QMC calculations with chiral EFT interactions

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Outline

Chiral EFT and **many-body forces**

Three-nucleon forces and neutron-rich nuclei

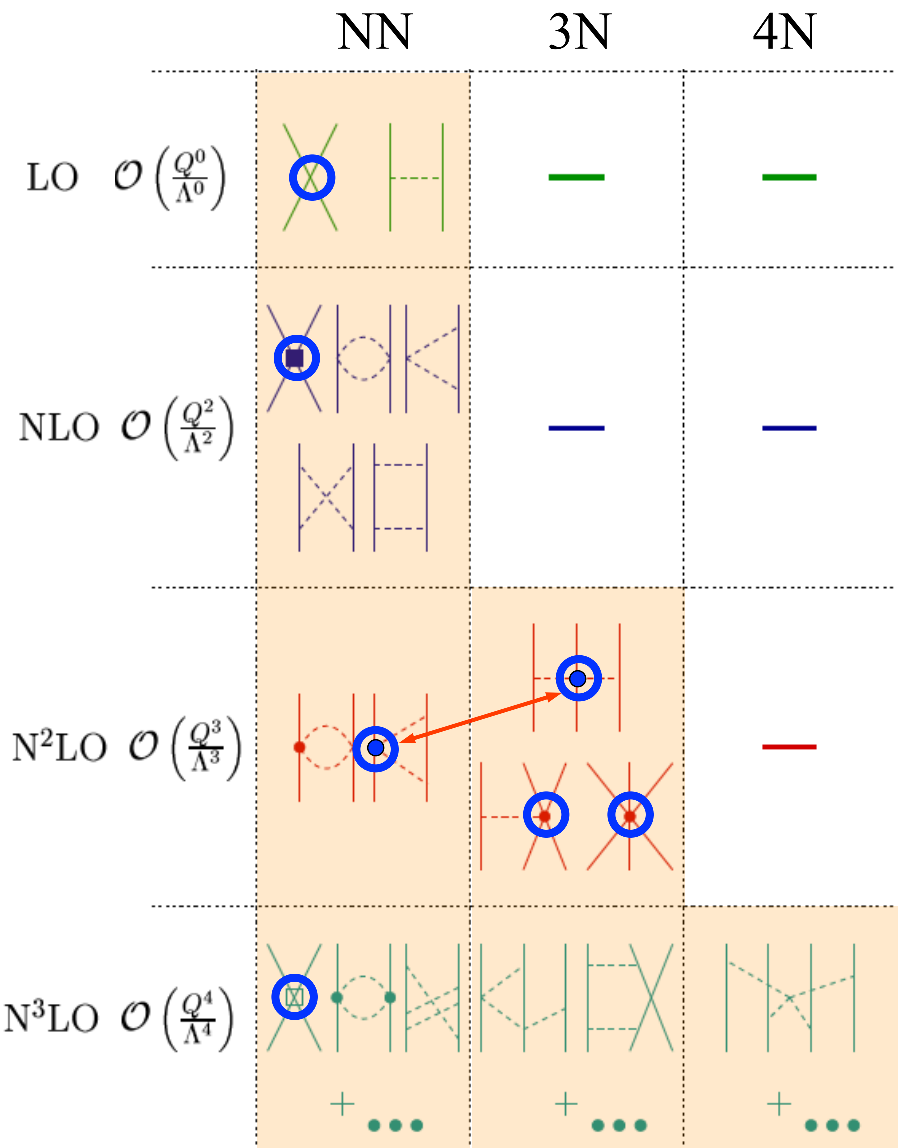
Neutron matter from chiral EFT interactions

need for nonperturbative benchmark,
which parts of chiral EFT interactions are perturbative?

