Nuclear symmetry energy from neutron drops

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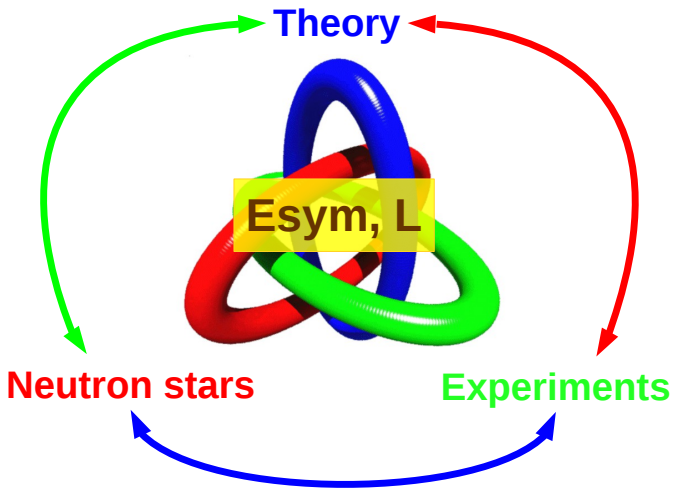
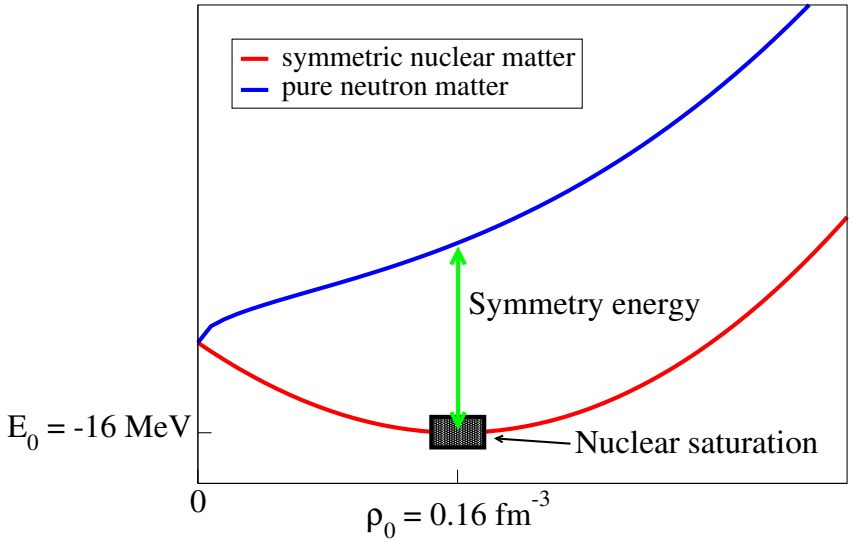
Nuclear symmetry energy



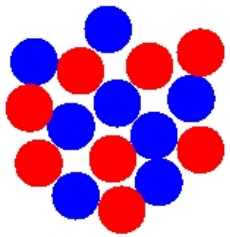


The Nuclear (A)Symmetry Energy cannot directly be measured, but it is related to many properties of nuclei and neutron stars.

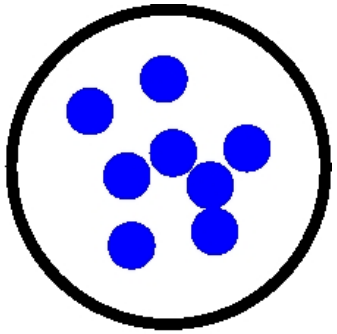
It is very important then to find indirect ways and relations to other observables to constrain it!

Neutron drops

Why study neutron drops?
Are they nothing more than a pure simple toy model?



NP self–bound



N confined

Neutron drops are interesting because:

- Provide a strong benchmark for microscopic calculations
- Model neutron-rich nuclei
- Calibrate density functionals for neutron-rich systems (useful to check $\nabla\rho$ terms in different geometries)
- Predictions of few neutron resonances
- Connections with skin thickness and symmetry energy

Outline

- The model and the method
- Microscopic calculations compared to density functionals
- Correlation between neutron drop radii and skin of nuclei
- Correlation radii-symmetry energy
- 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.

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

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

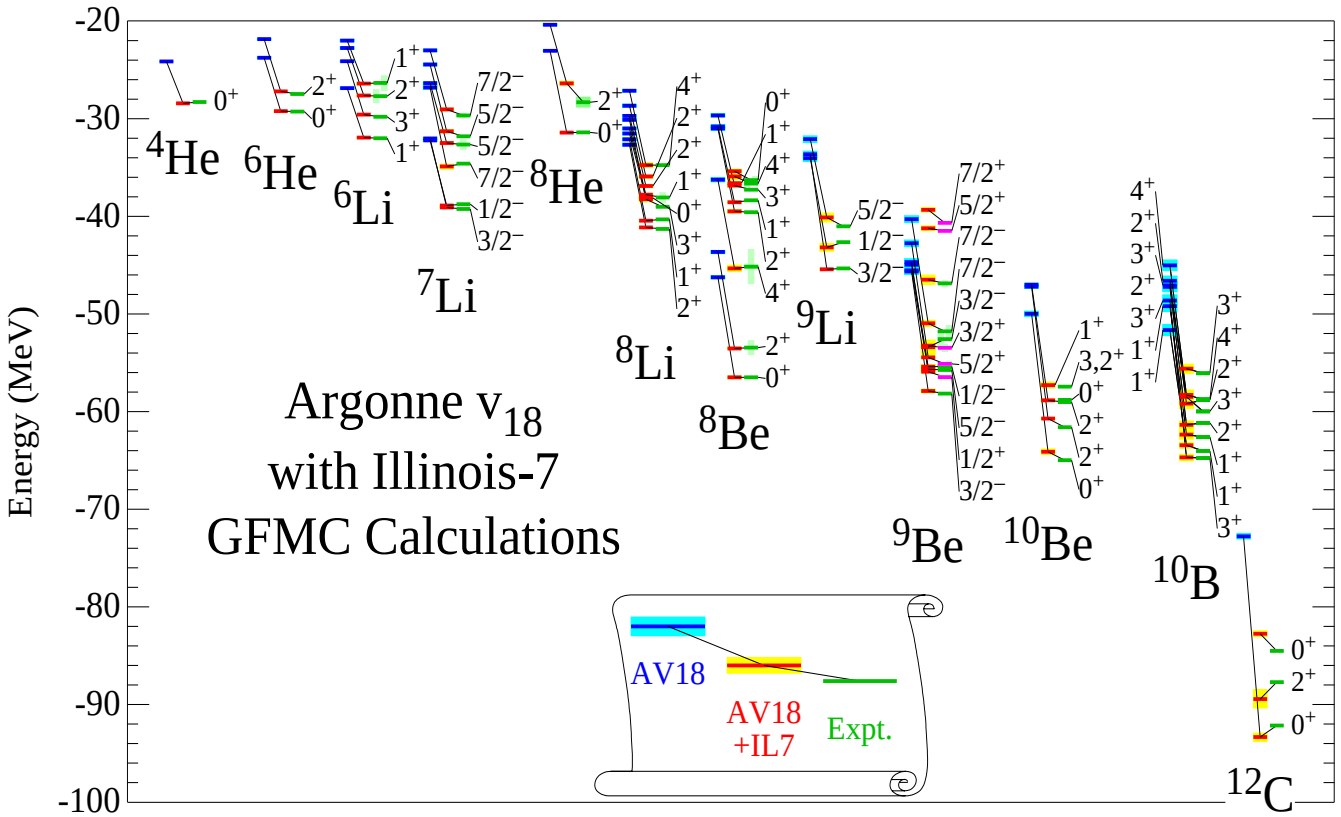
- Importance sampling: $G(R,R',t) \to G(R,R',t)\,\Psi_I(R')/\Psi_I(R)$
- Constrained-path approximation to control the sign problem. Unconstrained-path calculation possible in several cases (exact).

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 2-3 %.

See Carlson, et al., Rev. Mod. Phys. 87, 1067 (2015)

Light nuclei spectrum computed with GFMC



Carlson, et al., Rev. Mod. Phys. 87, 1067 (2015)

Also radii, densities, matrix elements, ...

Local chiral Hamiltonians used here also good to describe nuclei (see Lonardoni et al., PRL and PRC (2018)).

Neutron drops

We confine neutrons by adding an external potential:

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

V_{ext} is a Wood-Saxon or Harmonic well:

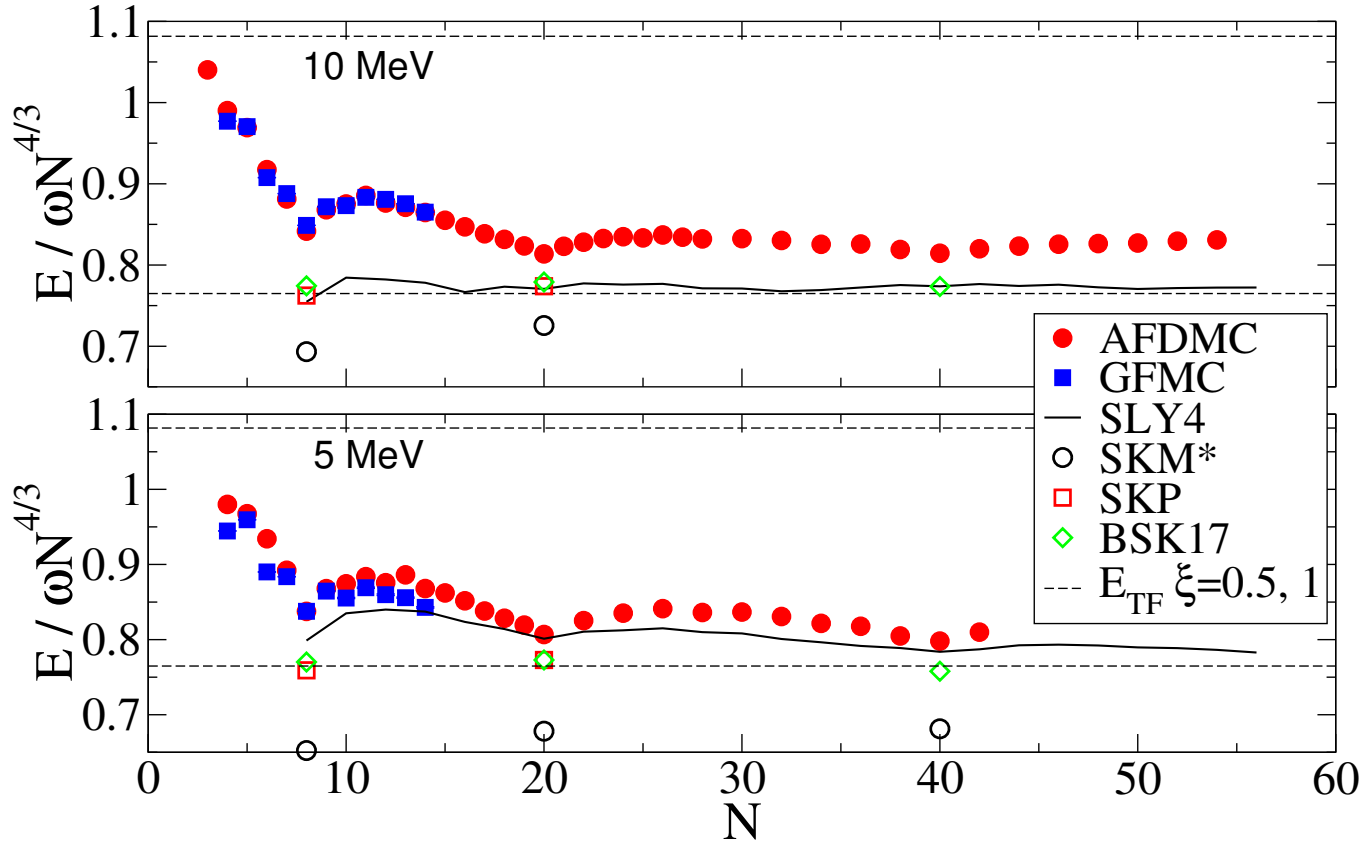
$$V_{WS} = -\frac{V_0}{1 + exp[(r-R)/a]}$$

