Quantum Monte Carlo calculations of nuclei and nuclear matter

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Los Alamos NATIONAL LABORATORY EST. 1943

NUCLEI Nuclear Computational Low-Energy Initiative

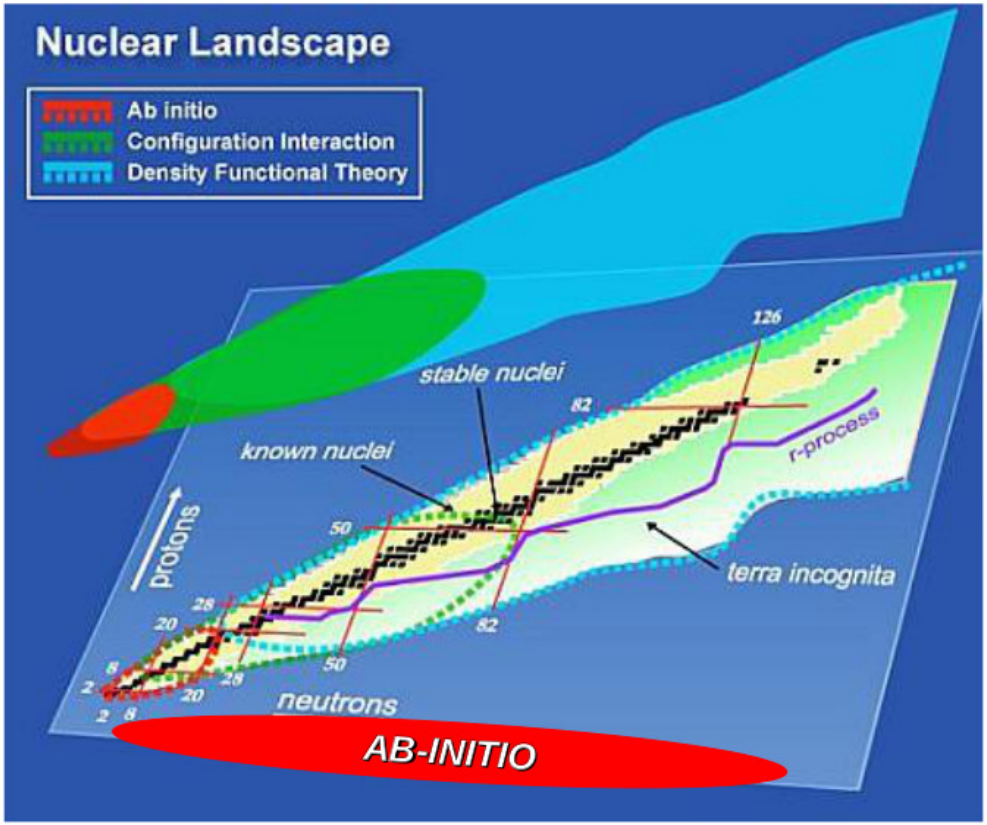
U.S. DEPARTMENT OF ENERGY

www.computingnuclei.org

NERSC National Energy Research Scientific Computing Center

U.S. DEPARTMENT OF ENERGY INCITE LEADERSHIP COMPUTING

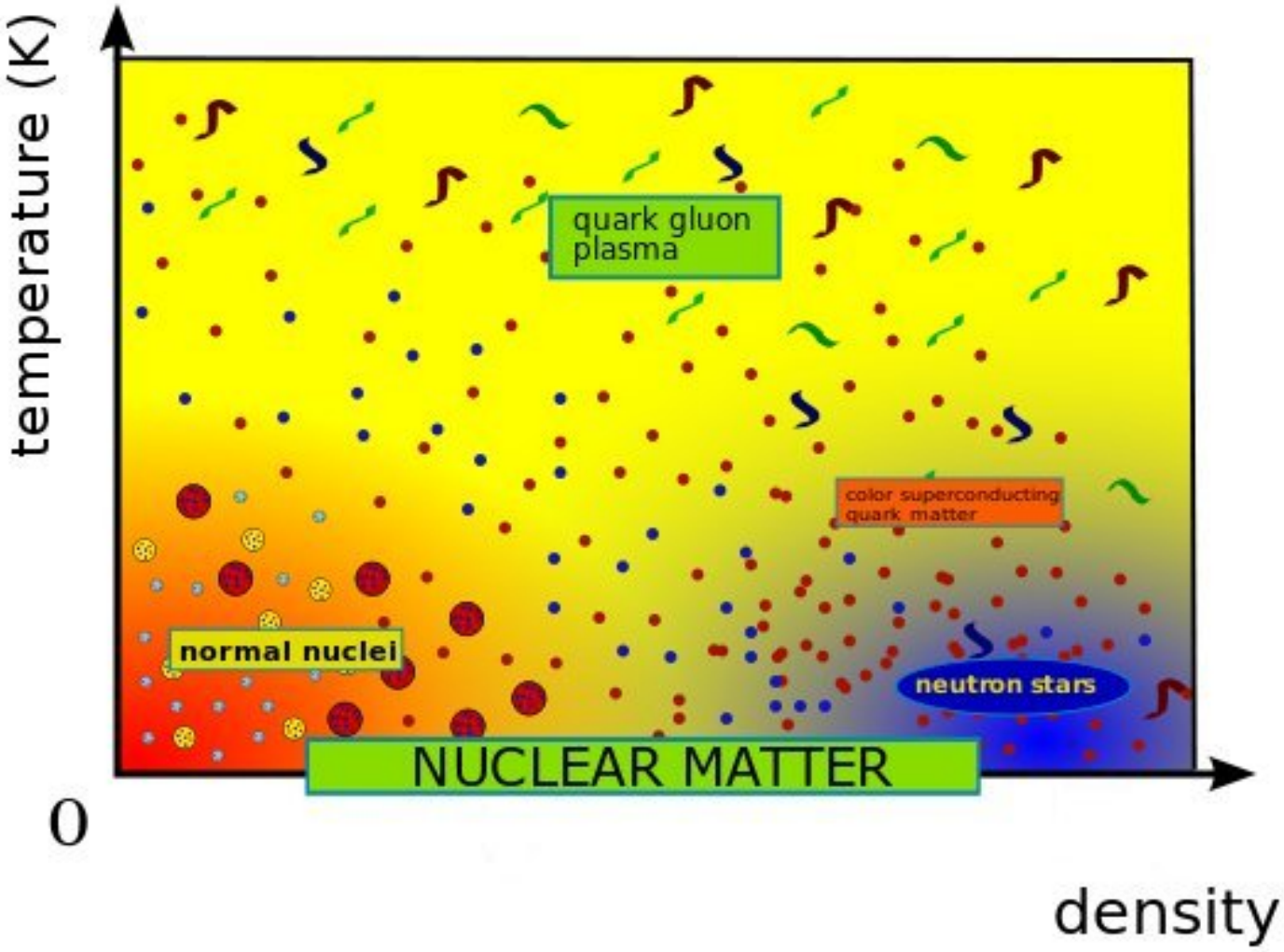
Nuclei



www.unedf.org

Large nuclei and inhomogeneous matter are mainly investigated using density functional theory. Ab-initio methods for big systems are needed to validate DFT.

Homogeneous neutron matter



Outline

- The model and the method
- Nuclei
- Equation of state of neutron matter
- Symmetry energy and neutron stars
- Nuclear matter
- Electro-weak interactions in ^{12}C
- 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:

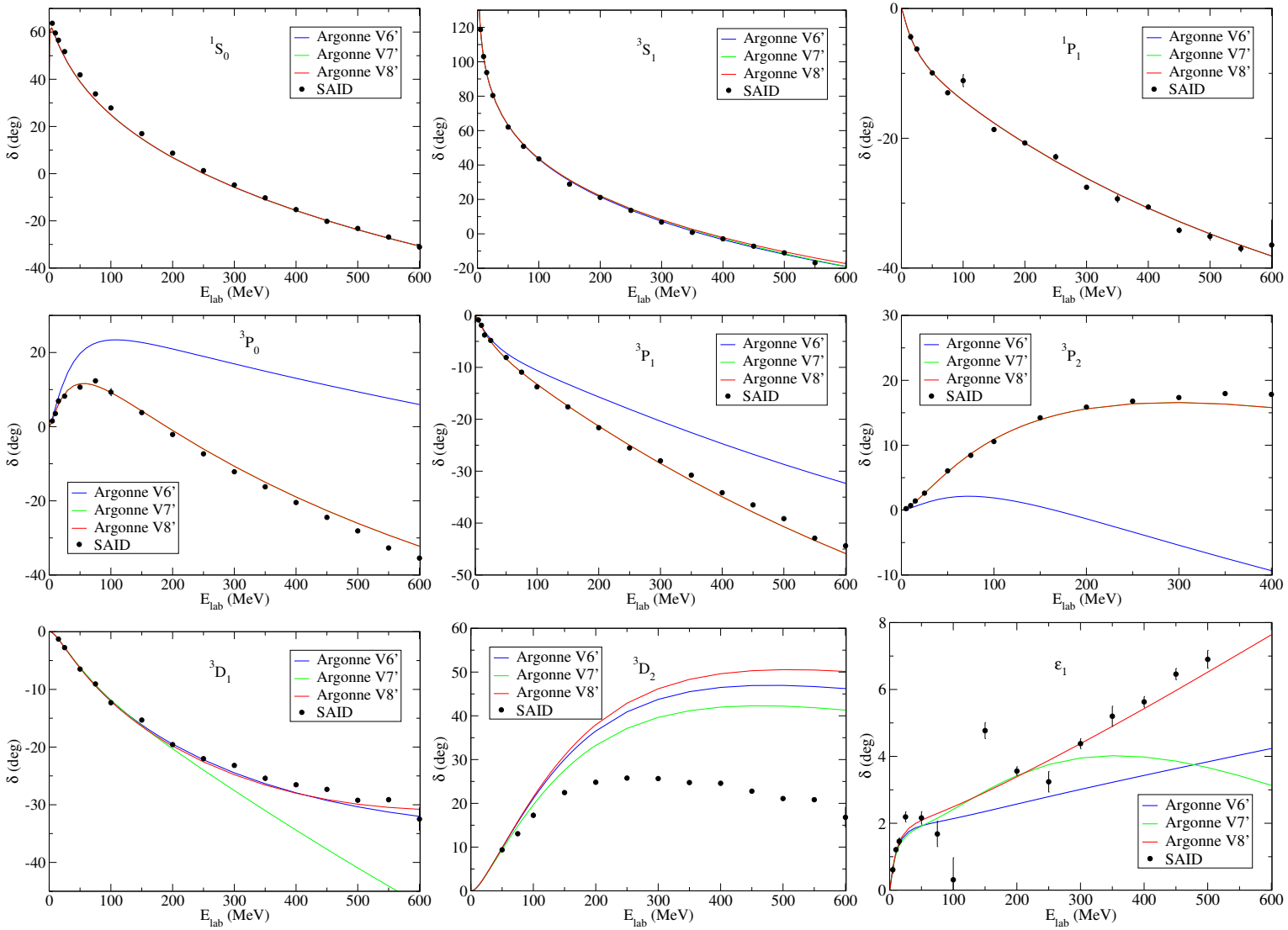
$$v_{ij} = \sum O_{ij}^{p=1,8} v^p(r_{ij}), \quad O_{ij}^p = (1, \vec{\sigma}_i \cdot \vec{\sigma}_j, S_{ij}, \vec{L}_{ij} \cdot \vec{S}_{ij}) \times (1, \vec{\tau}_i \cdot \vec{\tau}_j)$$

Argonne AV6' (no LS), AV7' (no LS-τ), AV8'.

Local chiral forces up to N^{2}LO has the same spin/isospin operatorial structure than AV7' - Gezerlis, Tews, et al. PRL (2013).

