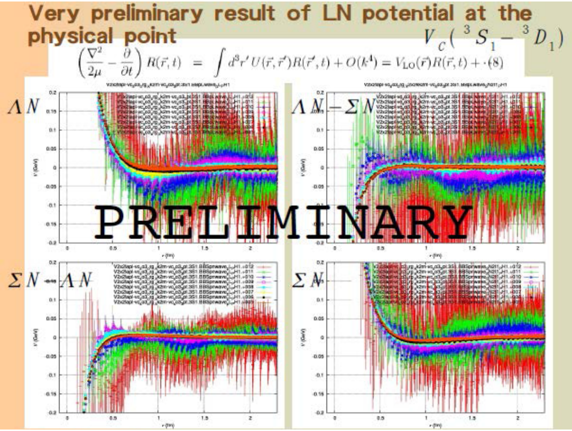
Hyperons

Future, more ΛN experiments and/or Lattice QCD.
Example: phase-shifts calculated with Lattice QCD.



Beane *et al.*, Nuclear Physics A794, 62 (2007)

Future, more ΛN experiments and/or Lattice QCD.
Example: attempt to extract the potential with Lattice QCD:



HAL QCD collaboration.

Summary

- EOS of pure neutron matter qualitatively well understood.
- Λ-nucleon data very limited, but ΛNN seems very important. Good reproduction of (limited) experimental data.
- Role of Λ in neutron stars far to be understood.
  My opinion: there is no puzzle. Just, too many pieces are missing...

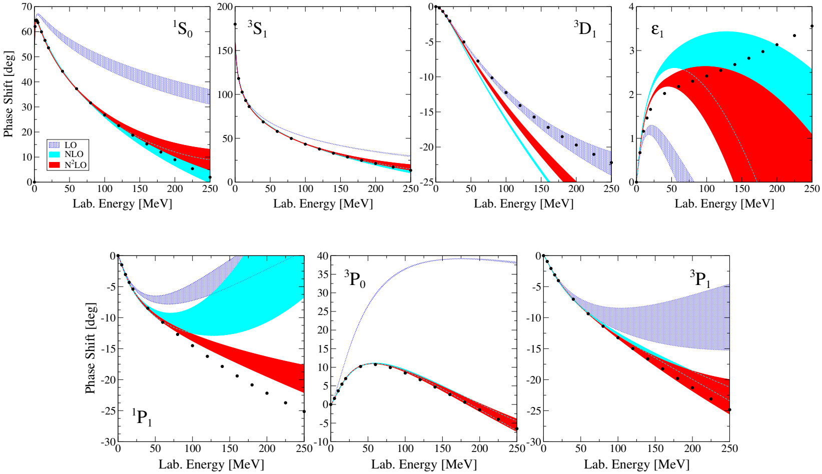
*M*y wishes:

- Accurate and precise measurement of E_{sym} and L.
- New observations of neutron stars (mass and radii, GW).
- More ΛN experimental data needed. Input from Lattice QCD?
- Light and medium Λ-nuclei measurements needed, especially $N \neq Z$.

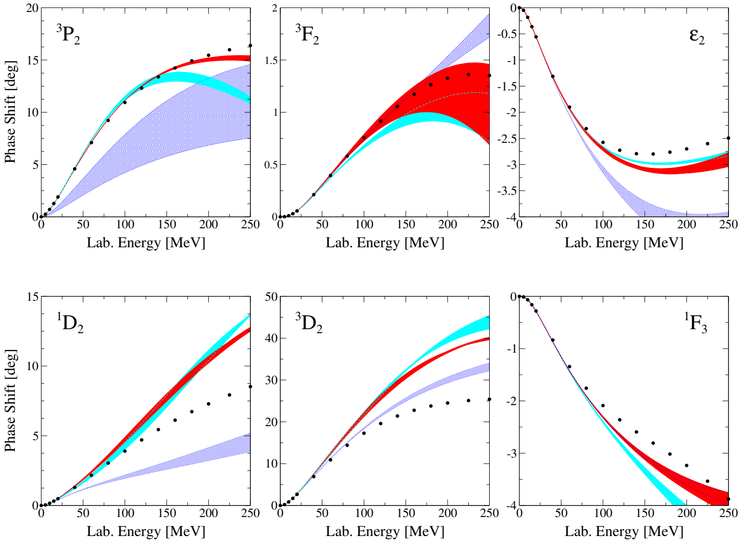
Acknowledgments:
J. Carlson, D. Lonardoni (LANL); A. Steiner (UT/ORL); S. Reddy, I. Tews (INT); A. Lovato, B. Wiringa (ANL); F. Pederiva (Trento); A. Gezerlis (Guelph); J. Lynn, A. Schwenk (Darmstadt)