$$V_{HO} = \frac{1}{2}m\omega^2 r^2$$

$\Longrightarrow$ different geometries and densities.

Neutron drops, harmonic oscillator well

External well: harmonic oscillator with $\hbar\omega$=5, 10 MeV.

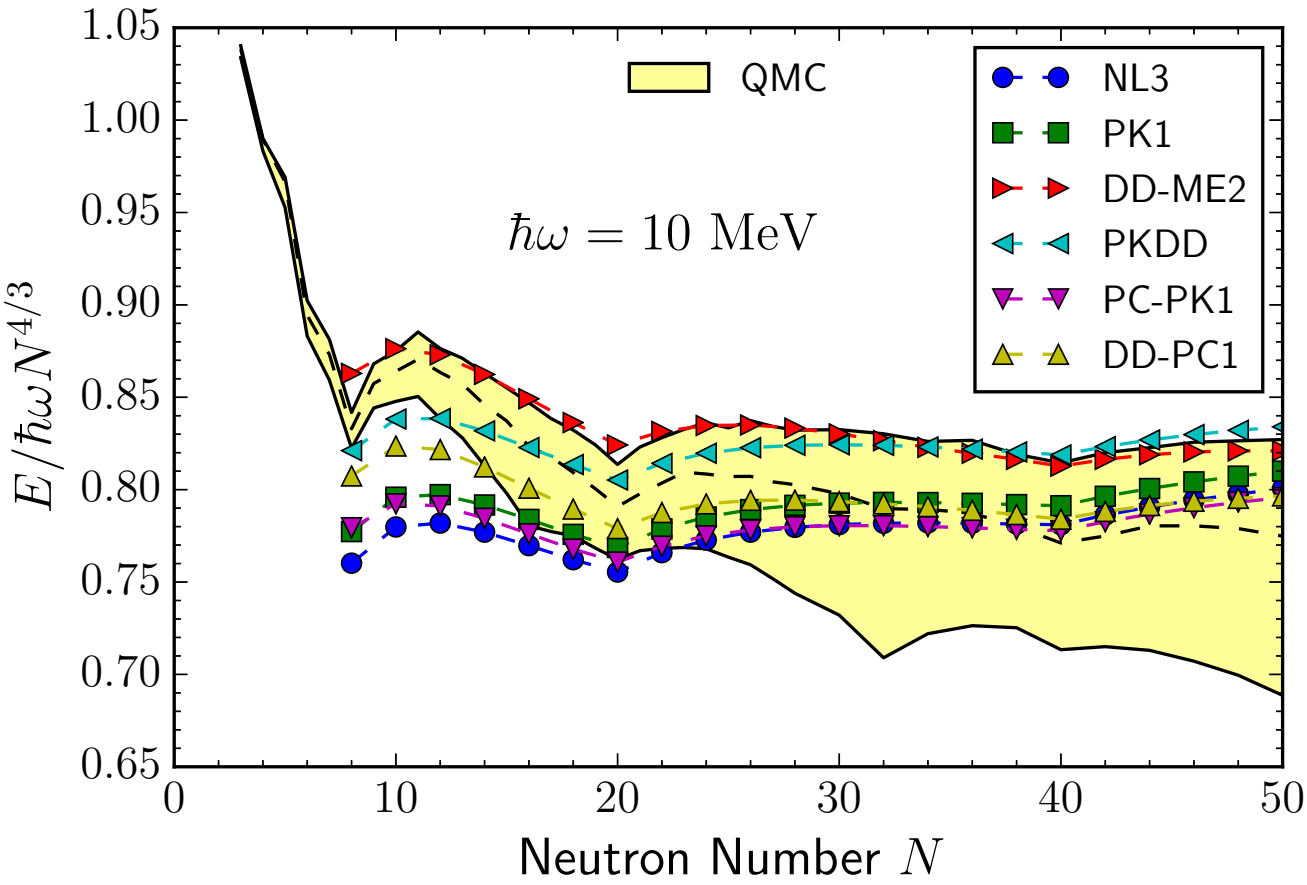


Skyrme systematically overbind neutron drops.

Gandolfi, Carlson, Pieper, PRL 106, 012501 (2011).

Neutron drops

Comparison with other functionals. QMC: AV8'+UIX, AV8', AV8'+IL7 (from Maris, *et al.*, PRC 2013)

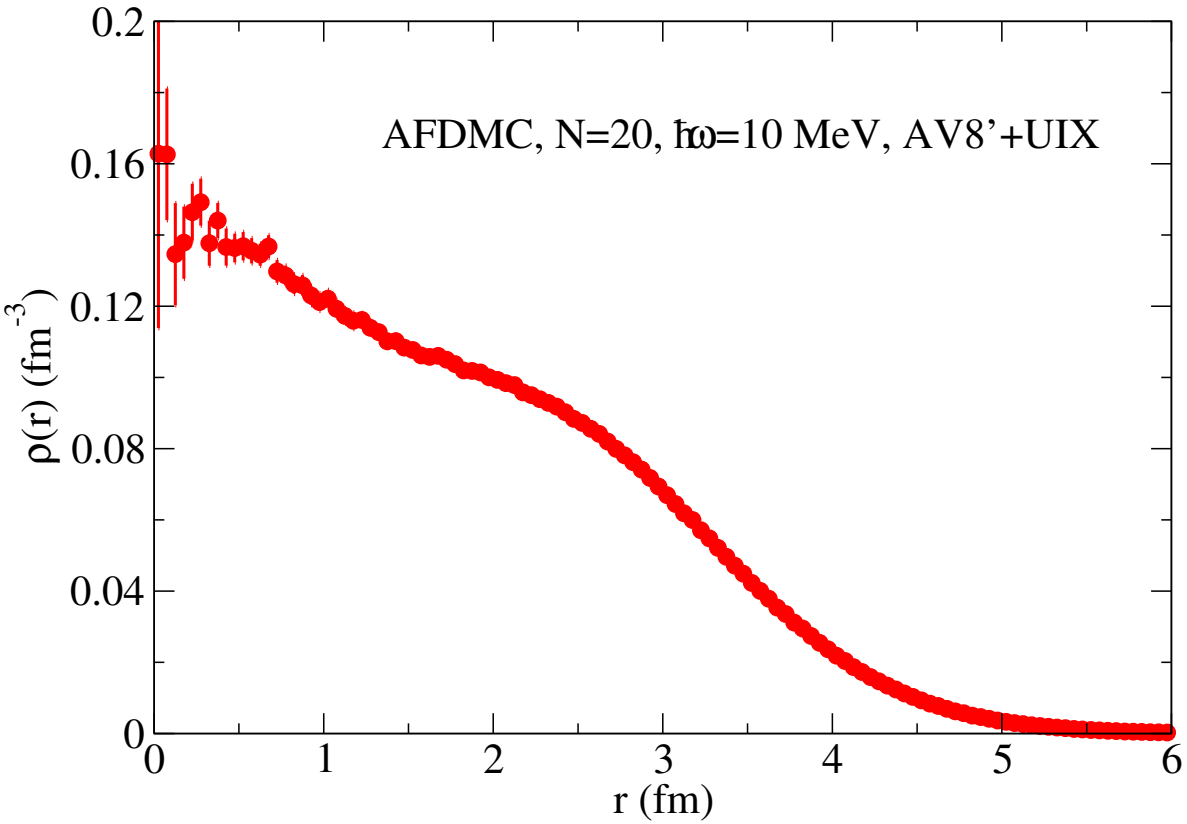


Zhao, Gandolfi, PRC 94, 054005 (2016)

Neutron drops - radii

Note: tune V_{ext} or N to have central density about 0.16(2) fm^{-3}.