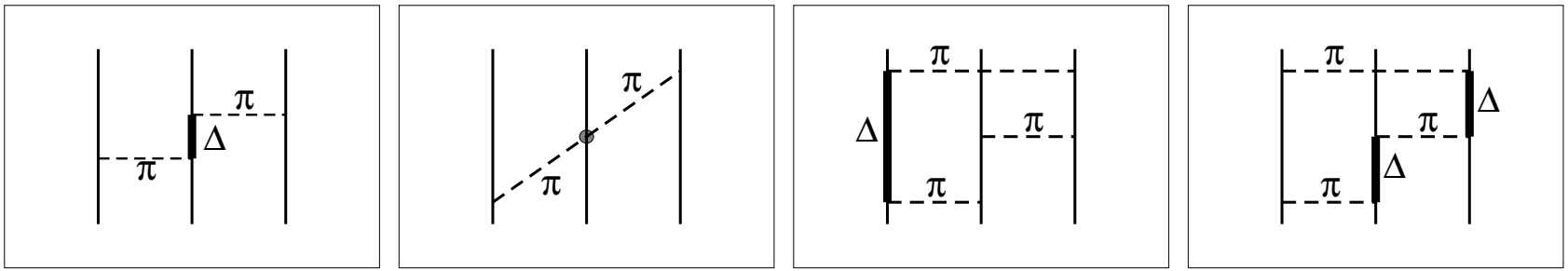
Nuclear Hamiltonian

Phase shifts, Argonne AV6', AV7' and AV8'



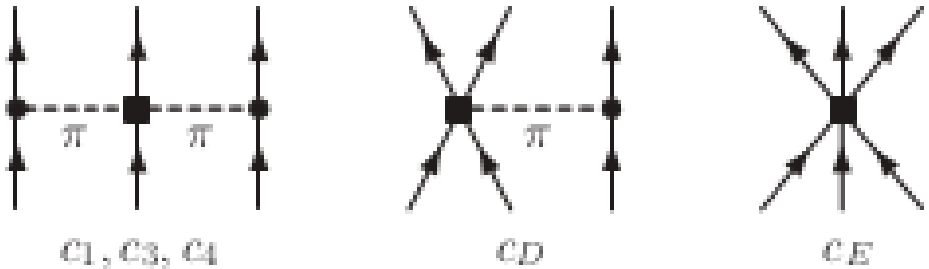
Three-body forces

Urbana–Illinois V_{ijk} models processes like



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

Chiral forces at N^{2}LO:



Quantum Monte Carlo

We want to solve:

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

In the limit of $t \to \infty$ it approaches to the lowest energy eigenstate (not orthogonal to $\psi(R,0)$).

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.

For a given (local) Hamiltonian, these methods solve the ground–state within a systematic uncertainty of **1–2%** in a **non-perturbative way.**

Quantum Monte Carlo

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, local) 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!

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 deal to large 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.

Simple wave function:

$$\Psi(R) = \prod_{i<j} f(r_{ij}) \Phi(R,S)$$

good for pure neutron systems, tensor correlations in T=1 are small.

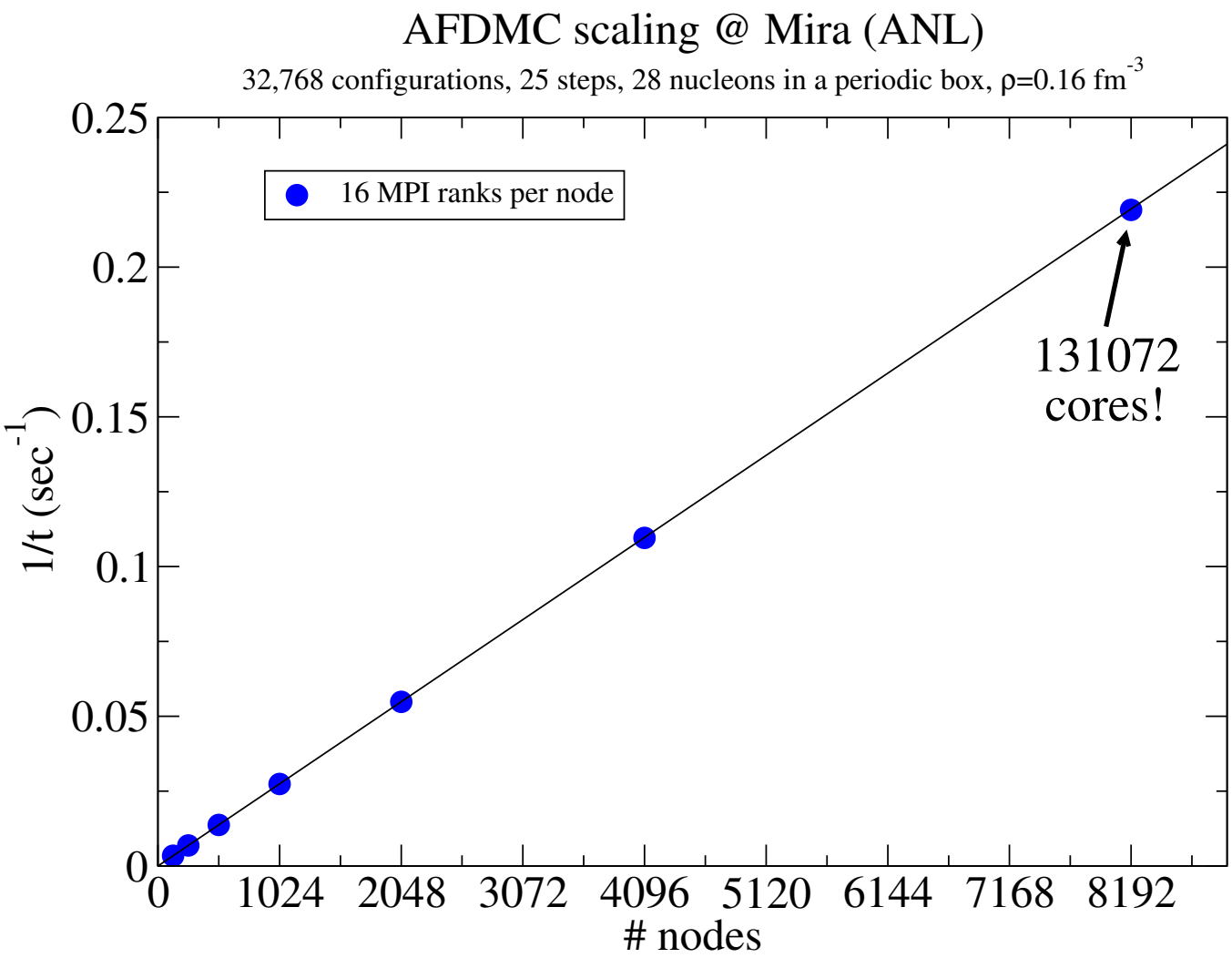
However, the T=0 tensor force is very strong, and it's hard to generate the many-body correlations from the above wave function. Improvement:

$$\Psi(R) = \prod_{i<j} f(r_{ij}) \left[1 + \sum_{i<j} [f_{\sigma\tau}(r_{ij}) \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j \boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_j + f_{t\tau}(r_{ij}) S_{ij}] \right] \Phi(R,S)$$

where $S_{ij} = 3\boldsymbol{\sigma}_i \cdot \hat{r}_{ij} \boldsymbol{\sigma}_j \cdot \hat{r}_{ij} - \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j$.

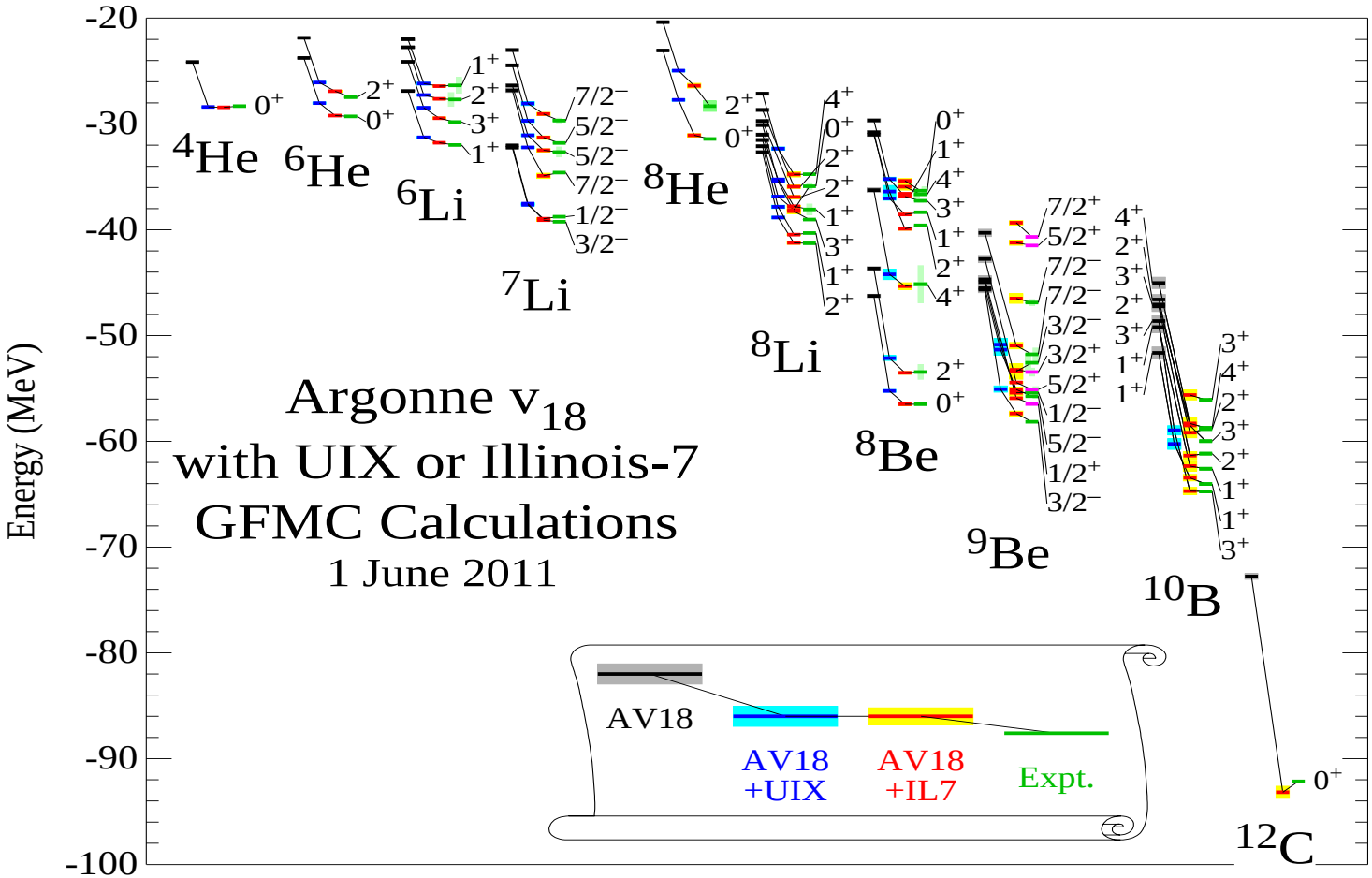
Note: the above wave function is much more computationally demanding, is not as good as GFMC, but its overlap with the ground-state is much higher.

AFDMC efficiency



Note: MPI only so far.

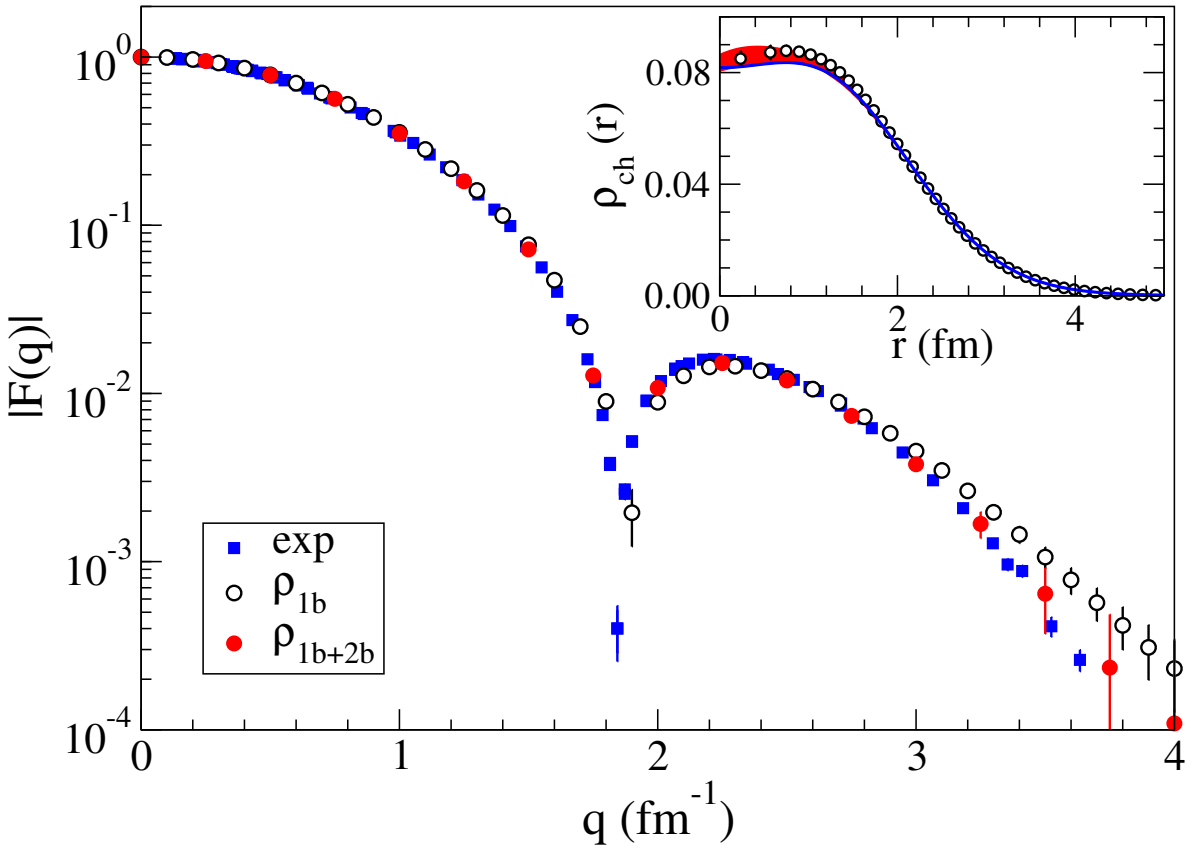
Light nuclei spectrum computed with GFMC



Carlson, Pieper, Wiringa, many papers

Charge form factor of ^{12}C

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



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

Test case: ^{4}He

Preliminary results!