QMC calculations with chiral EFT interactions

Chiral effective field theory for nuclear forces

Separation of scales: low momenta $\frac{1}{\lambda} = Q \ll \Lambda_b$ breakdown scale ~500 MeV



limited resolution at low energies, can expand in powers $(Q/\Lambda_b)^n$

expansion parameter ~ 1/3 for nuclei

include long-range pion physics

few short-range couplings, fit to experiment once

systematic: can work to desired accuracy and obtain **error estimates**

consistent **electroweak interactions** and **matching to lattice QCD**

Weinberg, van Kolck, Kaplan, Savage, Wise, Epelbaum, Kaiser, Machleidt, Meissner,…

Chiral effective field theory and **many-body forces**

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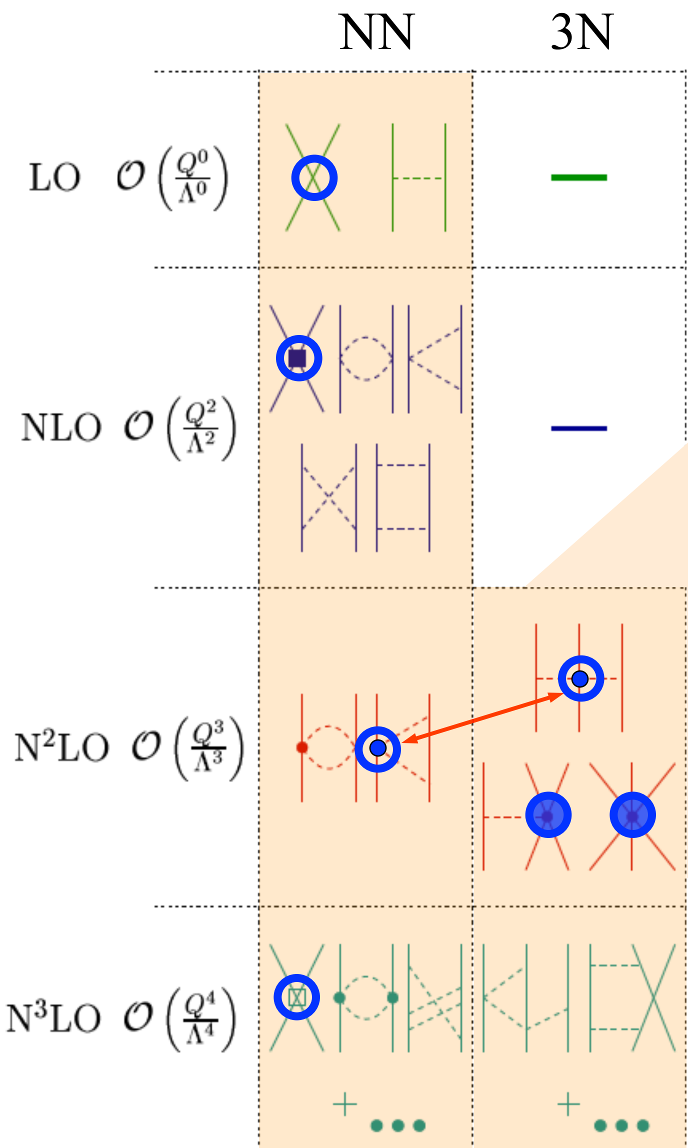
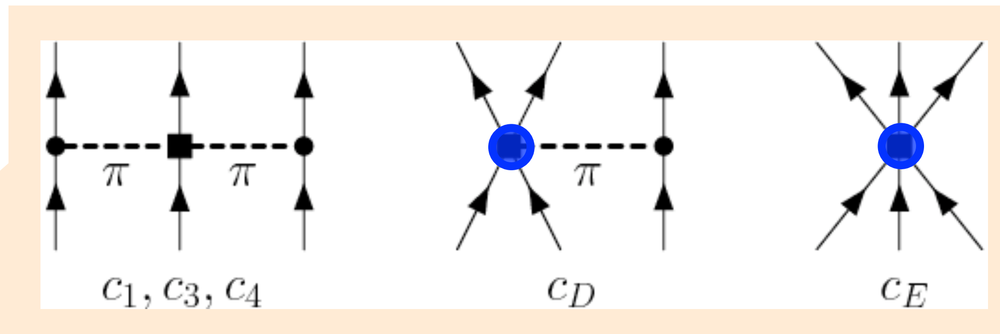


consistent NN-3N interactions

3N,4N: only 2 new couplings to N^{3}LO



c_i from πN and NN Meissner et al. (2007)

$$c_1 = -0.9^{+0.2}_{-0.5}\,,\ c_3 = -4.7^{+1.2}_{-1.0}\,,\ \ c_4 = 3.5^{+0.5}_{-0.2}$$