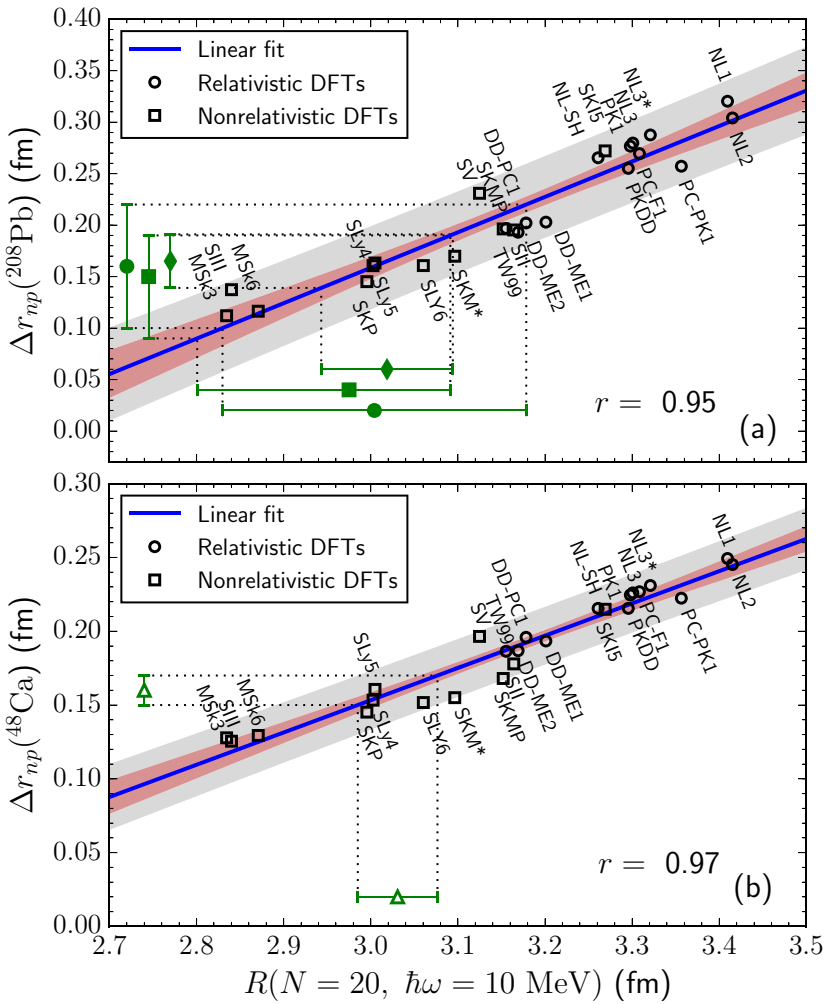
For example, this is given by putting 20 neutrons in an external trap with $\hbar\omega$=10 MeV:



Rms radius: $\sqrt{< r^2 >} = 3.14(1)$ fm

Neutron drops radii and skin

Correlation between neutron drops radii and the skin thickness of ^{208}Pb and ^{48}Ca from relativistic mean field:

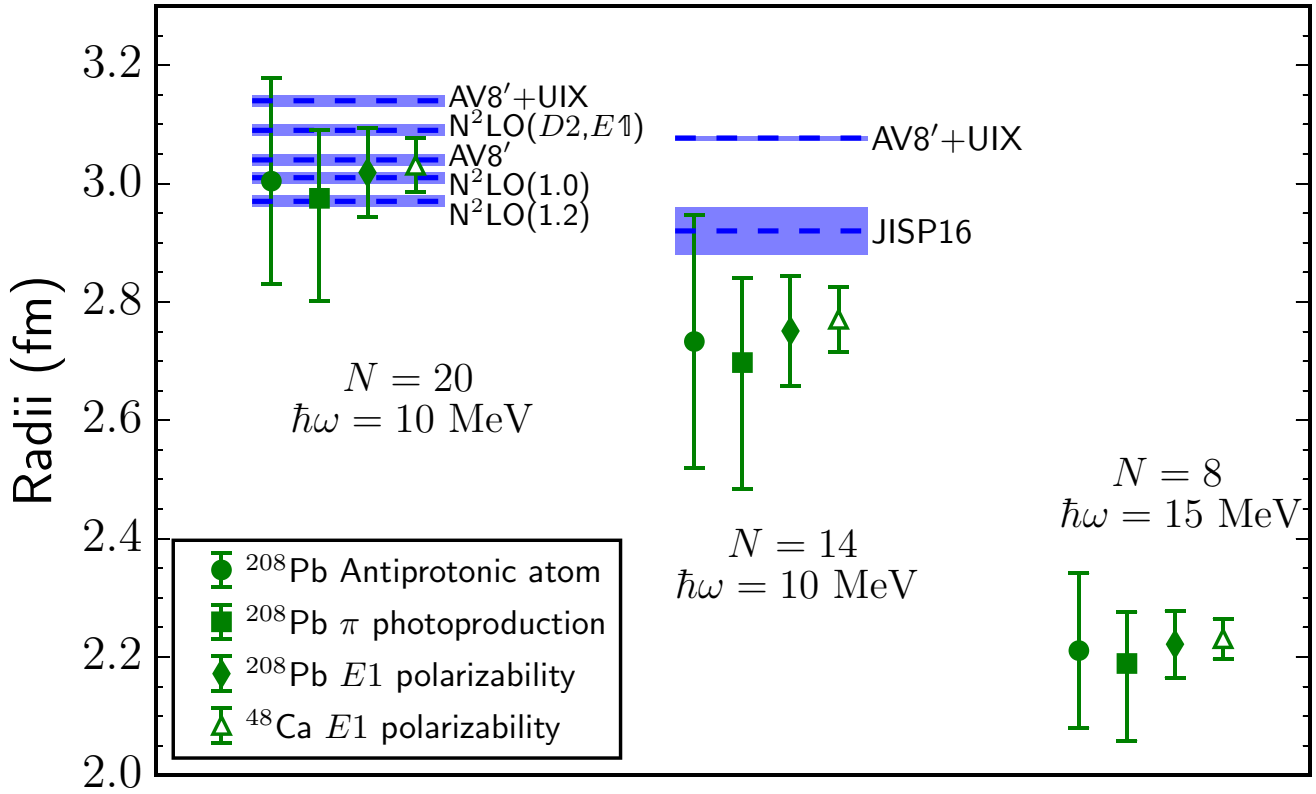


Zhao, Gandolfi, PRC 94, 054005 (2016)

Green points: antiprotonic atoms, pion photoproduction, electric dipole polarizability

Neutron drops

Radii: AFDMC calculations with various Hamiltonians, compared to what might be extracted from experiments:

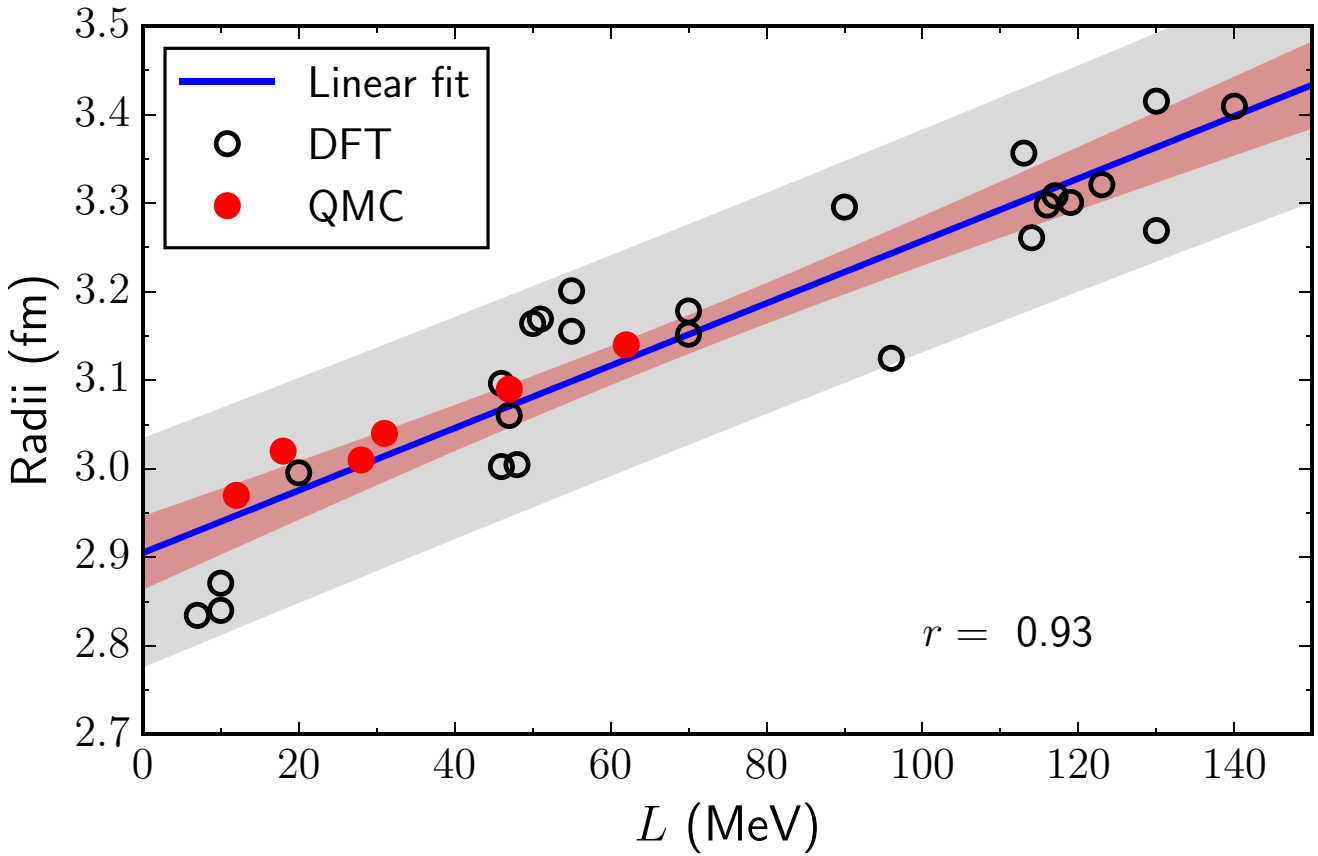


Zhao, Gandolfi, PRC 94, 054005 (2016)

Note, $N = 14$ has central density of about 0.12 fm^{-3}, N=8 we don't know yet...