Hamiltonian	AFDMC	GFMC
AV6'	-27.09(3)	-26.85(2)
AV7'	-25.7(2)	-26.2(1)
N^{2}LO (R_0=1.0 fm)	-24.41(3)	-24.56(1)
N^{2}LO (R_0=1.2 fm)	-25.77(2)	-25.75(1)

Binding energies for ^{4}He using different two-body interactions.

talk by Joel Lynn this afternoon

Nuclei

Preliminary results!

	AV6'	AV7'	exp
^{4}He	-27.09(3)	-25.7(2)	-28.295
^{16}O	-115.6(3)	-90.6(4)	-127.619
^{40}Ca	-322(2)	-209(1)	-342.051

Note: Coulomb energy (repulsive) missing in AFDMC.
About 10 to 40% of binding energy missing.

Even more preliminary: ^{16}O binding energy:

	R_0=1.2 fm	R_0=1.0 fm
LO	-1210.1(3)	-269.9(4)
NLO	-87.4(2)	-35.9(7)
N^{2}LO	-116.1(2)	-91.1(3)

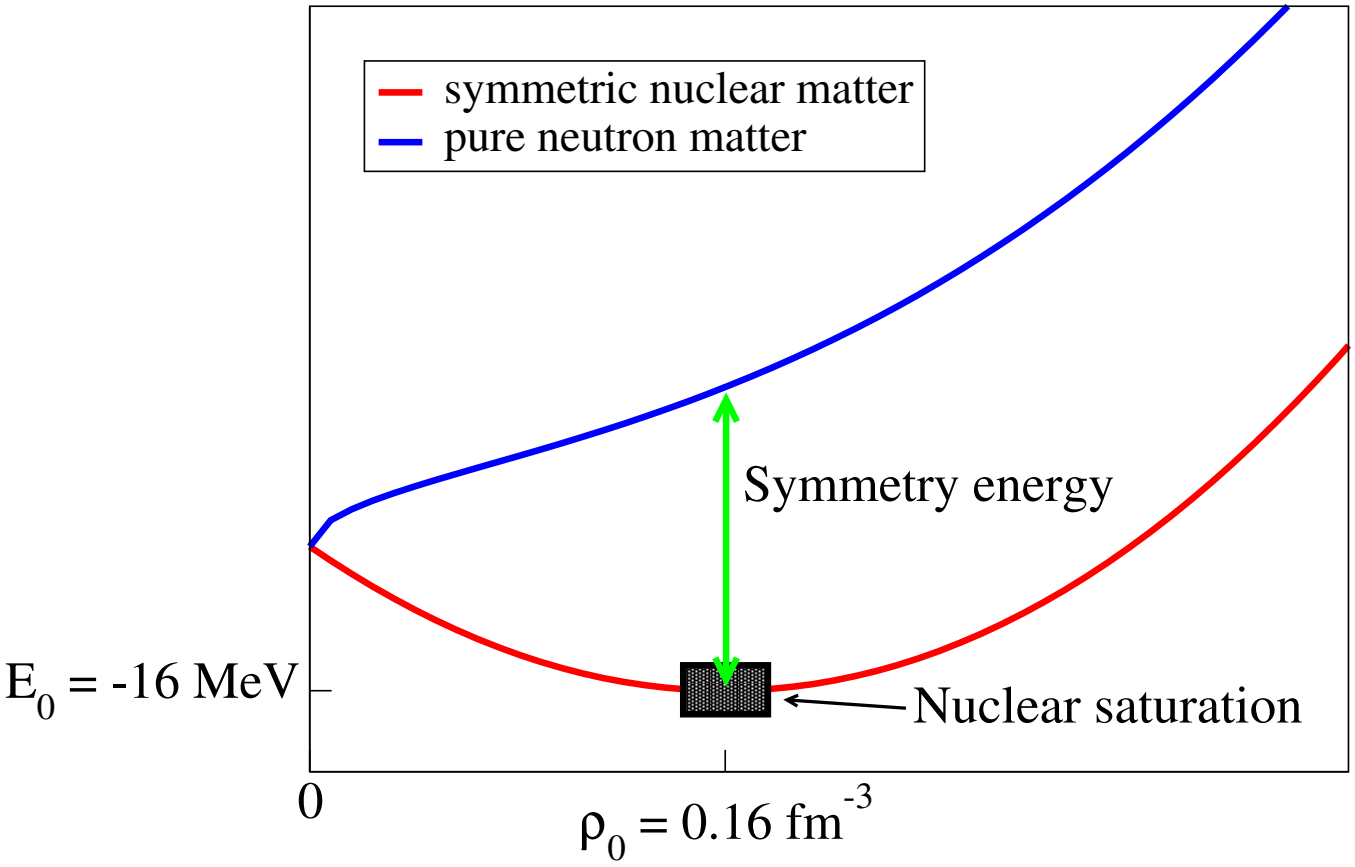
Neutron matter equation of state

Assumptions/observations:

- EOS of neutron matter useful to study the symmetry energy and its slope at saturation.
- The two-nucleon interaction reproduces well scattering data.
- The three-neutron force ($T = 3/2$) very weak in light nuclei, while $T = 1/2$ is the dominant part (but zero in neutron matter).
  No direct $T = 3/2$ experiments available!

We can bridge neutron star properties and the symmetry energy in a microscopic non-perturbative framework using QMC!

What is the Symmetry energy?



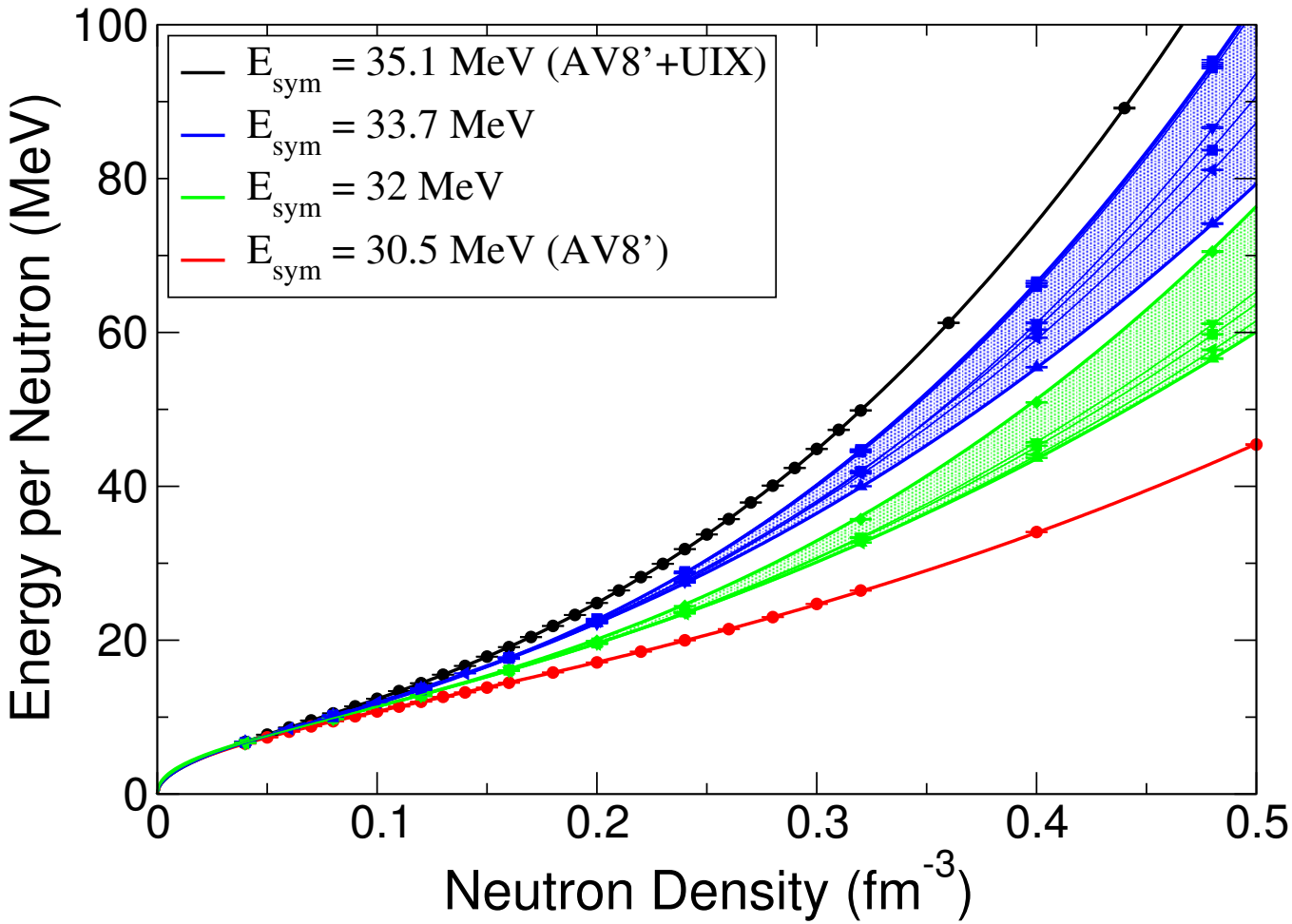
Assumption from experiments:

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

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

Neutron matter

Equation of state of neutron matter using Argonne forces:

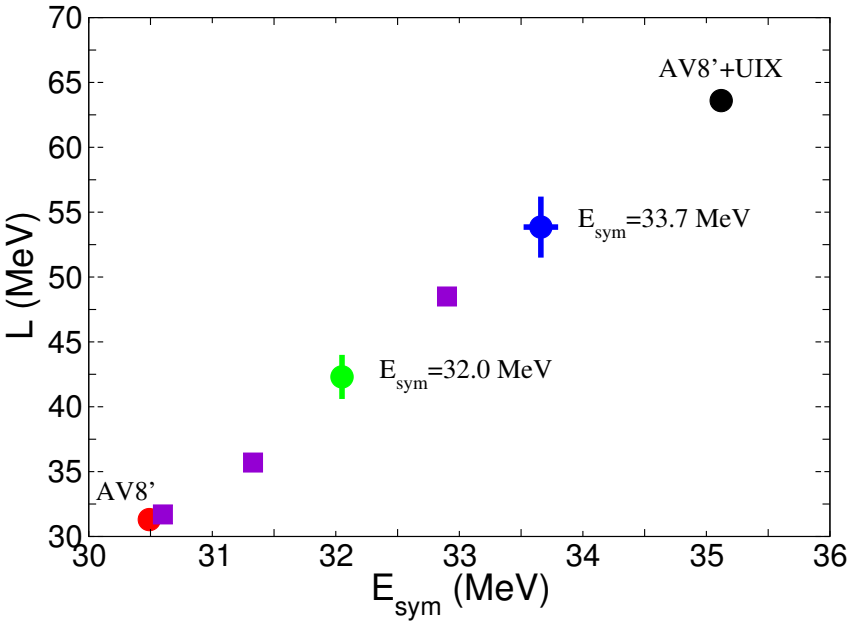


Gandolfi, Carlson, Reddy, PRC (2012)