single-Δ: $c_1=0$, $c_3=-c_4/2=-3$ GeV^{-1}

c_D, c_E fit to ^{3}H, ^{4}He properties only

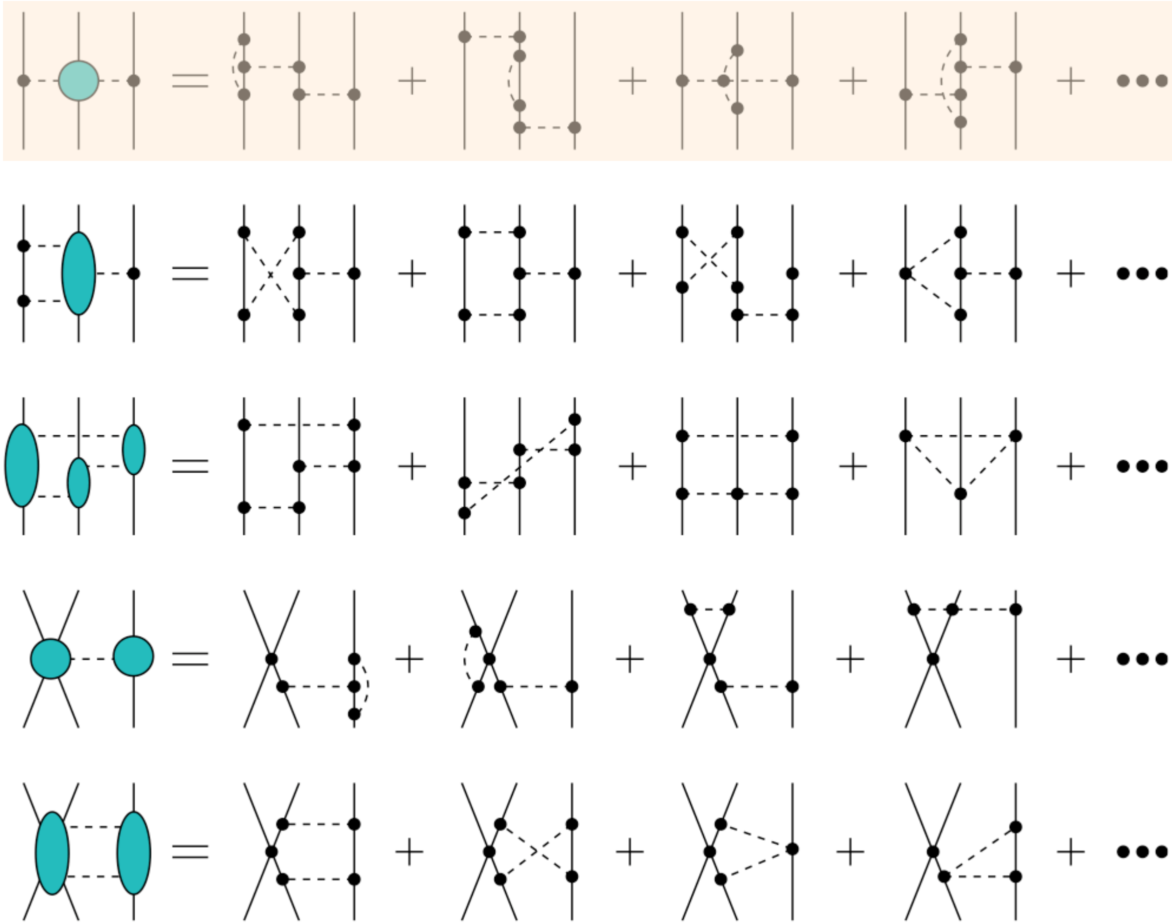
Weinberg, van Kolck, Kaplan, Savage, Wise, Epelbaum, Kaiser, Machleidt, Meissner,…

Subleading chiral 3N forces

parameter-free N^3LO Bernard et al. (2007,2011), Ishikawa, Robilotta (2007)

one-loop contributions:

2π-exchange, 2π-1π-exchange, rings, contact-1π-, contact-2π-exchange



decrease c_i strengths
$\delta c_3 = -\delta c_4 = 1\ \mathrm{GeV}^{-1}$
comparable to
N^2LO uncertainty