Neutron drops

Radius of 20 neutrons in a $\hbar\omega = 10$ MeV harmonic trap as a function of L (from the EOS)



Zhao, Gandolfi, PRC 94, 054005 (2016)

Conclusions

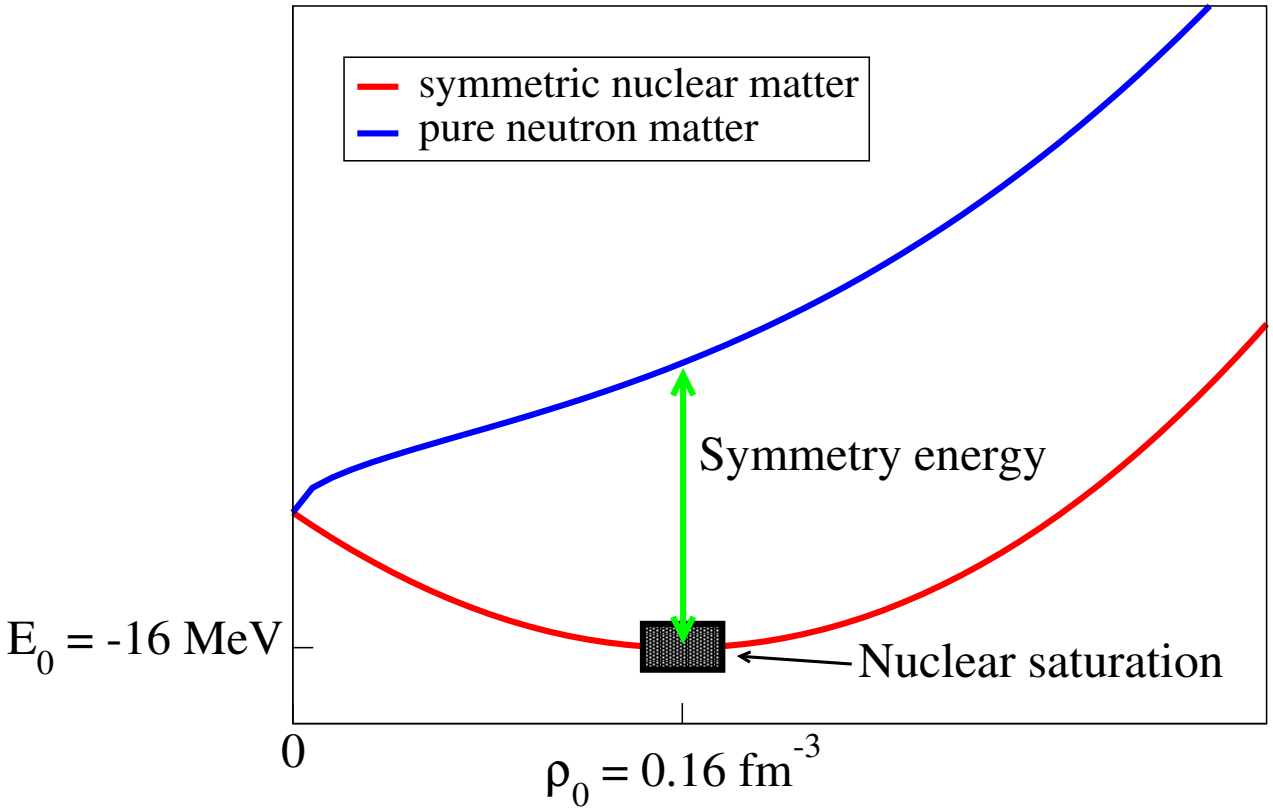
Neutron drops can provide new constraints to skin thickness of nuclei and symmetry energy:

- Using different density functionals we can find correlations between different observables.
- Neutron drops radii and skin of nuclei are correlated.
- Microscopic calculations can provide strong constraints on neutron drops radii.
- Neutron drops radii and symmetry energy (and slope) are correlated. Both at the DFT level, but also from microscopic calculations.

Thanks for the attention

Extra slides

What is the Symmetry energy?



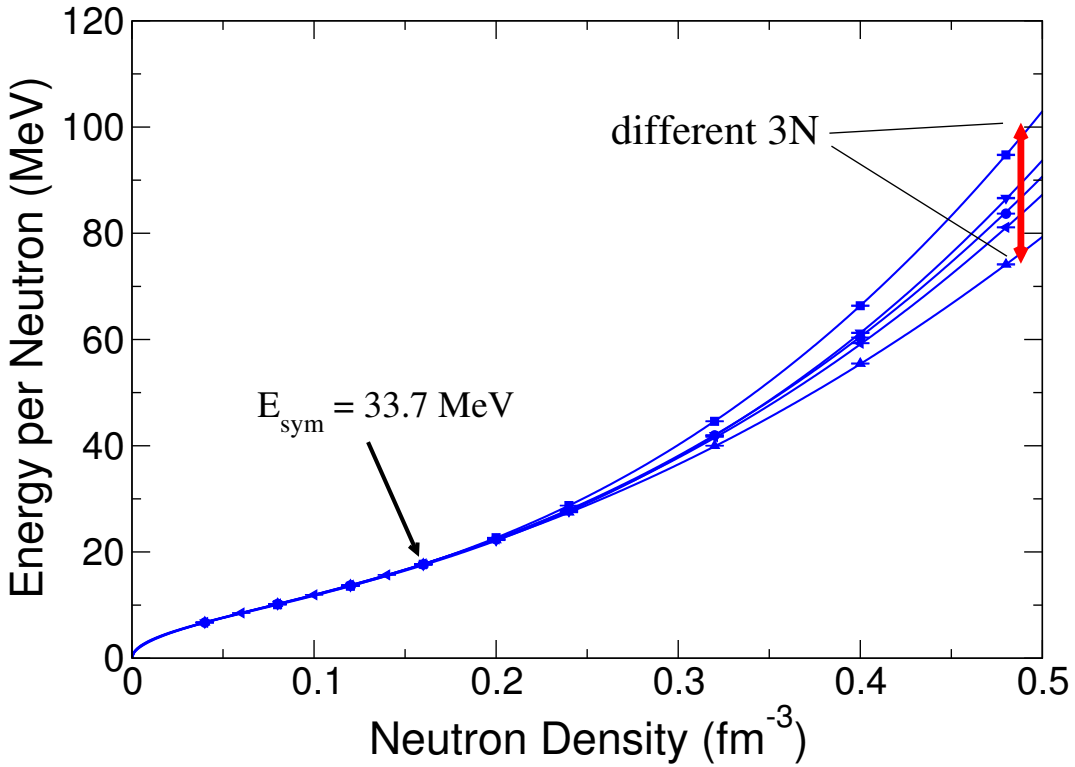
Assumption from experiments:

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

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

Neutron matter

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

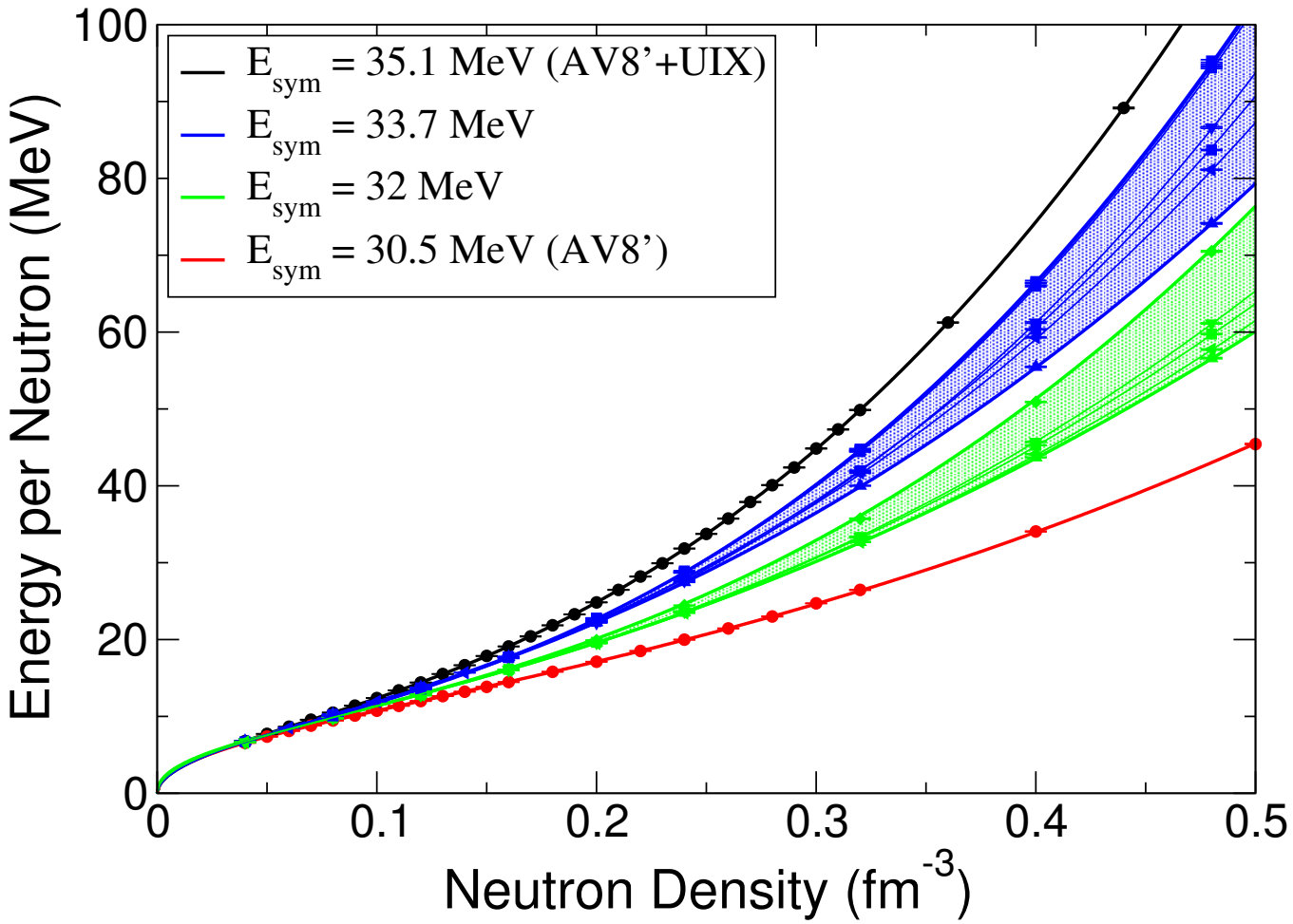


different 3N:

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

Neutron matter and symmetry energy

We then try to change the neutron matter energy at saturation:

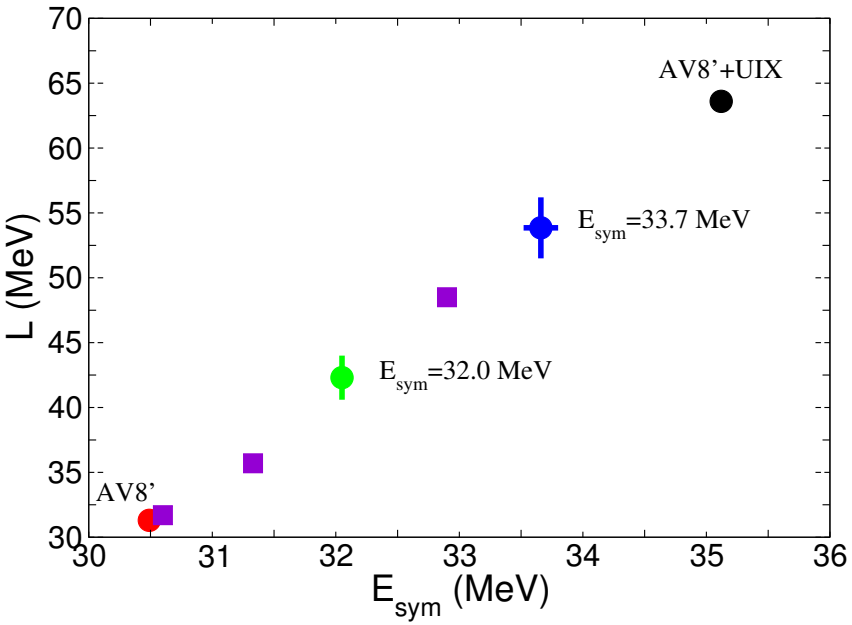


Gandolfi, Carlson, Reddy, PRC (2012).