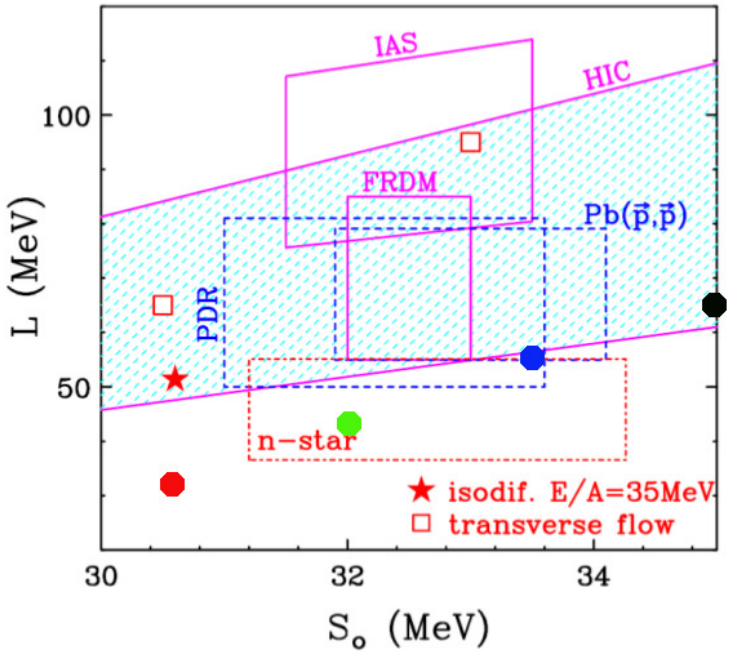
Neutron matter and symmetry energy

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)

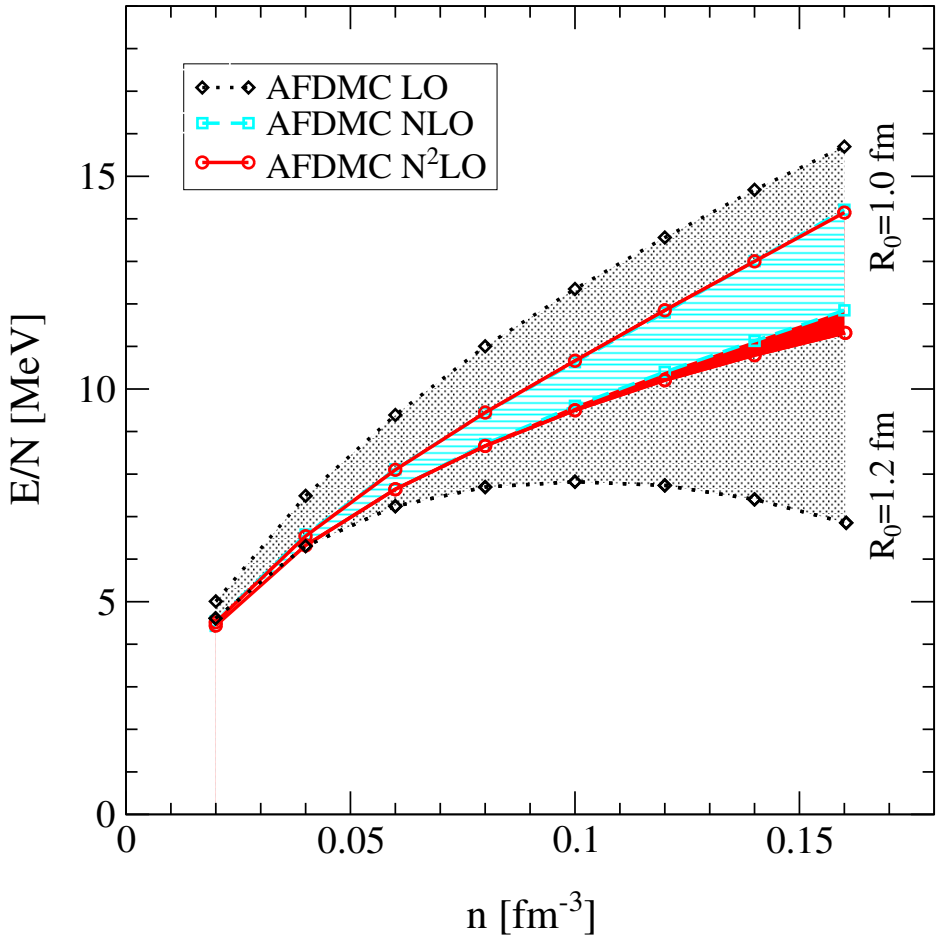


Tsang *et al.*, PRC (2012)

Very weak dependence to the model of 3N force for a given E_{sym}.
Chiral Hamiltonians give compatible results.

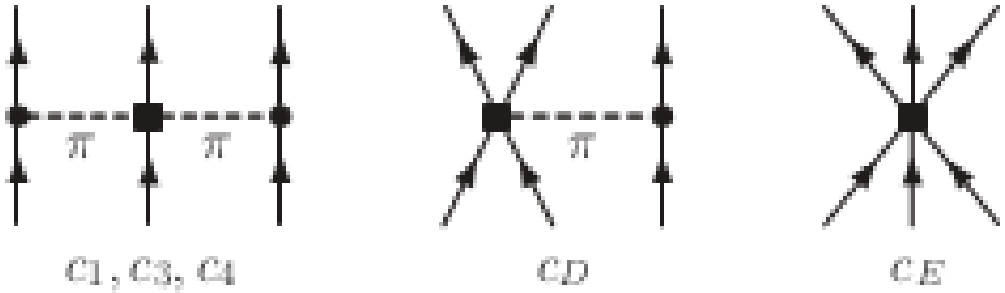
Neutron matter

Equation of state of neutron matter using NN chiral forces:



Gezerlis, Tews, *et al.*, PRL (2013), and arXiv:1406.0454 (2014)

Chiral three-body forces



For a finite cutoff, there are "induced" V_D and V_E diagrams that contribute in pure neutron matter.

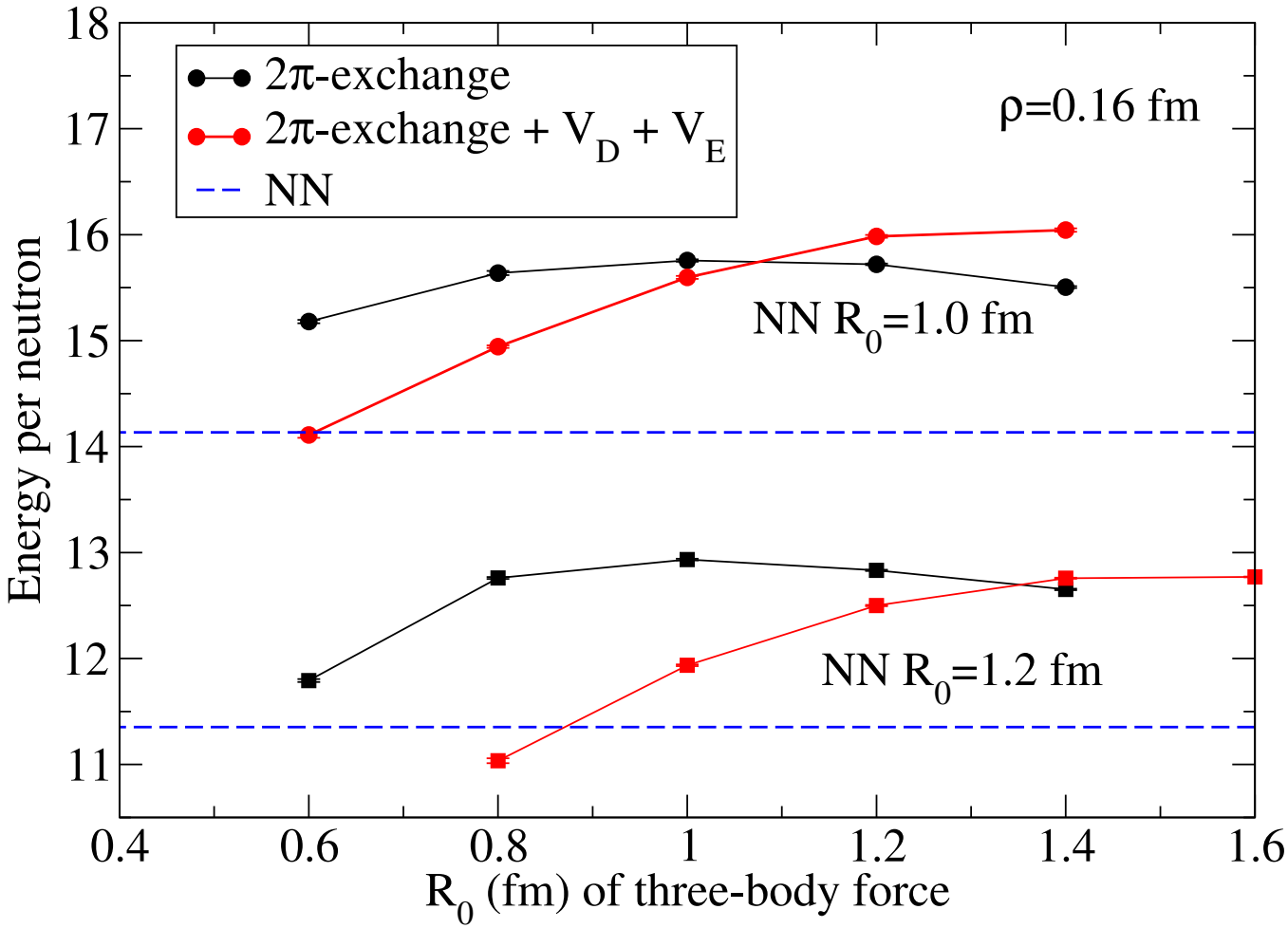
They have been often neglected in existing neutron matter calculations!

All the above terms have been written in coordinate space, and included into AFDMC.

Neutron matter with chiral forces

Preliminary!

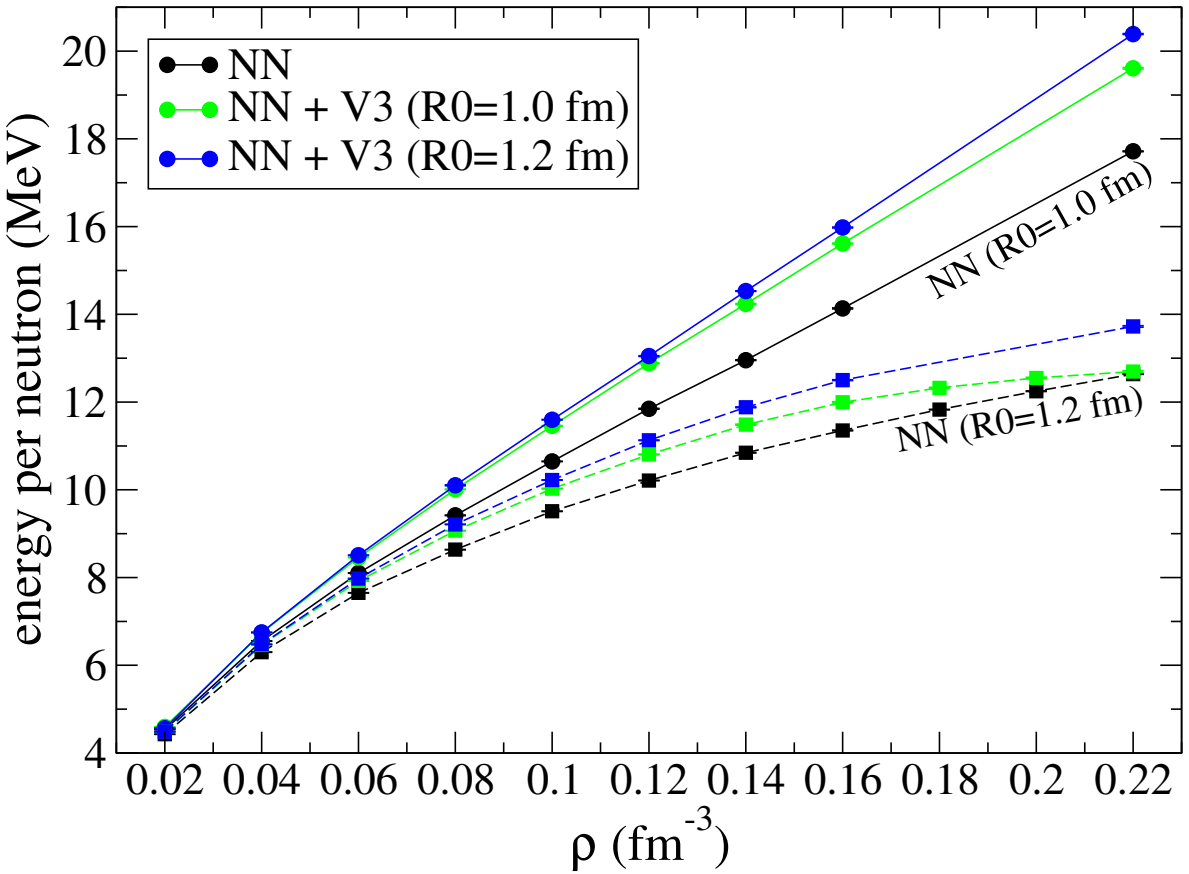
Contribution of "induced" V_D and V_E terms:



Neutron matter with chiral forces

Preliminary!