1/m corrections: spin-orbit parts, interesting for A_y puzzle

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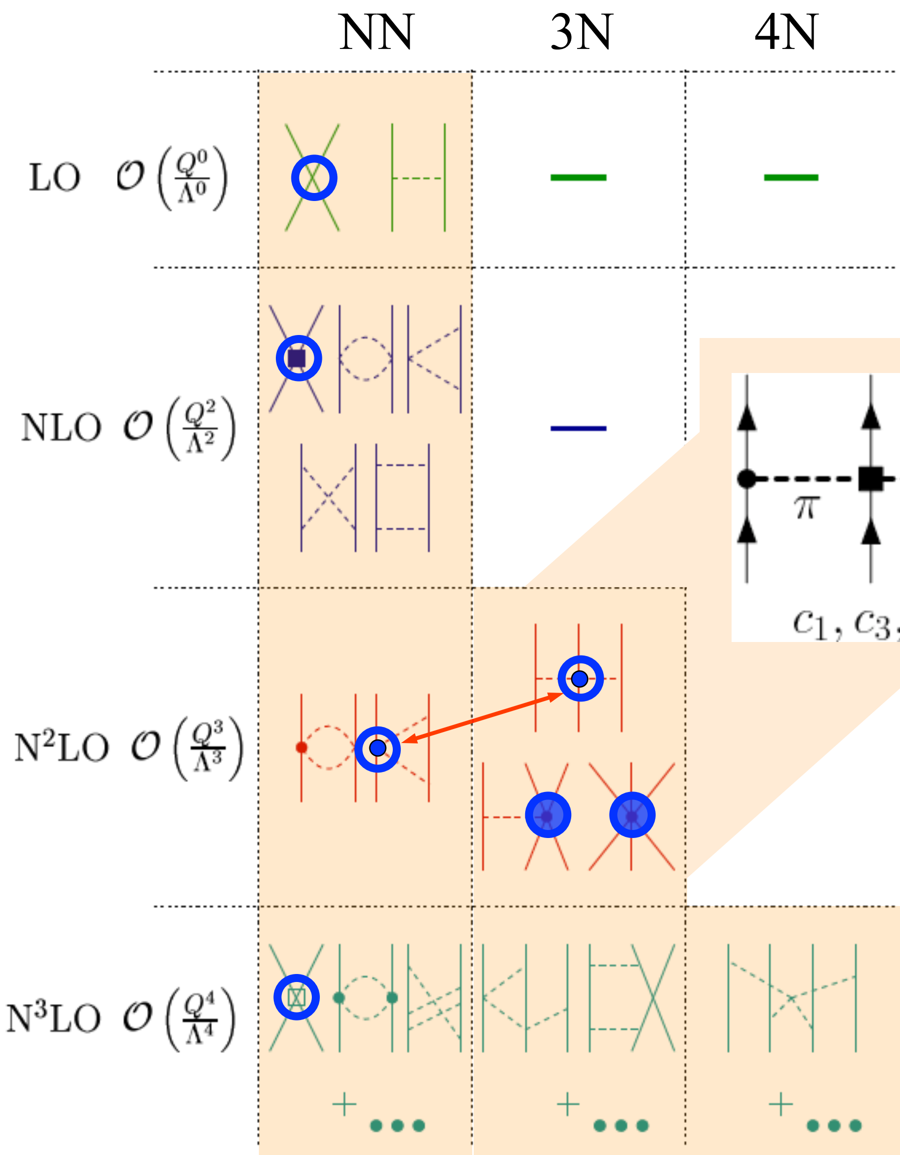
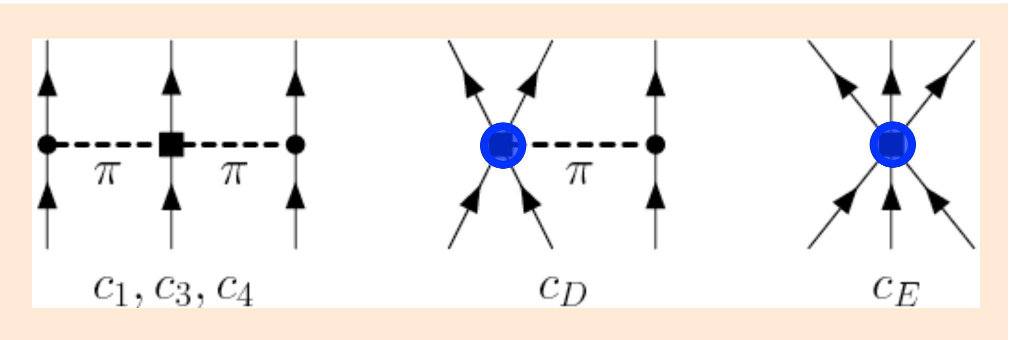


c_D, c_E don't contribute for neutrons because of Pauli principle and pion coupling to spin, also for c_4