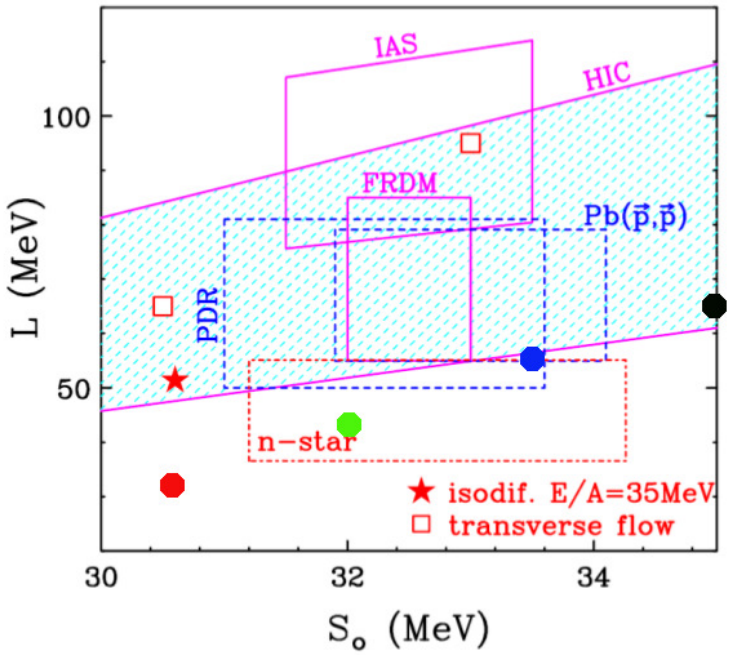
Neutron matter and symmetry energy

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)

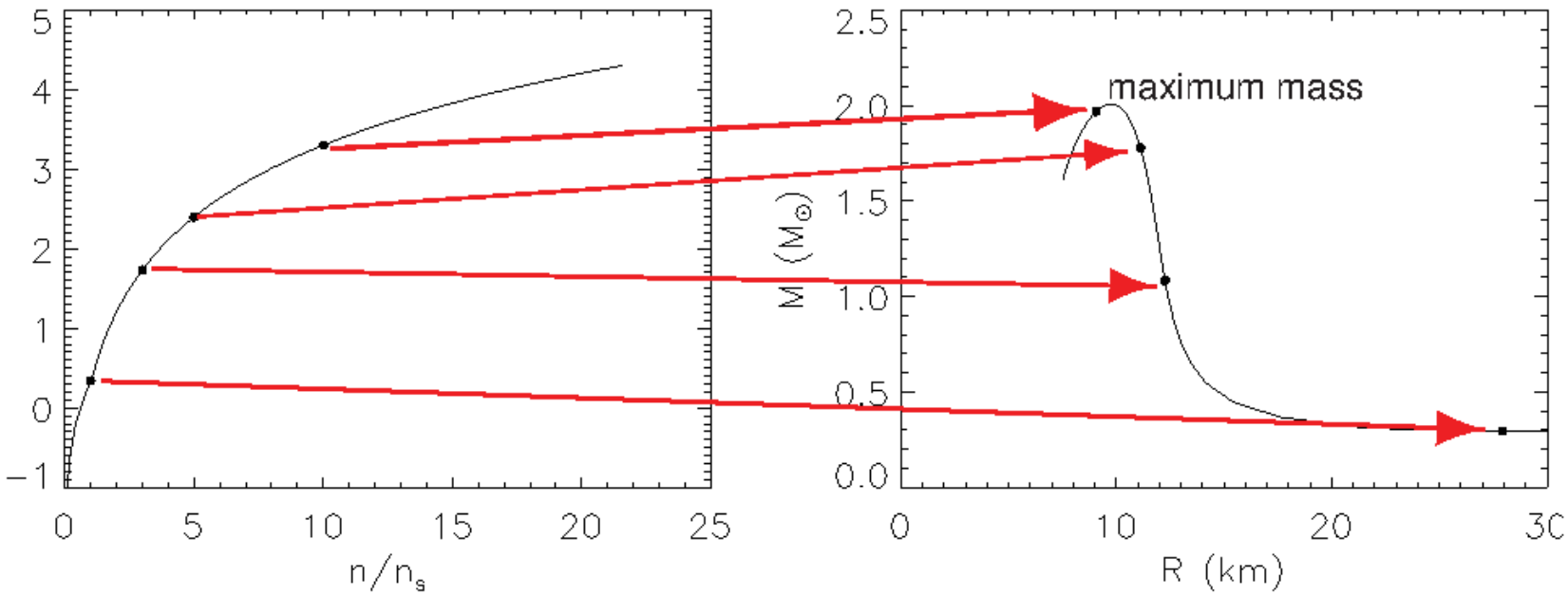
Very weak dependence to the model of 3N force for a given E_{sym}.
Knowing E_{sym} or L useful to constrain 3N! (within this model...)

Neutron matter and neutron star structure

TOV equations:

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

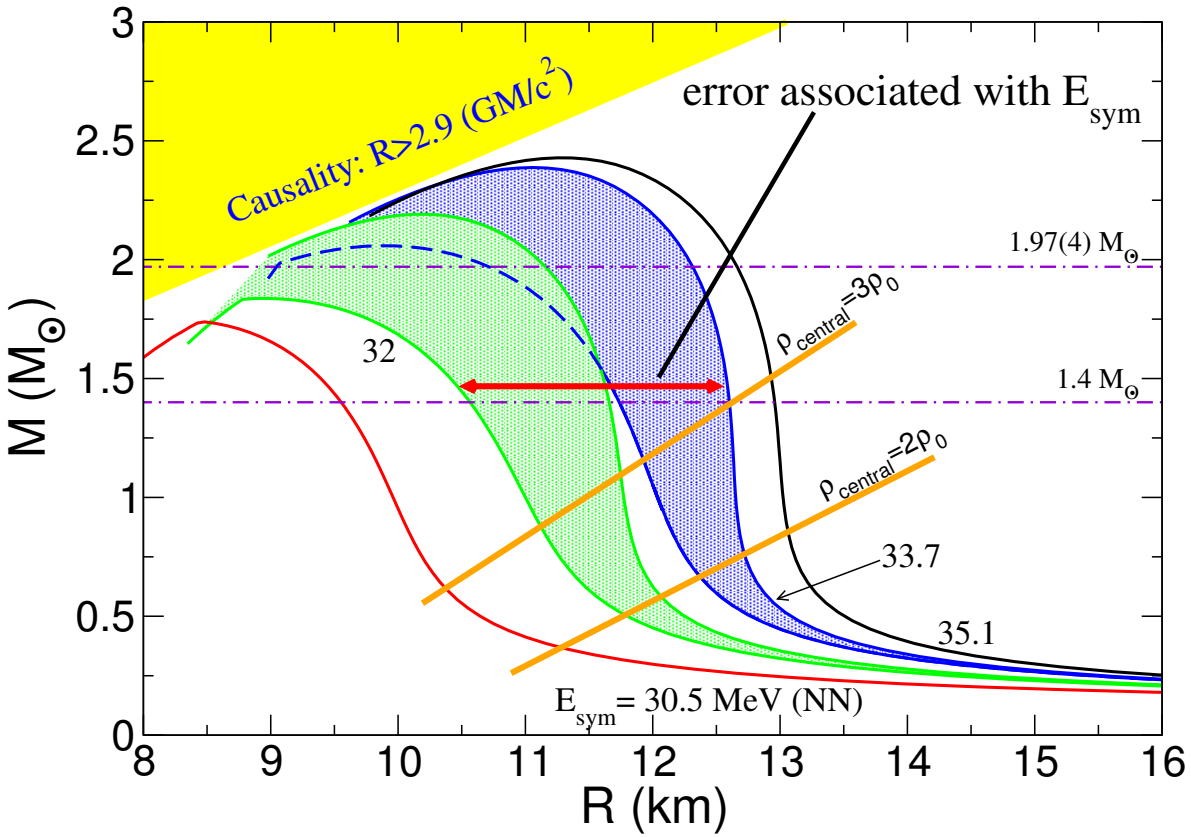
$$\frac{dm(r)}{dr} = 4\pi\epsilon r^2,$$



J. Lattimer

Neutron star structure

EOS used to solve the TOV equations.