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

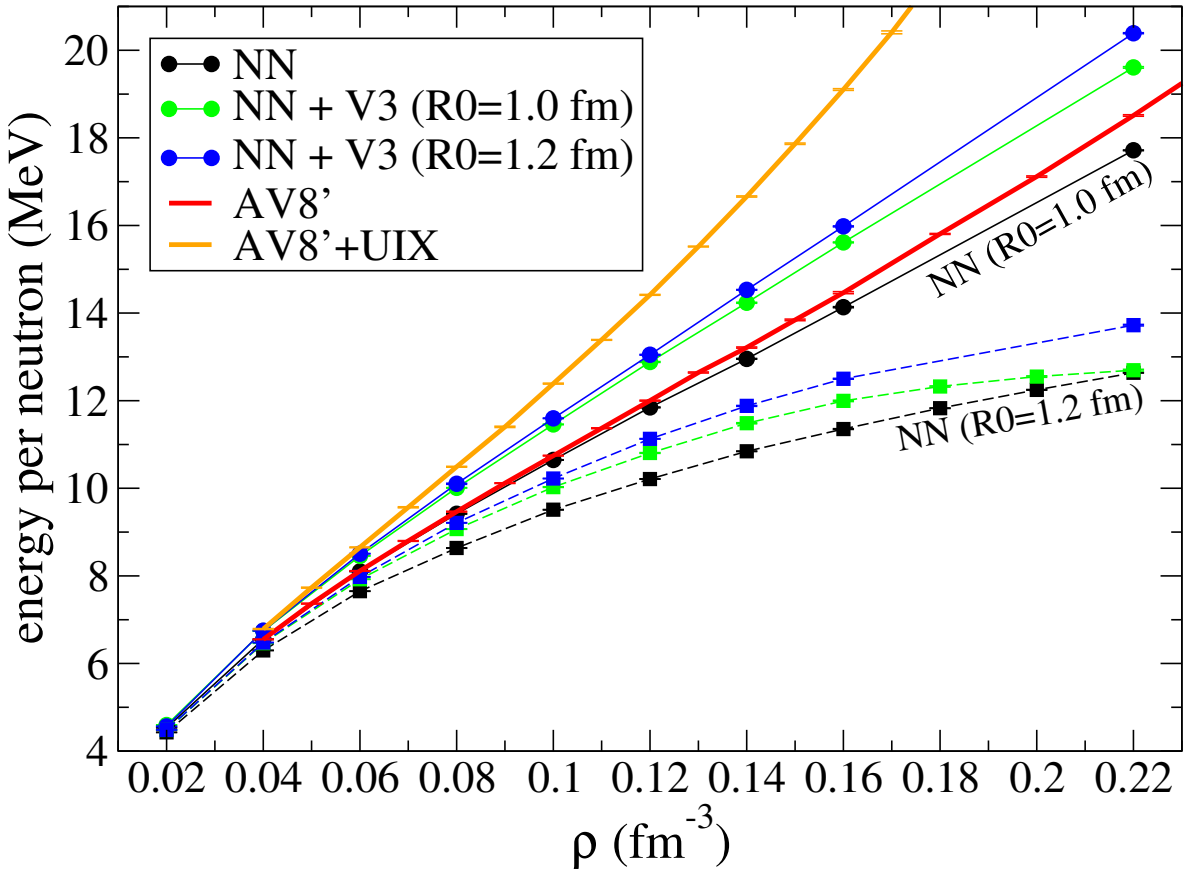


Note: the "real" V_D and V_E terms are not included yet.

Neutron matter with chiral forces

Preliminary!

Equation of state of neutron matter, a comparison.

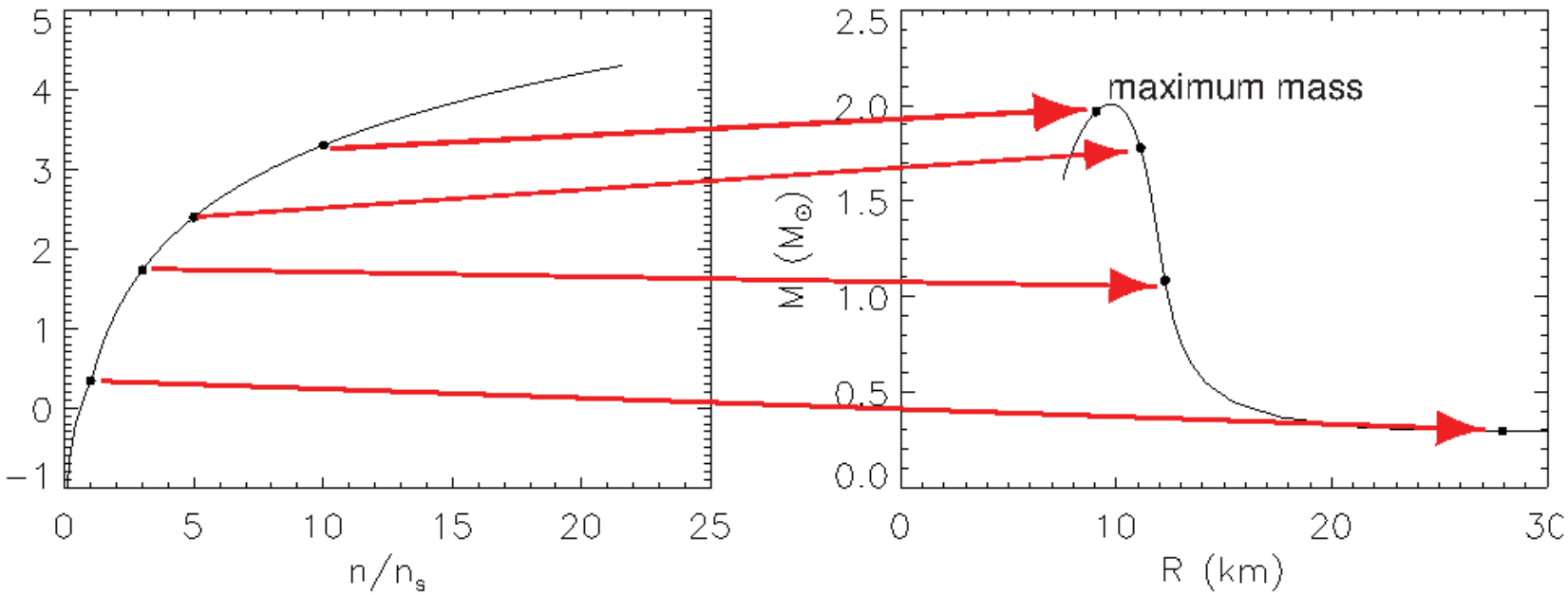


Neutron matter and neutron star structure

TOV equations:

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

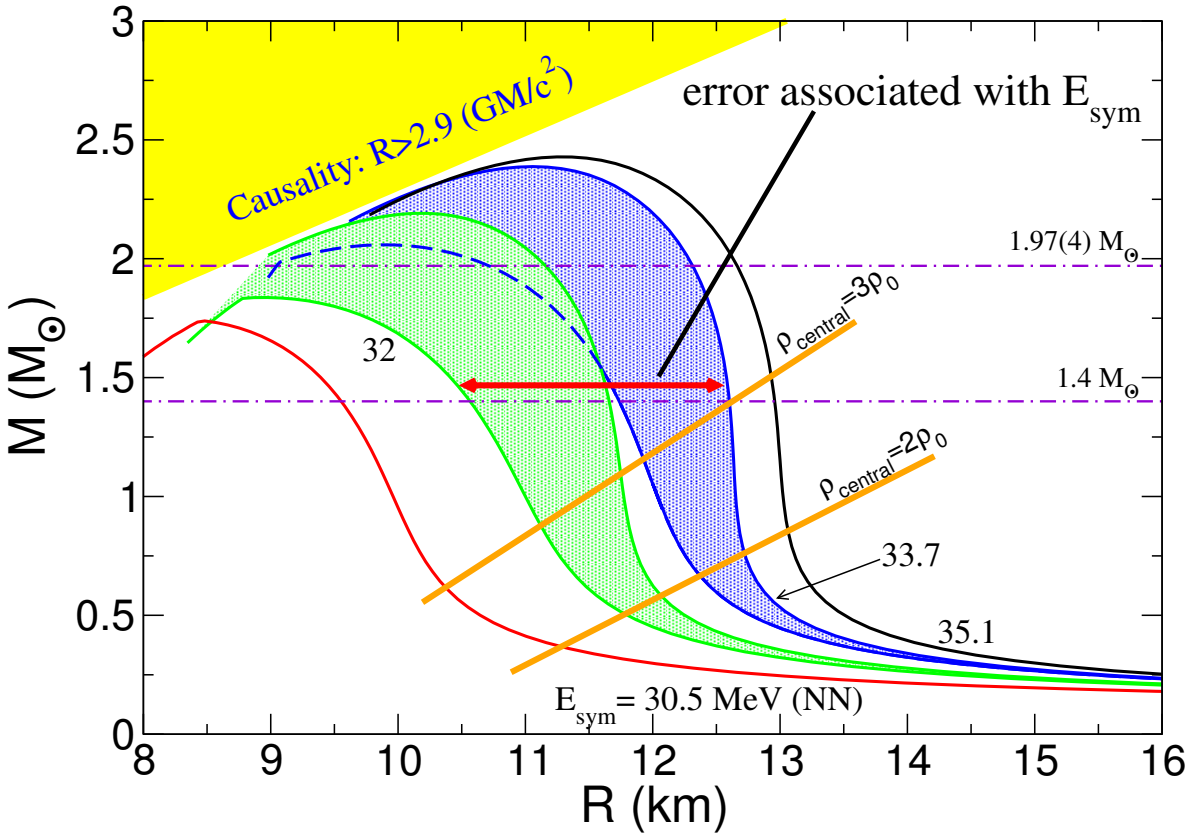
$$\frac{dm(r)}{dr} = 4\pi\epsilon r^2,$$



J. Lattimer

Neutron star structure

EOS used to solve the TOV equations.

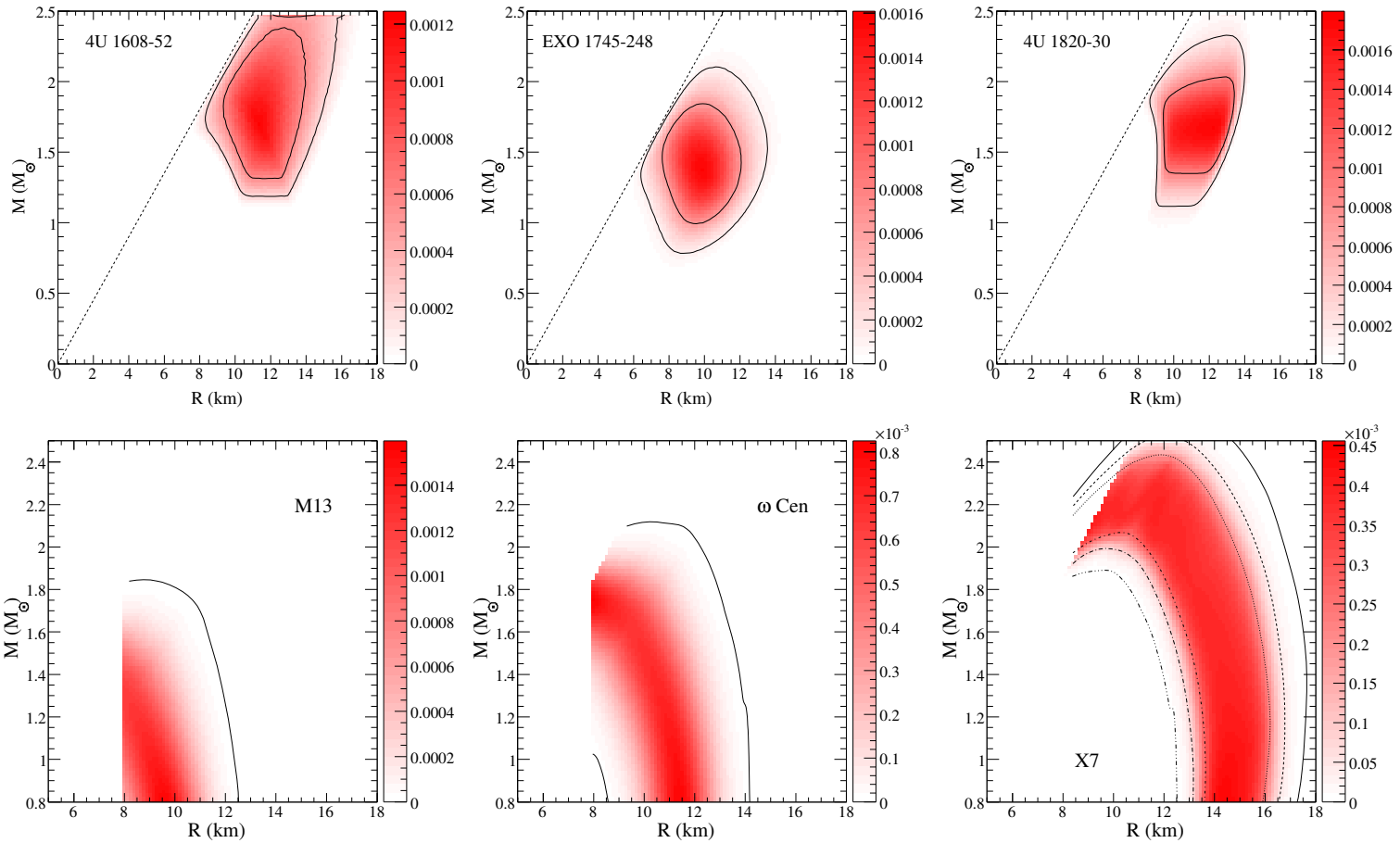


Gandolfi, Carlson, Reddy, PRC (2012).