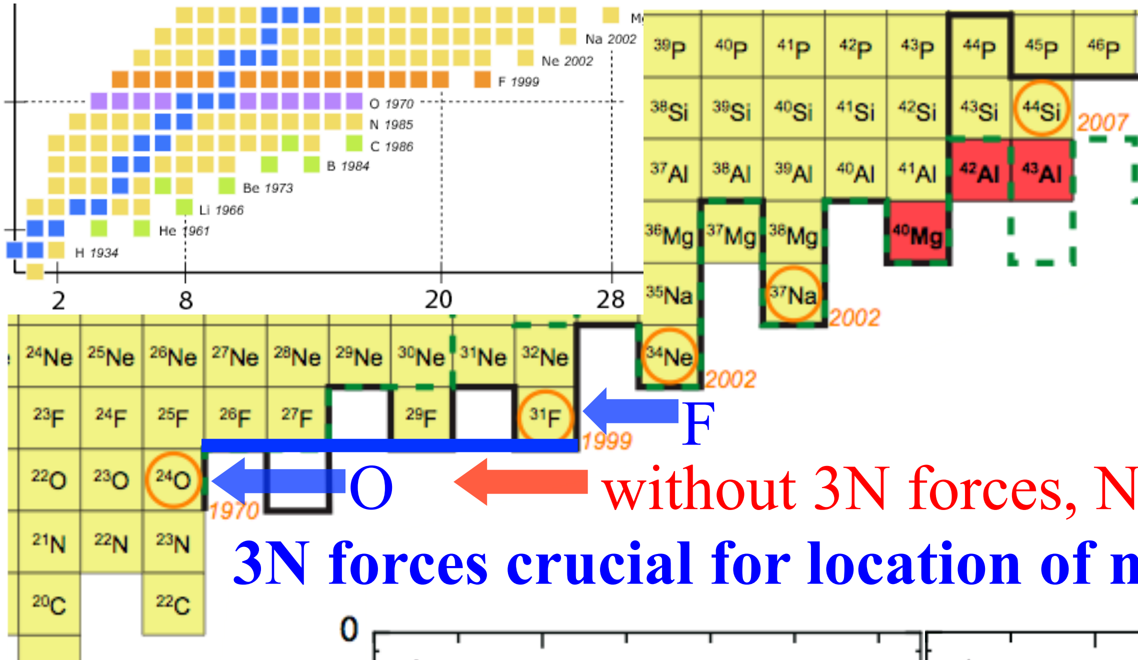
Hebeler, AS (2010)



all 3- and 4-neutron forces are predicted to N³LO!

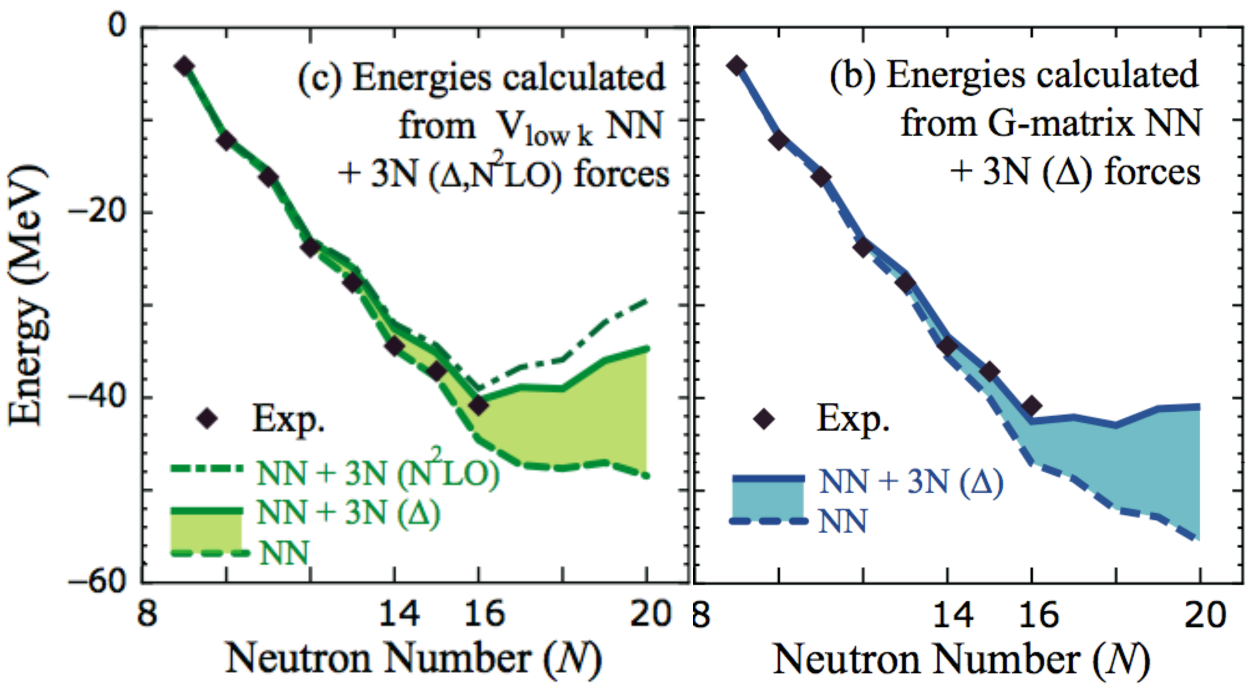
Weinberg, van Kolck, Kaplan, Savage, Wise, Epelbaum, Kaiser, Machleidt, Meissner,…