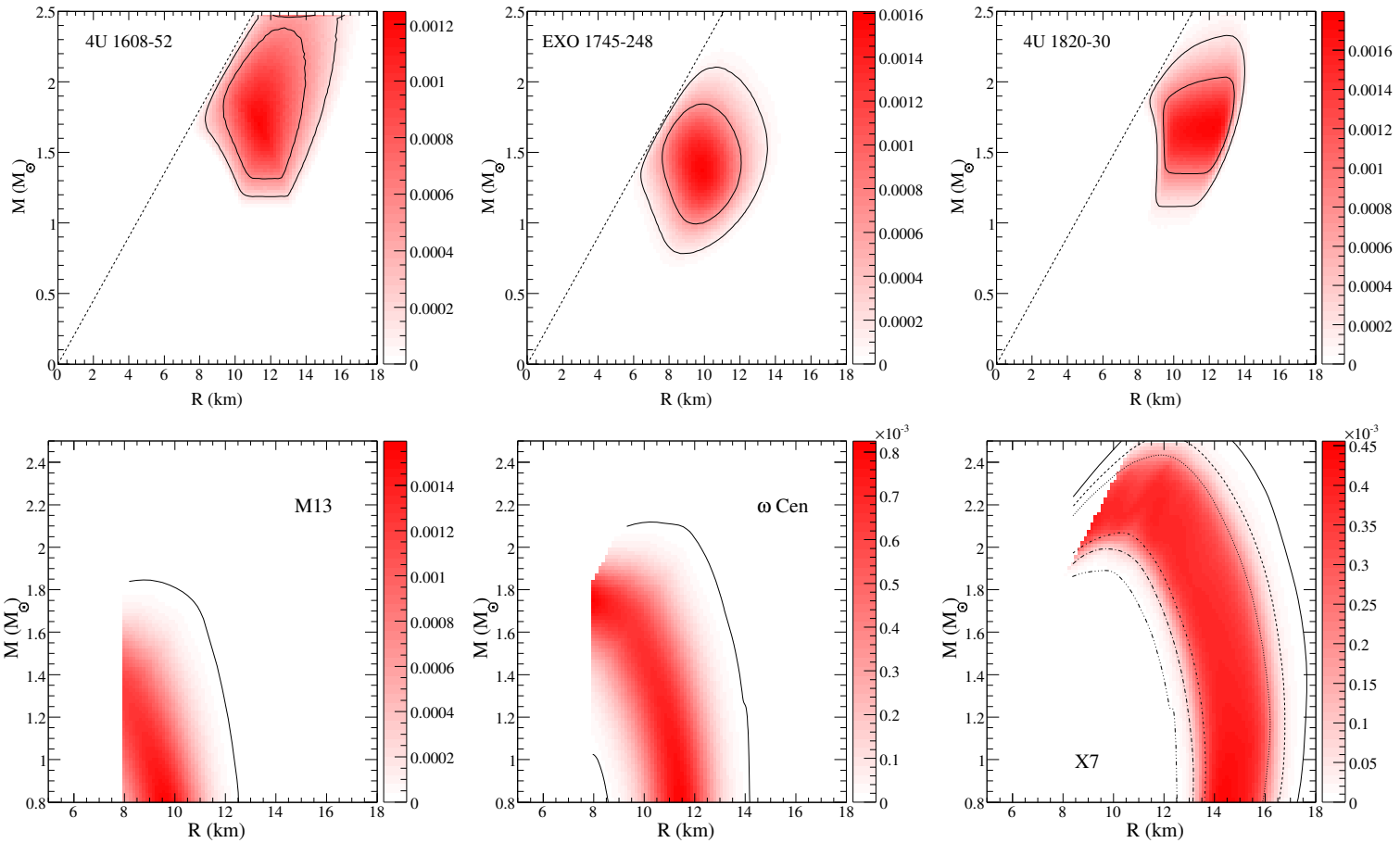


Gandolfi, Carlson, Reddy, PRC (2012).

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

Observations of the mass-radius relation are becoming available:



Steiner, Lattimer, Brown, ApJ (2010)

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

Neutron star matter

Neutron star matter model:

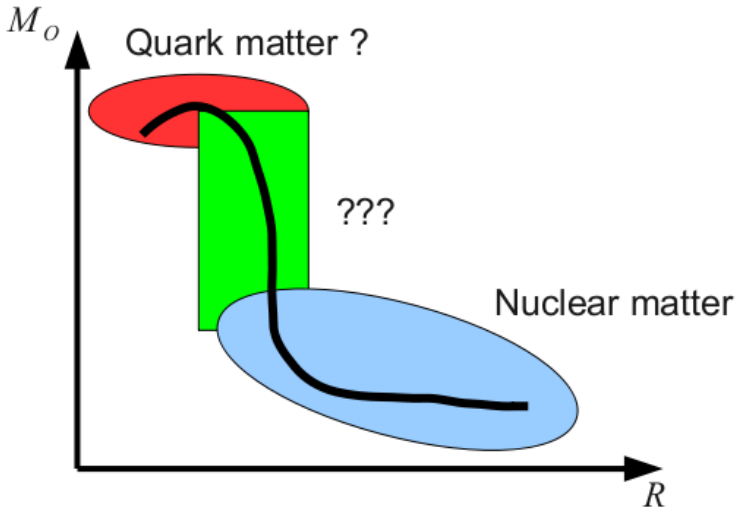
$$E_{NSM} = a\left(\frac{\rho}{\rho_0}\right)^{\alpha} + b\left(\frac{\rho}{\rho_0}\right)^{\beta}, \quad \rho < \rho_t$$

(form suggested by QMC simulations),

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

i) two polytropes

ii) polytrope+quark matter model

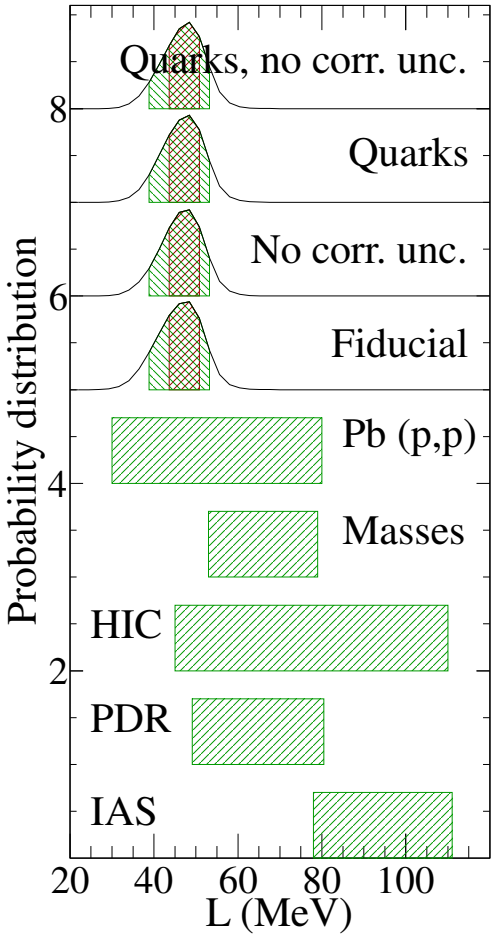


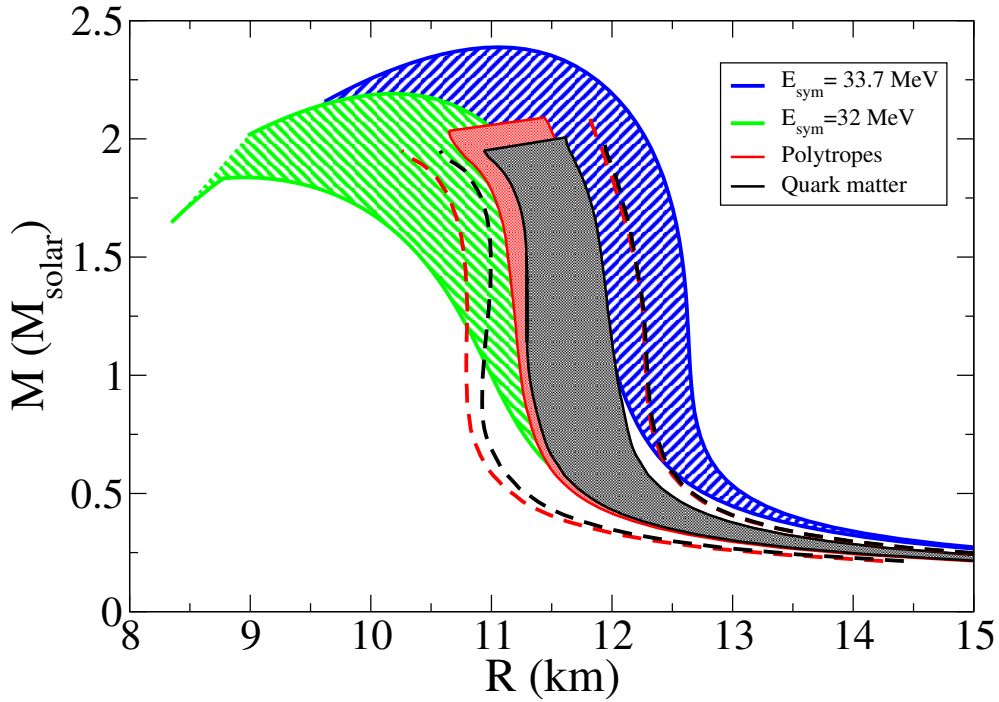
Neutron star radius sensitive to the EOS at nuclear densities!

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).

Uncertainties on observations not included!

Scattering data and neutron matter

Two neutrons have

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

that correspond to

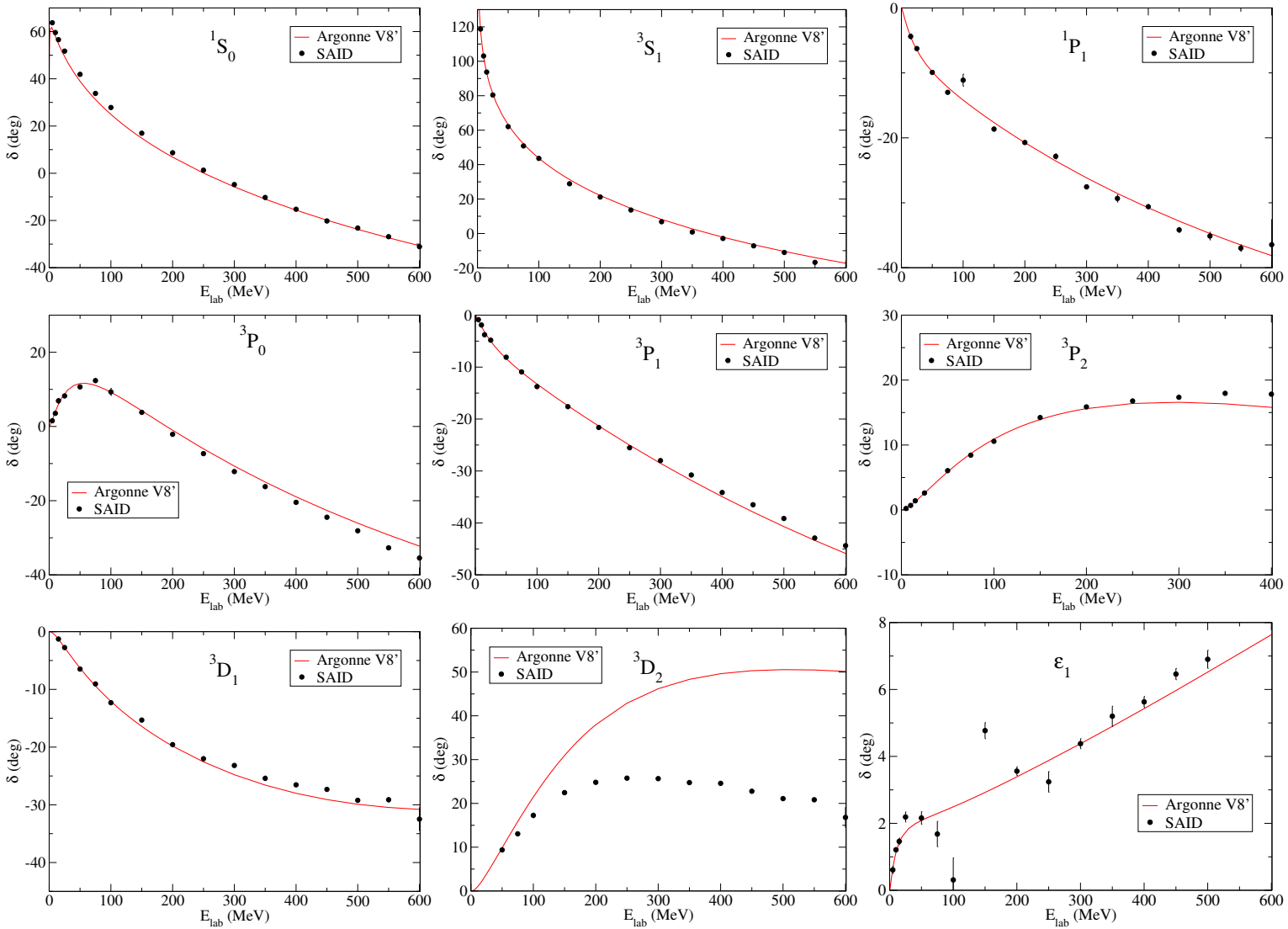
$$k_F \rightarrow \rho \approx (E_{lab}\, m/2)^{3/2}/2\pi^2\,.$$