Accurate measurement of E_{sym} would 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 'measure' the EOS and constrain E_{sym} and L.

Neutron star matter

Neutron star matter model:

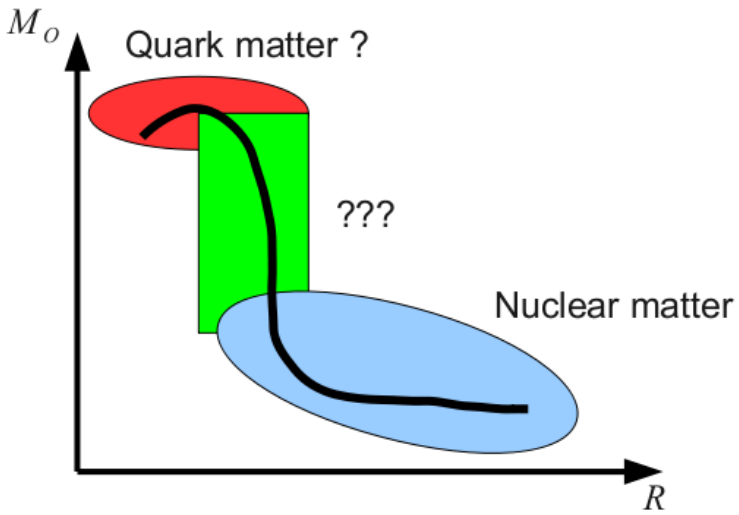
$$E_{NSM} = a\left(\frac{\rho}{\rho_0}\right)^{\alpha} + b\left(\frac{\rho}{\rho_0}\right)^{\beta}, \quad \rho < \rho_t$$

(form suggested by QMC simulations),

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

i) two polytropes

ii) polytrope+quark matter model

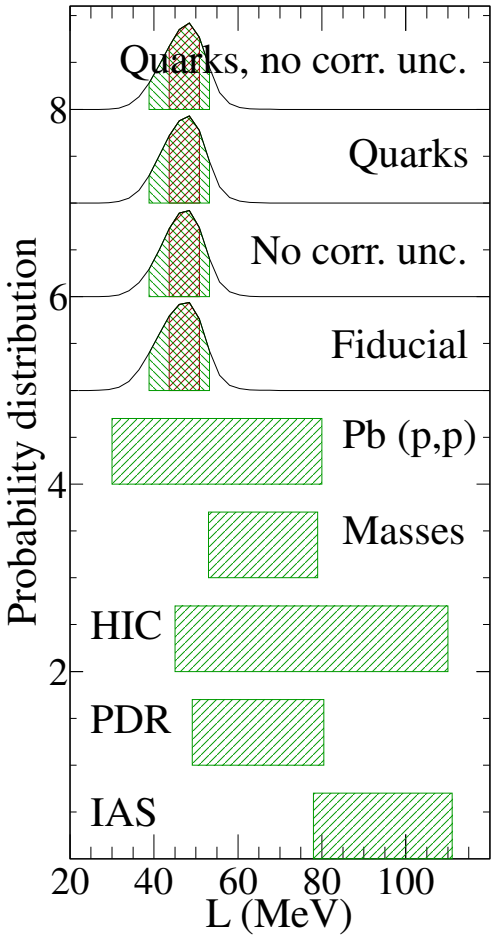


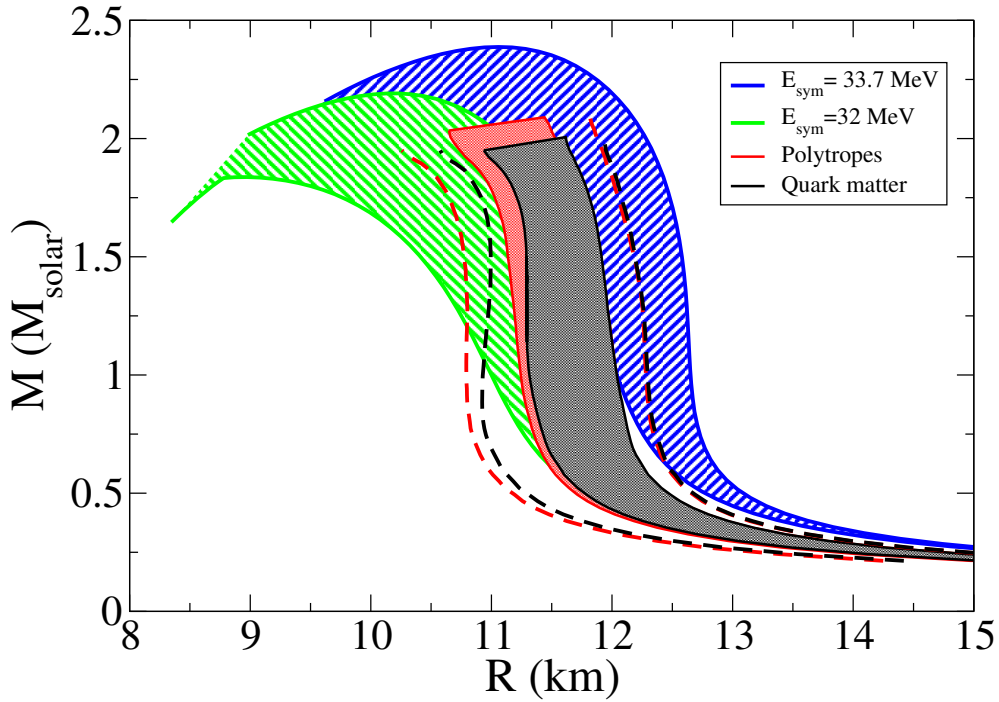
Direct way to extract E_{sym} and L from neutron stars observations:

$$E_{sym} = a + b + 16\,, \quad L = 3(a\alpha + b\beta)$$

Neutron star matter really matters!

Here an 'astrophysical measurement'





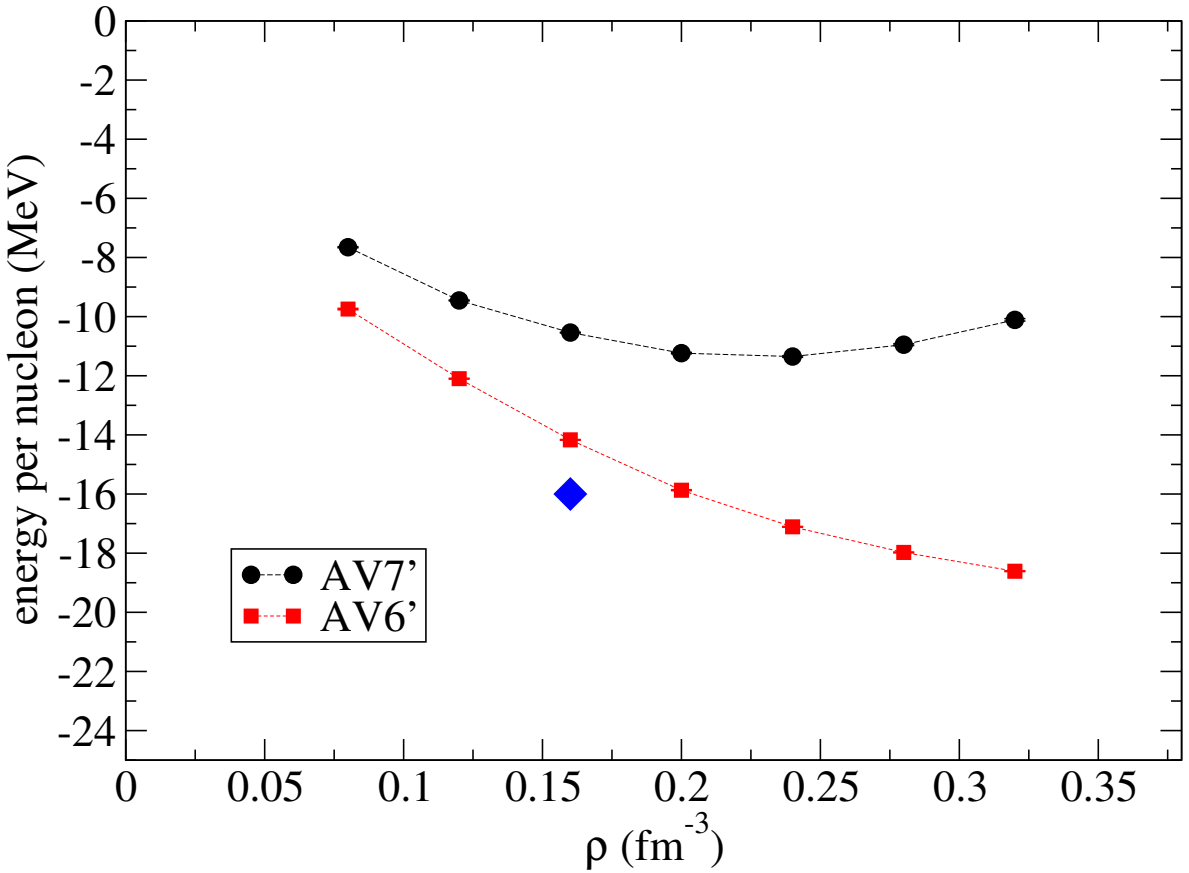
$32 < E_{sym} < 34\ MeV,\ 43 < L < 52\ MeV$

Steiner, Gandolfi, PRL (2012).

Nuclear matter

Preliminary results!

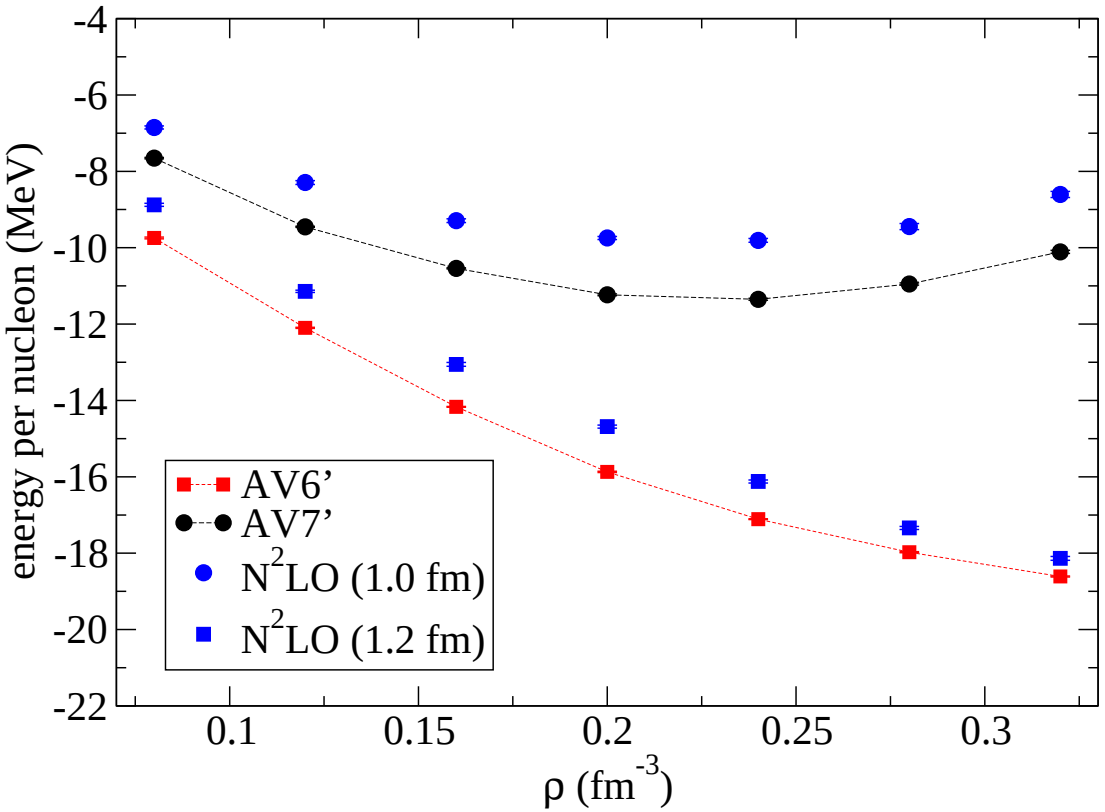
EOS of symmetric nuclear matter using Argonne AV6' and AV7':