The oxygen anomaly Otsuka et al. (2010)



without 3N forces, NN interactions too attractive

3N forces crucial for location of neutron dripline



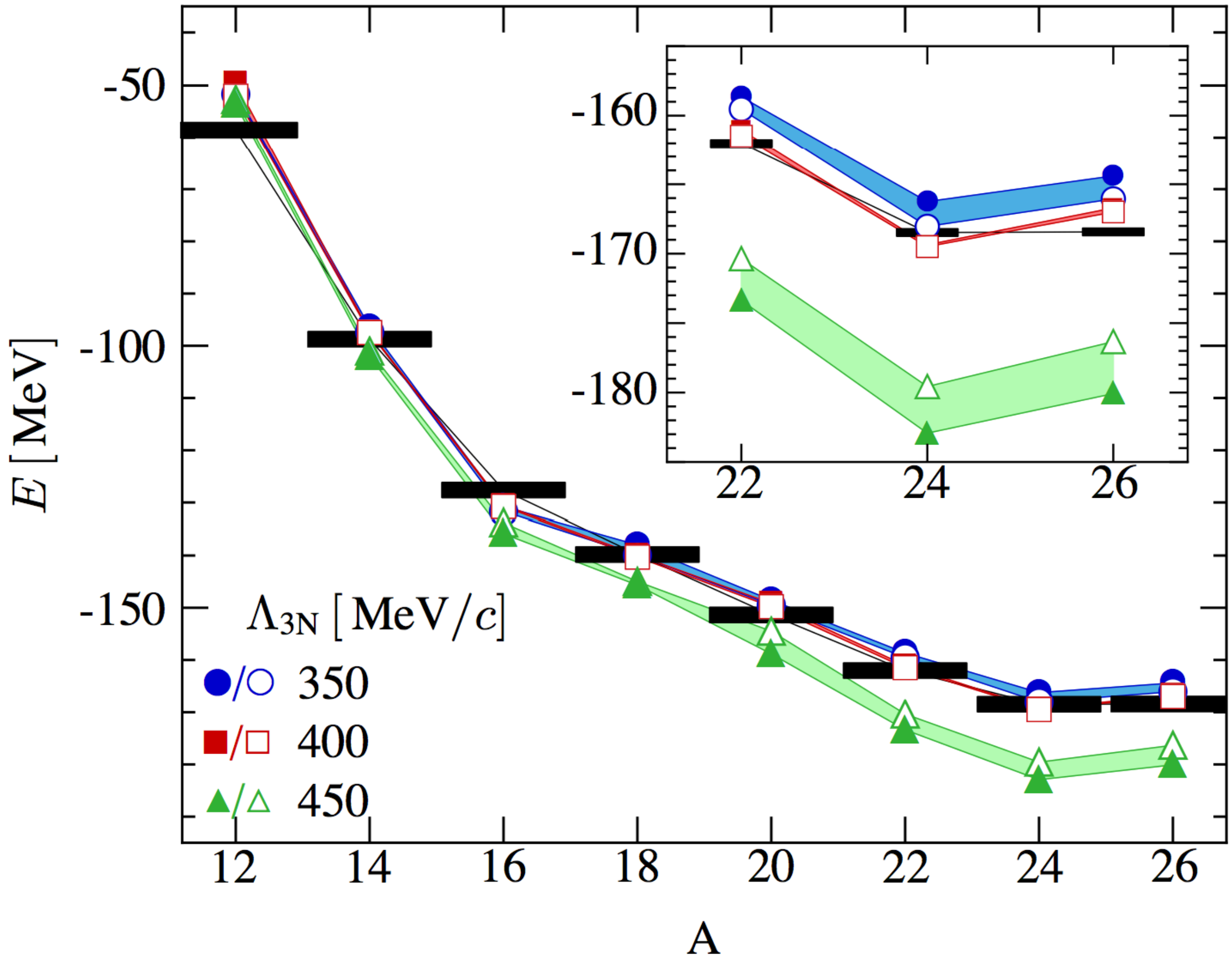
New ab-initio methods extend reach

impact of 3N forces confirmed in ab-initio calculations:

Coupled Cluster theory with phenomenological 3N forces Hagen et al. (2012)