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}

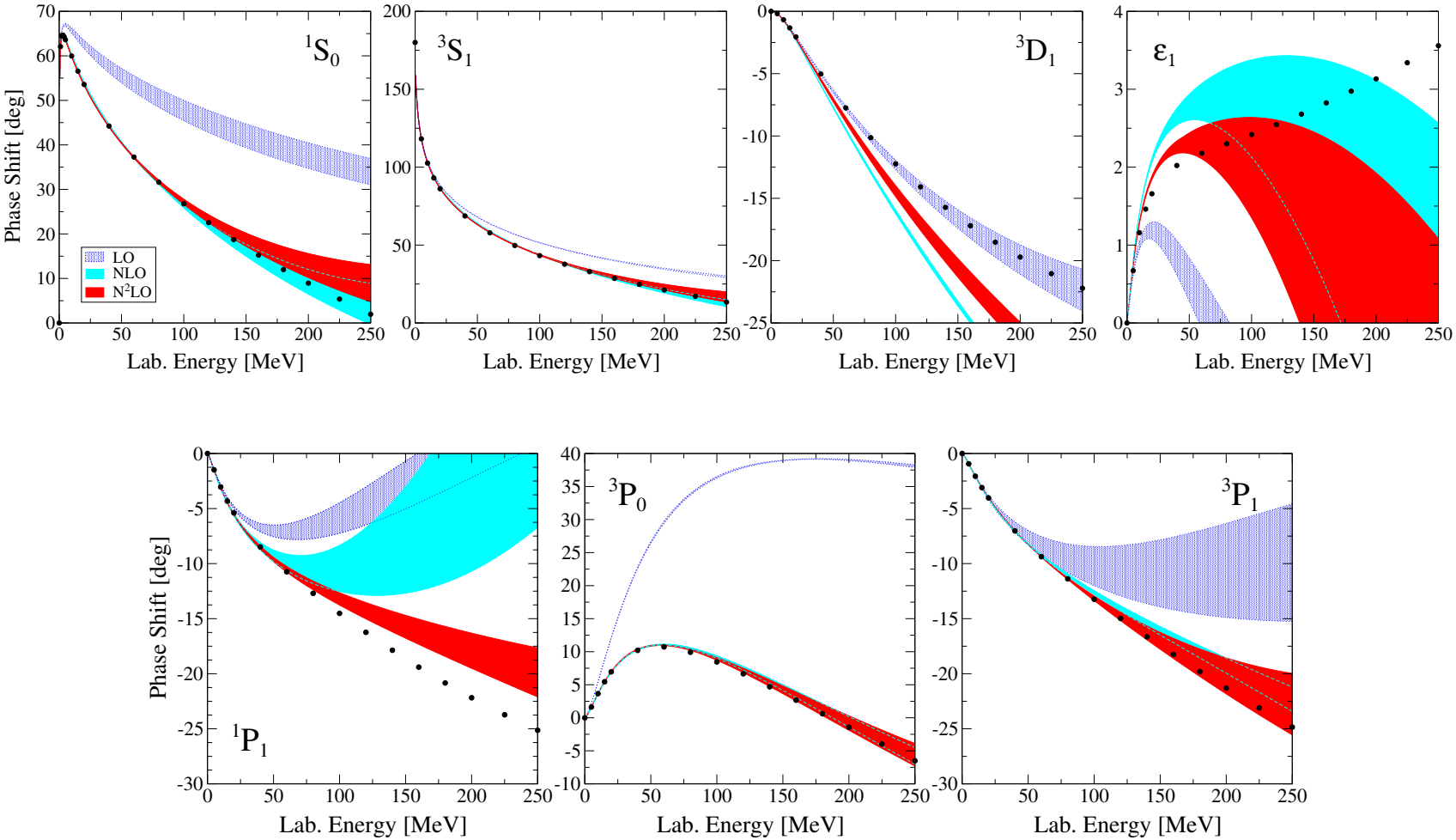
Phase shifts, AV8'



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

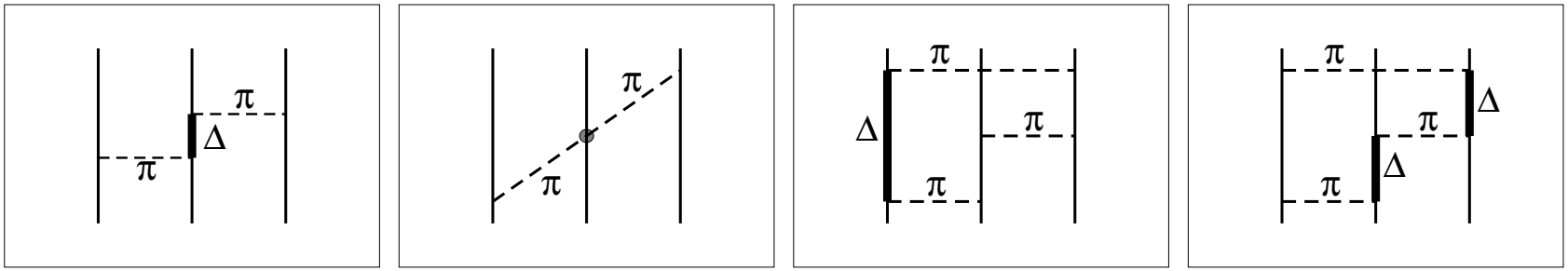
Nuclear Hamiltonian

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



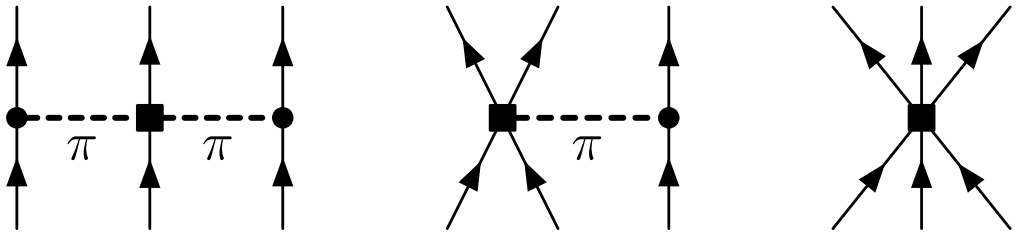
Three-body forces

Urbana–Illinois V_{ijk} models processes like



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

Chiral forces at N^{2}LO:



c_1, c_3, c_4 c_D c_E

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

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

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:

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

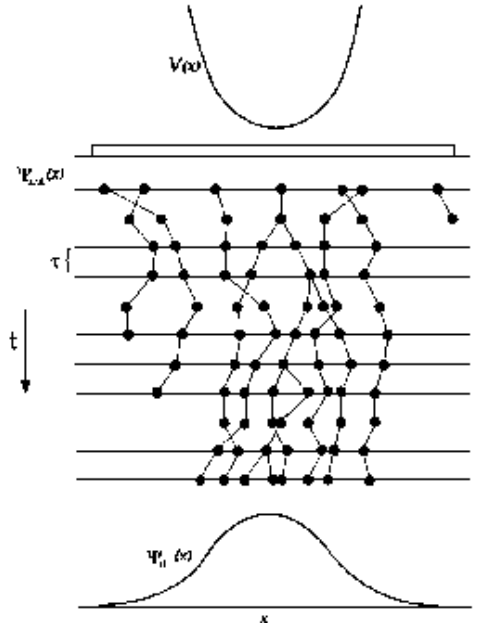
Algorithm for each time-step:

- 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:

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

where the new operators are

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

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

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

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

Three-body forces

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

For example:

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

The above form can be included in the AFDMC propagator.

Three-body forces

$$V_a^{2\pi,PW} = A_a^{2\pi,PW} \sum_{i<j<k} \sum_{cyc} \{\vec{\tau}_i \cdot \vec{\tau}_k, \vec{\tau}_j \cdot \vec{\tau}_k\} \{\sigma_i^\alpha \sigma_k^\gamma, \sigma_k^\mu \sigma_j^\beta\} \mathcal{X}_{i\alpha k\gamma} \mathcal{X}_{k\mu j\beta}$$

$$= 4A_a^{2\pi,PW} \sum_{i<j} \vec{\tau}_i \cdot \vec{\tau}_j \sigma_i^\alpha \sigma_j^\beta \sum_{k\neq i,j} \mathcal{X}_{i\alpha k\gamma} \mathcal{X}_{k\gamma j\beta} \,, \tag{1}$$

$$V_c^{2\pi,PW} = A_c^{2\pi,PW} \sum_{i<j<k} \sum_{cyc} [\vec{\tau}_i \cdot \vec{\tau}_k, \vec{\tau}_j \cdot \vec{\tau}_k][\sigma_i^\alpha \sigma_k^\gamma, \sigma_k^\mu \sigma_j^\beta] \mathcal{X}_{i\alpha k\gamma} \mathcal{X}_{k\mu j\beta}$$

$$= -4A_c^{2\pi,PW} \sum_{i<j<k} \sum_{cyc} \tau_i^\eta \tau_j^\xi \tau_k^\phi \epsilon_{\eta\xi\phi} \sigma_i^\alpha \sigma_j^\beta \sigma_k^\nu \epsilon_{\nu\gamma\mu} \mathcal{X}_{i\alpha k\gamma} \mathcal{X}_{k\mu j\beta} \tag{2}$$