Nuclear matter

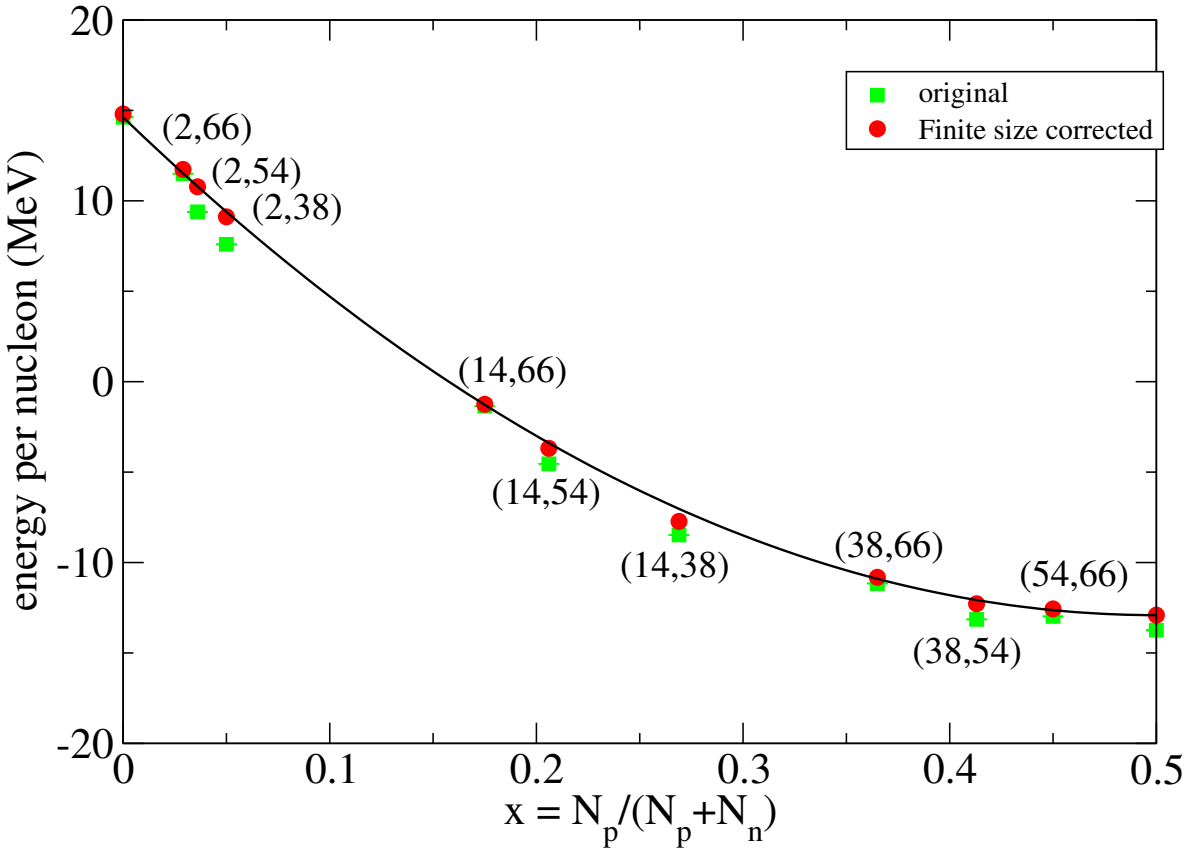
Preliminary results!

EOS of symmetric nuclear matter with chiral forces:



Nuclear matter

Preliminary results! Asymmetric nuclear matter, AV6':



Symmetry energy $\simeq$ 28.8 MeV.

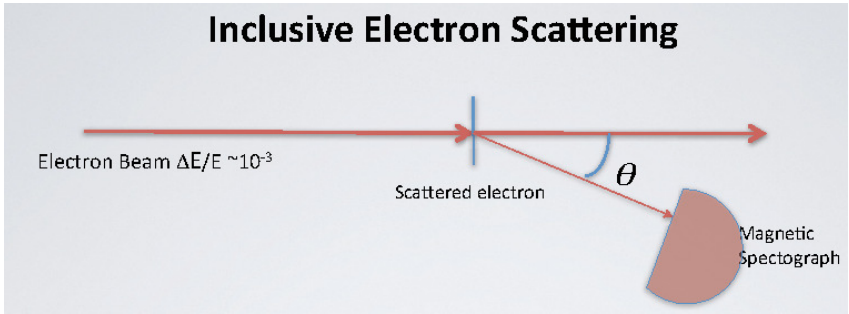
Experiments/neutron stars suggest that it should be larger than 30-31 MeV. $\Rightarrow V_3(PNM) - V_3(SNM) > 1 - 2$ MeV.

Quadratic dependence to isospin-asymmetry look fine.

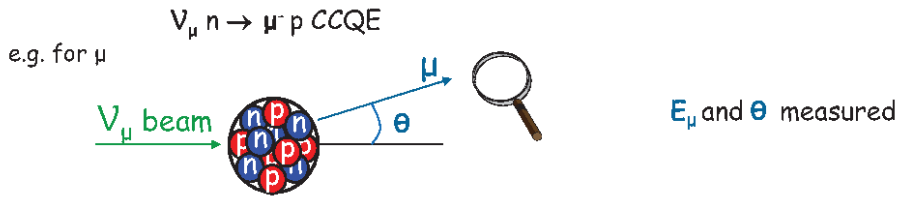
Introduction: ν energy and cross-section

Knowledge of energy-dependent ν and $\bar{\nu}$ cross sections is crucial to extract Δm^2, mixing angles and δ_{CP} from oscillation experiments.

Electron energy easy:



E_ν difficult to reconstruct:



Reconstructed neutrino energy

$$\overline{E_\nu} = \frac{E_\mu - m_\mu^2/(2M)}{1 - (E_\mu - P_\mu \cos\theta)/M}$$

via two-body kinematics

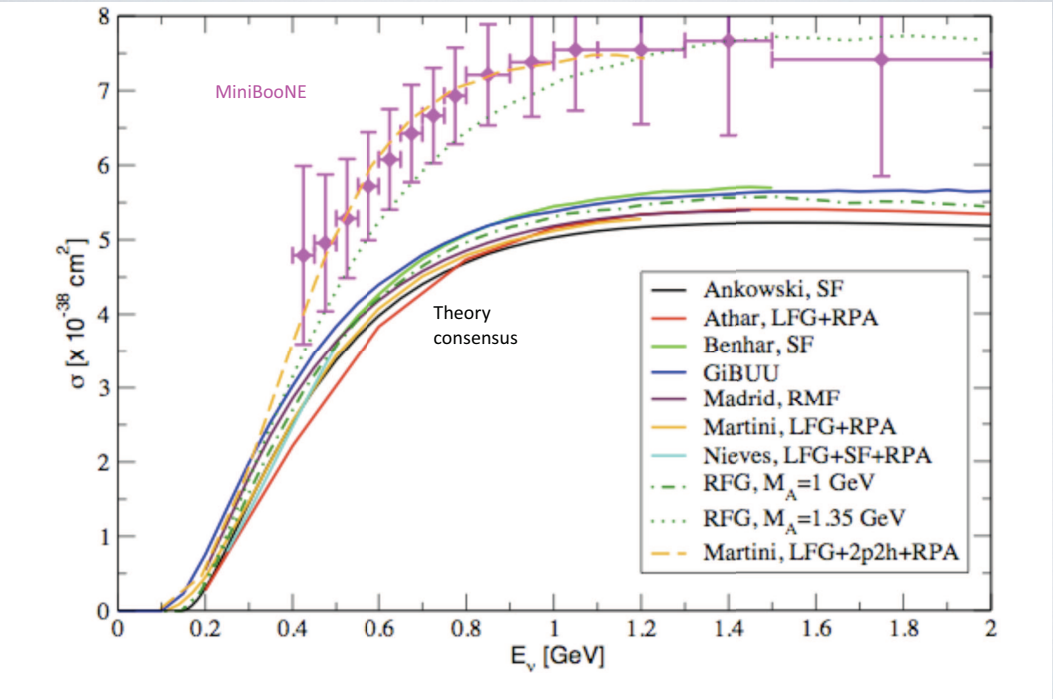
Initial/final state interaction commonly neglected. Neutral current process even more difficult.

Charge-change quasi-elastic cross-section in ^{12}C

Experimental vs theory **disagreement**

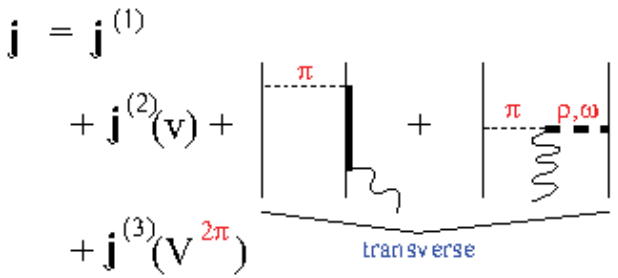
What is Observed? CCQE

$$\nu_{\mu} + {}^{12}C \rightarrow \mu^{-} + 7p, 5n(\not{\pi})$$

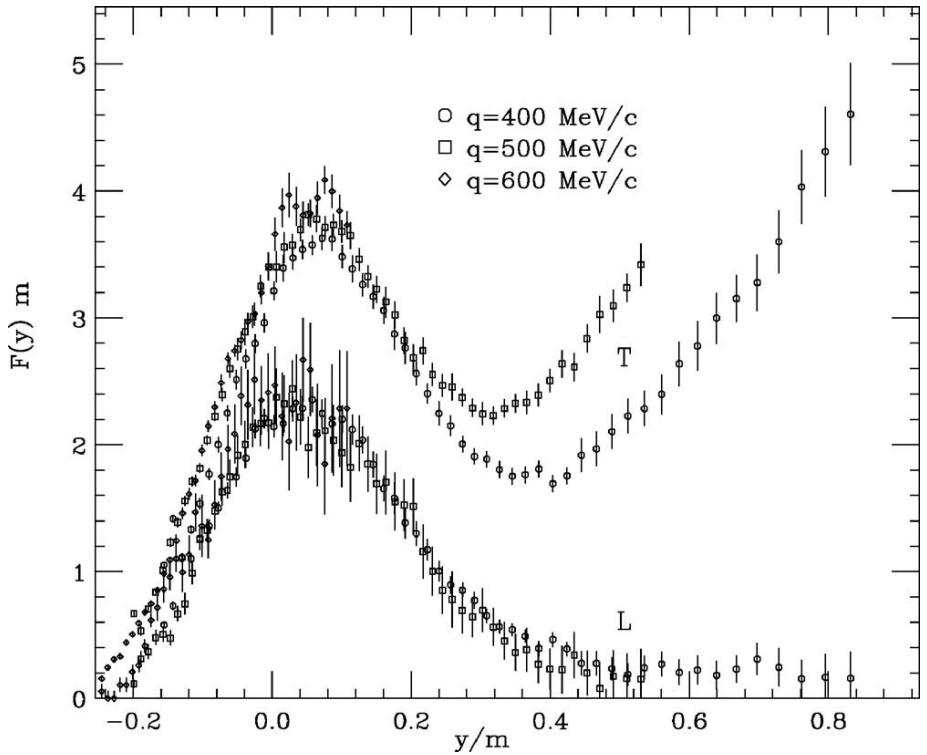


All the above theoretical calculations **do not** include two-body processes.
No nucleon-nucleon correlations included.