Extra slides

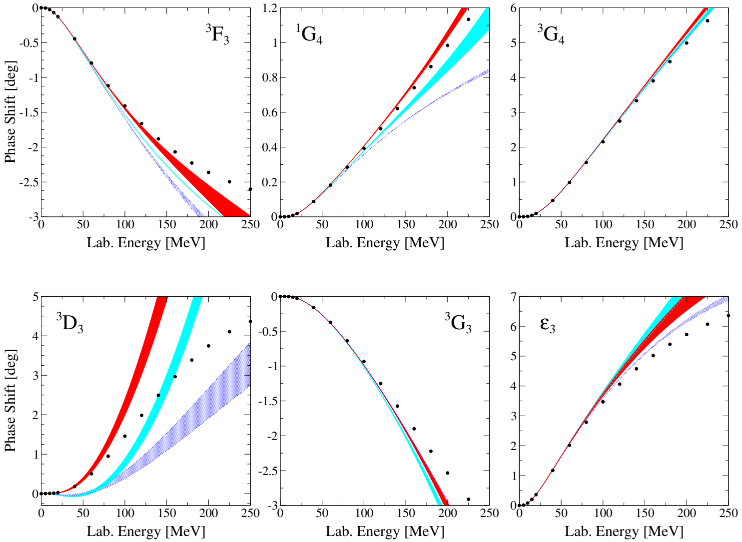
Phase shifts, LO, NLO and N^2LO with R_0=1.0 and 1.2 fm:



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

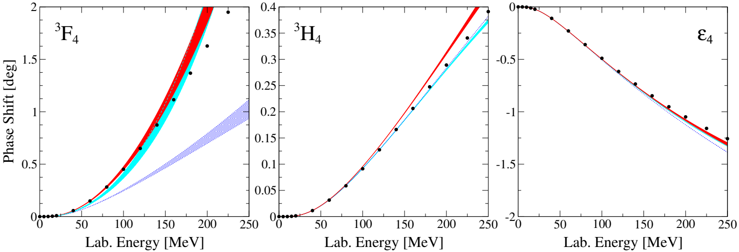


Phase shifts, LO, NLO and N^2LO with R_0=1.0 and 1.2 fm:



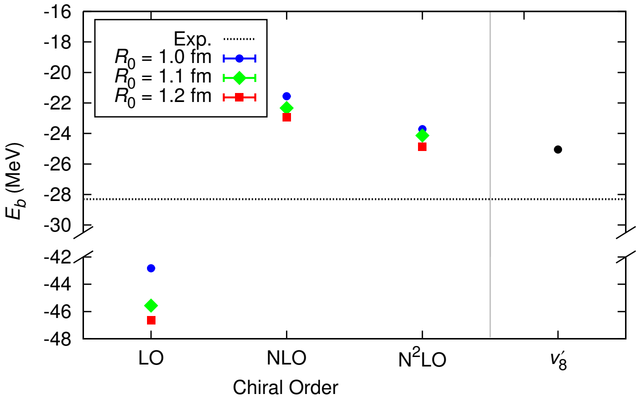
Nuclear Hamiltonian

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



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

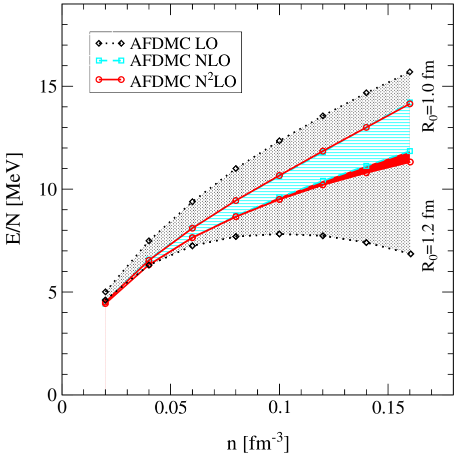
Binding energy of ^{4}He with only two-body interactions:



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

Neutron matter

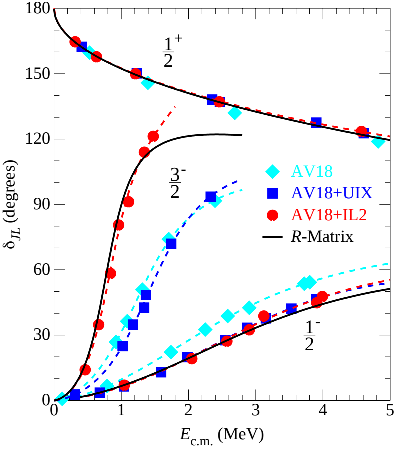
Equation of state of neutron matter using NN chiral forces:



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

Chiral three-body forces

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



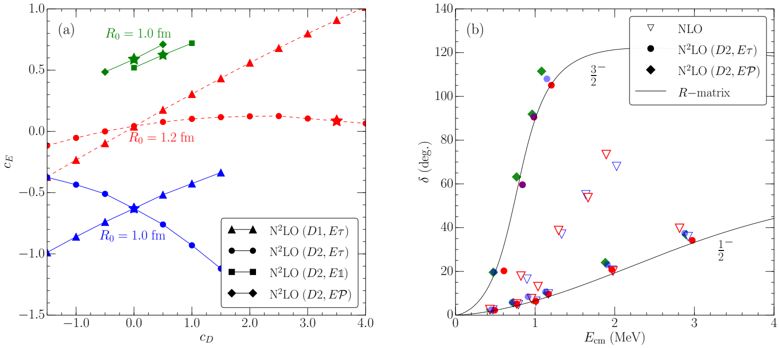
GFMC neutron-^{4}He results using Argonne Hamiltonians.

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

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

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

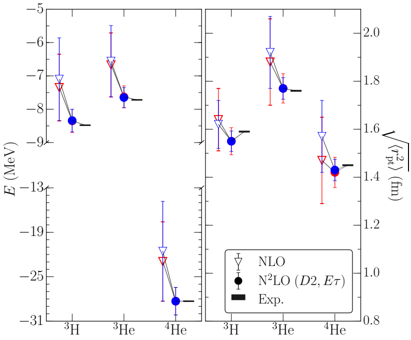
Cutoff R_0 taken consistently with the two-body interaction.



No fit 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

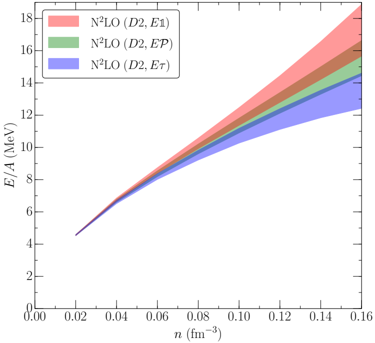


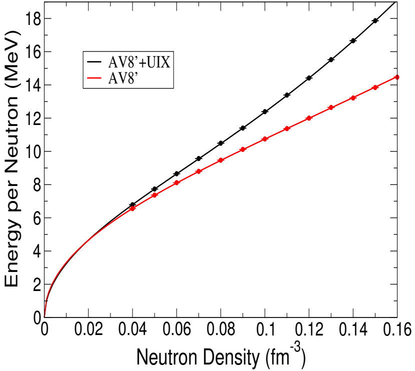
Error quantification: define $Q = \max\left(\frac{p}{\Lambda_b}, \ \frac{m_\pi}{\Lambda_b}\right)$ and calculate:

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

Epelbaum, Krebs, Meissner (2014).

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).

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 %.

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:

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

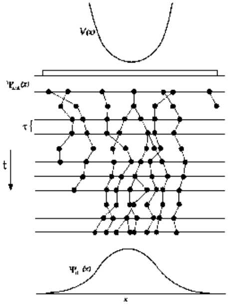
Algorithm for each time-step:

- 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:

$$O_{2\pi} = \sum_{cyc}\left[\{X_{ij},X_{jk}\}\{\tau_i\cdot\tau_j,\tau_j\cdot\tau_k\}+\frac{1}{4}[X_{ij},X_{jk}][\tau_i\cdot\tau_j,\tau_j\cdot\tau_k]\right]$$

$$= 2\sum_{cyc}\{X_{ij},X_{jk}\} = \sigma_i\sigma_k f(r_i,r_j,r_k)$$

The above form can be included in the AFDMC propagator.

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.

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.

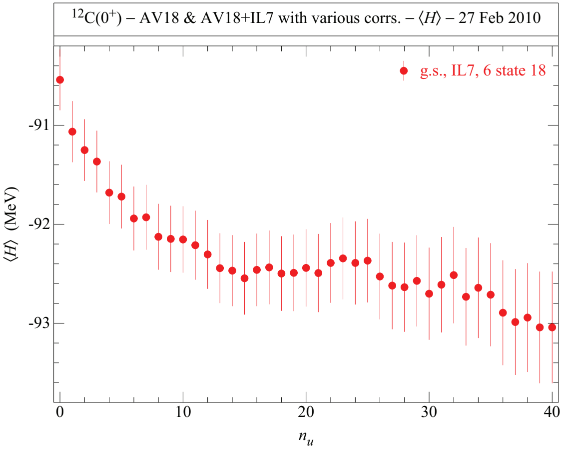
If Ψ is complex:

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

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

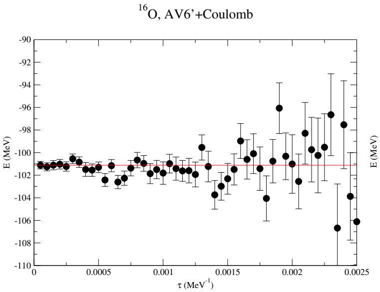
GFMC unconstrained-path propagation:



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.