$$= A_c^{2\pi,PW} \sum_{i<j<k} \sum_{cyc} [\vec{\tau}_i \cdot \vec{\tau}_k, \vec{\tau}_j \cdot \vec{\tau}_k][\sigma_i^\alpha \sigma_k^\gamma, \sigma_k^\mu \sigma_j^\beta] \left(X_{i\alpha k\gamma} - \delta_{\alpha\gamma} \frac{4\pi}{m_\pi^3} \Delta(r_{ik}) \right) \left(X_{k\mu j\beta} - \delta_{\mu\beta} \frac{4\pi}{m_\pi^3} \Delta(r_{kj}) \right) \tag{3}$$

$$= V_c^{\Delta\Delta} + V_c^{\Delta\delta} + V_c^{\delta\delta} \tag{4}$$

$$V^{2\pi,SW} = A^{2\pi,SW} \sum_{i<j<k} \sum_{cyc} \mathcal{Z}_{ik\alpha} \mathcal{Z}_{jk\alpha} \sigma_i^\alpha \sigma_j^\beta \vec{\tau}_i \cdot \vec{\tau}_j$$

$$= A^{2\pi,SW} \sum_{i<j} \sigma_i^\alpha \sigma_j^\beta \vec{\tau}_i \cdot \vec{\tau}_j \sum_{k\neq i,j} \mathcal{Z}_{ik\alpha} \mathcal{Z}_{jk\alpha} \tag{5}$$

$$V_D = A_D \sum_{i<j} \sigma_i^\alpha \sigma_j^\beta \vec{\tau}_i \cdot \vec{\tau}_j \sum_{k\neq i,j} \mathcal{X}_{i\alpha j\beta} [\Delta(r_{ik}) + \Delta(r_{jk})] \tag{6}$$

$$V_E = A_E \sum_{i<j} \vec{\tau}_i \cdot \vec{\tau}_j \sum_{k\neq i,j} \Delta(r_{ik}) \Delta(r_{jk}) \tag{7}$$

Three-body forces

$$H' = H - V_c^{2\pi,PW} + \alpha_1 V_a^{2\pi,PW} + \alpha_2 V_D + \alpha_3 V_E \,. \tag{8}$$

The Hamiltonian H' can be exactly included in the AFDMC propagation. The three constants α_i are adjusted in order to have:

$$\begin{aligned} \langle V_c^{\Delta\Delta} \rangle &\approx \langle \alpha_1 V_a^{2\pi,PW} \rangle \\ \langle V_c^{\Delta\delta} \rangle &\approx \langle \alpha_2 V_D \rangle \\ \langle V_c^{\delta\delta} \rangle &\approx \langle \alpha_3 V_E \rangle \end{aligned} \tag{9}$$

Once the ground state Ψ of H' is calculated with AFDMC as explained above, the expectation value of the Hamiltonian H is given by

$$\begin{aligned} \langle H \rangle &= \langle \Psi | H' | \Psi \rangle + \langle \Psi | H - H' | \Psi \rangle \\ &= \langle \Psi | H' | \Psi \rangle + \langle \Psi | V_c^{2\pi,PW} - \alpha_1 V_a^{2\pi,PW} - \alpha_2 V_D - \alpha_3 V_E | \Psi \rangle \end{aligned} \tag{10}$$

Variational wave function

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

$\rightarrow$ 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.

Variational wave function

$$\langle RS|\Psi_V\rangle = \langle RS|\Big[\prod_{i<j} f^c(r_{ij})\Big]\Big[1+\sum_{i<j} F_{ij} + \sum_{i<j<k} F_{ijk}\Big]|\Phi_{JM}\rangle\,,$$

$$\langle RS|\Phi_{JM}\rangle = \sum_n k_n \Big[\sum D\{\phi_\alpha(r_i,s_i)\}\Big]_{JM}\,,$$

$$\phi_\alpha(r_i,s_i) = \Phi_{nlj}(r_i)\left[Y_{lm_l}(\hat{r}_i)\xi_{sm_s}(s_i)\right]_{jm_j}\,,$$

In particular, we included orbitals in $1\mathrm{S}_{1/2}$, $1\mathrm{P}_{3/2}$, $1\mathrm{P}_{1/2}$, $1\mathrm{D}_{5/2}$, $2\mathrm{S}_{1/2}$, and $1\mathrm{D}_{3/2}$.

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.

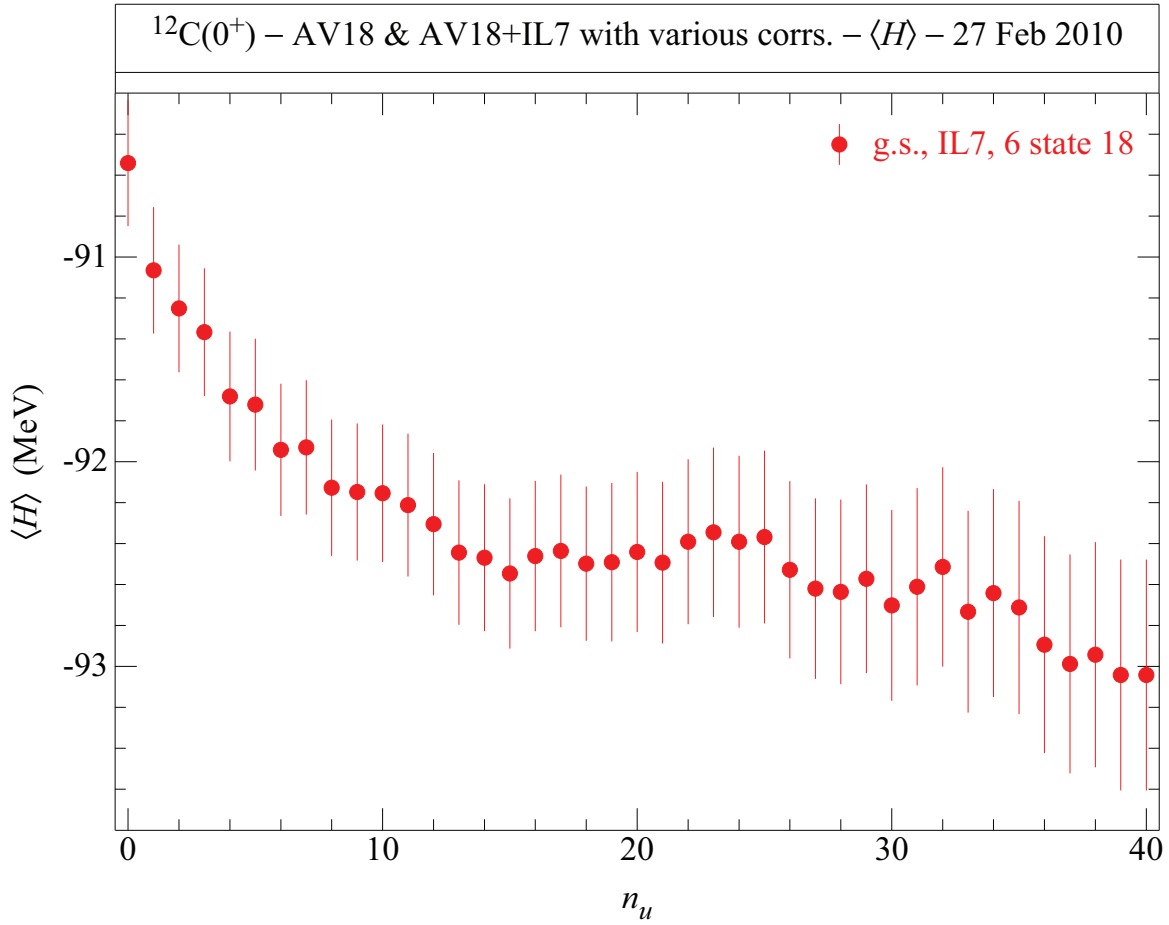
If Ψ is complex:

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

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

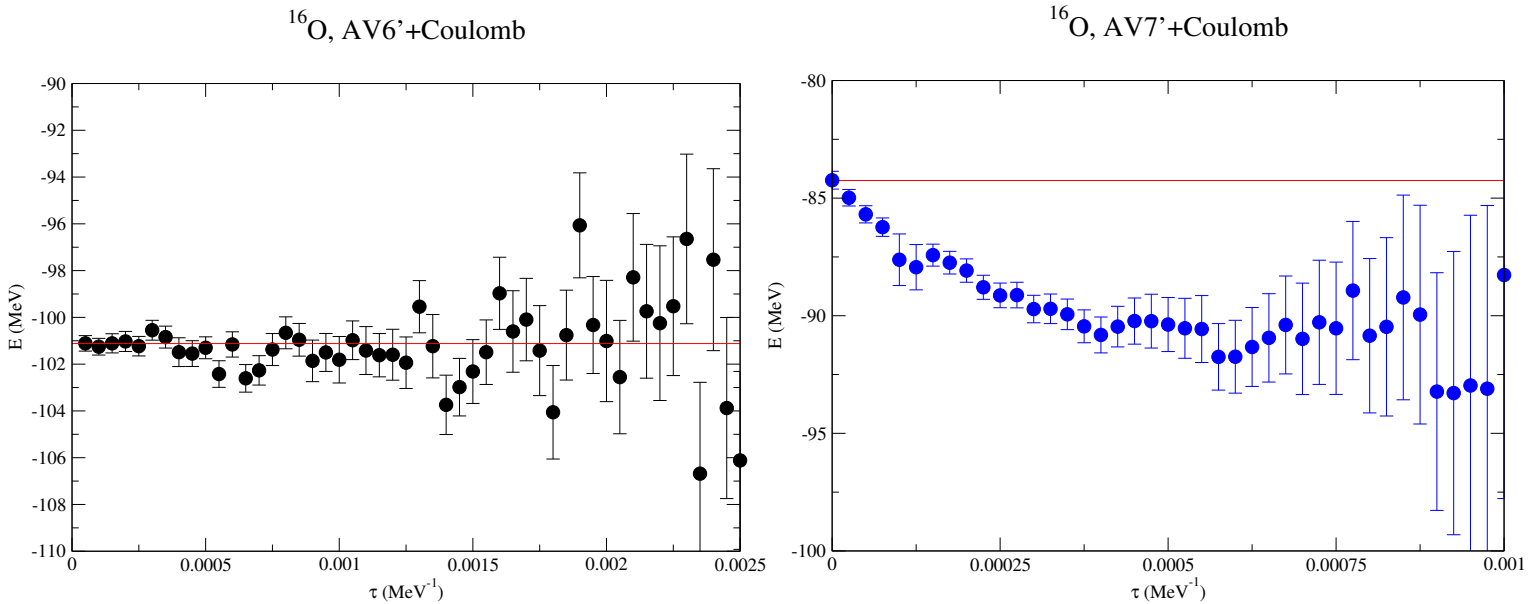
GFMC unconstrained-path propagation:



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.