Two-body processes



Example of two-body processes involved in electroweak currents

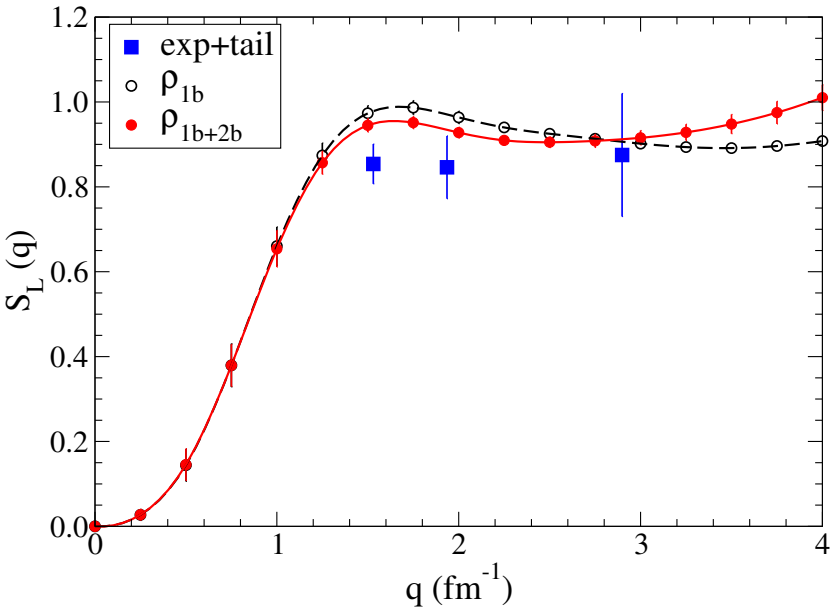


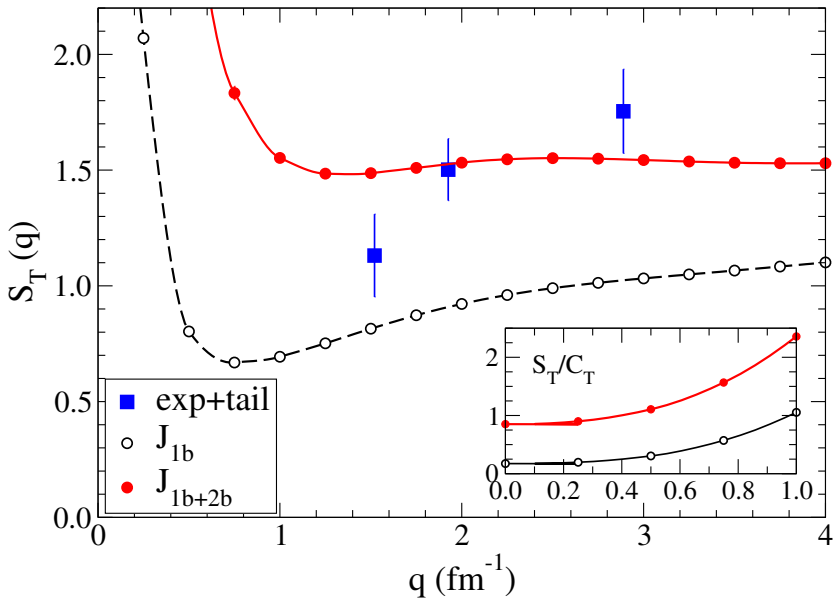
Rescaled longitudinal vs transverse electromagnetic response in ^{12}C

Without two-body processes, the longitudinal and transverse response is the same!

Electromagnetic sum-rules in ^{12}C

$$S_{L,T}(q) = C_{L,T} \int R_{L,T}(\omega, q) d\omega$$





$$S_L(q) = C_L \left(\langle \psi | \rho_q^\dagger \, \rho_q | \psi \rangle - |\langle \psi | \rho_q | \psi \rangle|^2 \right) \qquad S_T(q) = C_T \langle \psi | \vec{J}_q^\dagger \, \vec{J}_q | \psi \rangle$$

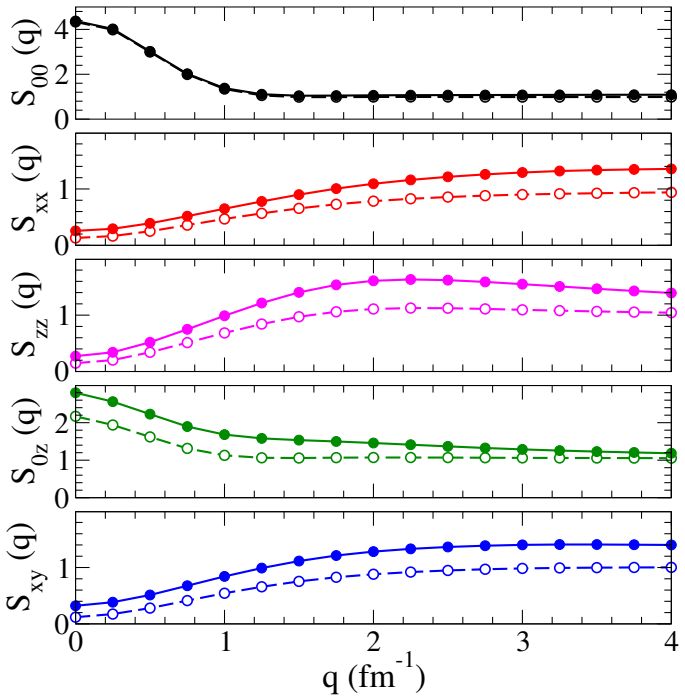
Lovato, Gandolfi, Butler, Carlson, Lusk, Pieper, Schiavilla, PRL (2013)

MEC currents (two-body operators) very important in S_T sum-rule.

Electroweak sum-rules in ^{12}C

Neutrino cross-section:

$$\left(\frac{d\sigma}{d\epsilon' d\Omega}\right)_{\nu/\overline{\nu}} = \frac{G^2}{2\pi^2}\, k'\epsilon'\, F(Z,k') \cos^2\frac{\theta}{2}\left[R_{00} + \frac{\omega^2}{q^2} R_{zz} - \frac{\omega}{q} R_{0z} + \left(\tan^2\frac{\theta}{2} + \frac{Q^2}{2\,q^2}\right) R_{xx+yy} \mp \tan\frac{\theta}{2}\sqrt{\tan^2\frac{\theta}{2} + \frac{Q^2}{q^2}}\, R_{xy}\right]$$



Lovato, Gandolfi, Carlson, Pieper, Schiavilla, PRL (2014).

Two-body operators enhance sum-rules up to 50%. Crucial for ν vs anti-ν

Summary

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

- Local chiral forces can be implemented in QMC.
- Three-neutron force is the bridge between E_{sym} and neutron star structure.
- Neutron matter equation of state calculated with several different Hamiltonians.
- Calculations of medium nuclei and nuclear matter is in progress. Role of three-body forces need investigation.
- Two-body processes dramatically important in electro-weak interactions.

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NUCLEI Nuclear Computational Low-Energy Initiative

www.computingnuclei.org

U.S. DEPARTMENT OF ENERGY

NERSC National Energy Research Scientific Computing Center

U.S. DEPARTMENT OF ENERGY INCITE LEADERSHIP COMPUTING

Extra slides

Overview

Recall: propagation in imaginary-time

$$e^{-(T+V)\Delta\tau}\psi \approx e^{-T\Delta\tau}e^{-V\Delta\tau}\psi$$

Kinetic energy is sampled as a diffusion of particles:

$$e^{-\nabla^2\Delta\tau}\psi(R) = e^{-(R-R')^2/2\Delta\tau}\psi(R) = \psi(R')$$

The (scalar) potential gives the weight of the configuration:

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

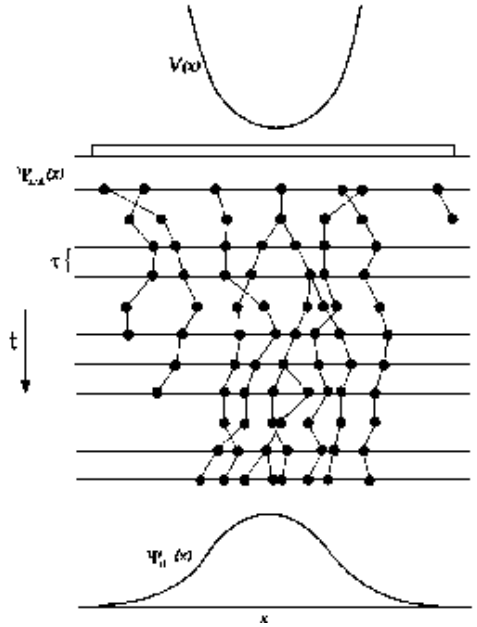
Algorithm for each time-step:

- do the diffusion: $R' = R + \xi$
- compute the weight w
- compute observables using the configuration R' weighted using w over a trial wave function ψ_T.

For spin-dependent potentials things are much worse!

Branching

The configuration weight w is efficiently sampled using the branching technique:



Configurations are replicated or destroyed with probability

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

Note: the re-balancing is the bottleneck limiting the parallel efficiency.

Wave function

The general form of the wave function is

$$\psi = \begin{vmatrix} \phi_1(1) & \phi_1(2) & \cdots & \phi_1(N) \\ \phi_2(1) & \phi_2(2) & \cdots & \phi_2(N) \\ \cdots & \cdots & \cdots & \cdots \\ \phi_N(1) & \phi_N(2) & \cdots & \phi_N(N) \end{vmatrix} = |S_{ij}|$$

where

$$\phi_i(j) = f_i^{\uparrow}(\vec{r}_j)a_j + f_i^{\downarrow}(\vec{r}_j)b_j$$

The Slater matrix must be diagonalized at each time step. With the inverse we can compute all the operators we need using:

$$\frac{O_i\psi}{\psi} = \sum_j S_{ij}^{-1} O\phi_j(i)$$

For example, O is ∇^2 to compute the kinetic energy, or σ_z to compute the spin, and so on.

Computational cost $\approx N^3$.

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

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

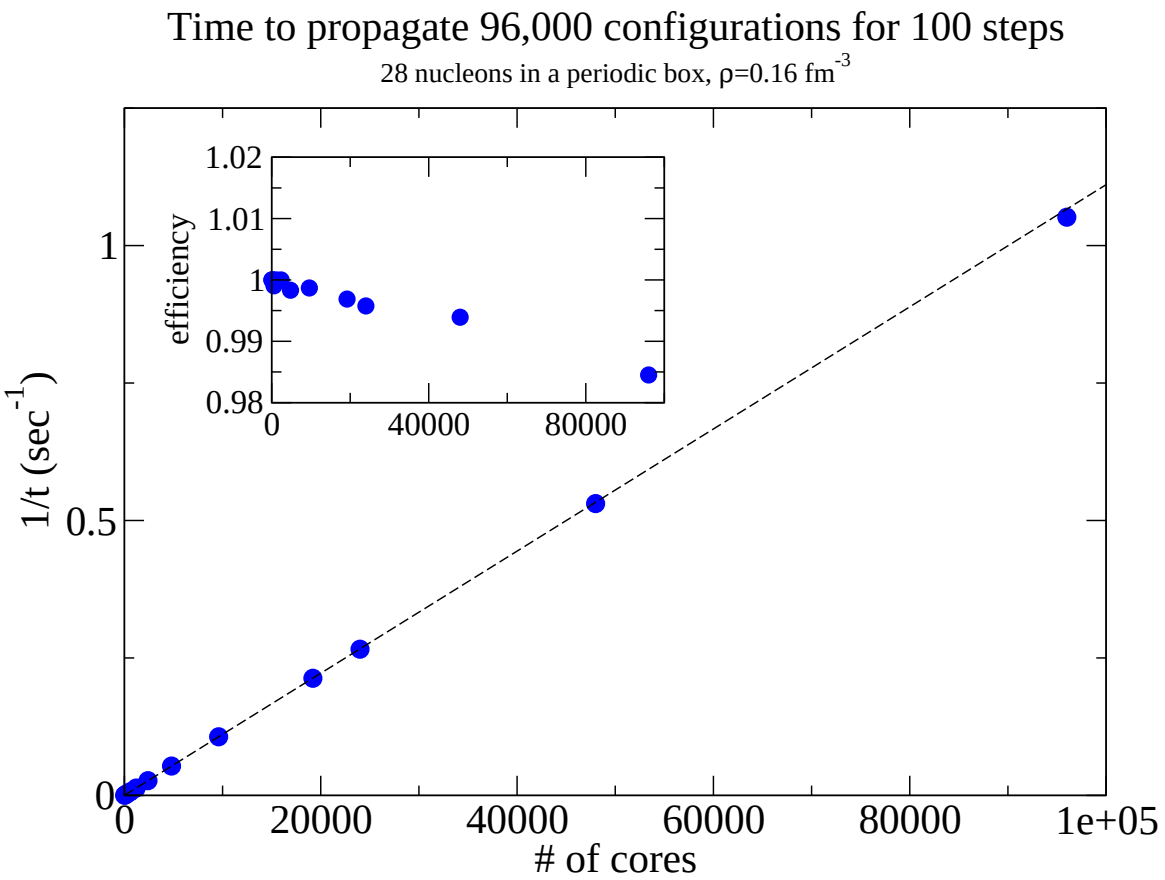
Now we can use the HS transformation to do the propagation:

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

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

AFDMC efficiency

Edison, NERSC:



Note: MPI only so far.