In-Medium Similarity RG based on chiral NN+3N Hergert et al. (2013)

Green's function methods based on chiral NN+3N Cipollone et al. (2013)

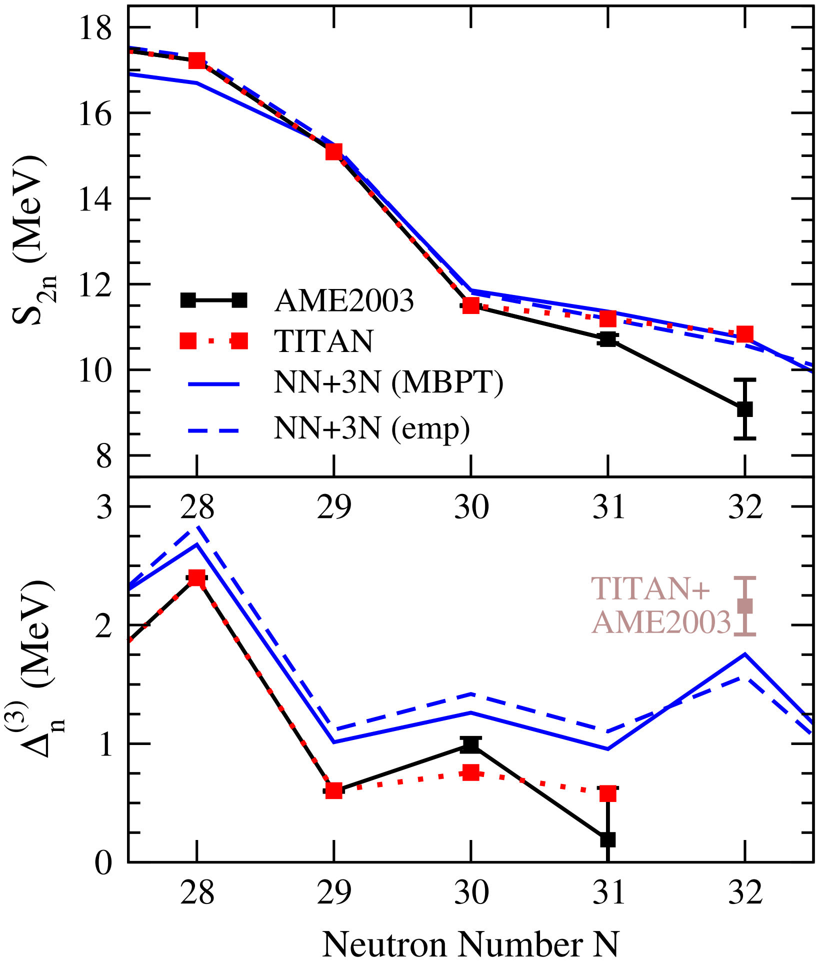


new ^{51,52}Ca TITAN measurements

^{52}Ca is 1.75 MeV more bound compared to atomic mass evaluation

Gallant et al. (2012)

behavior of 2n separation energy S_{2n} agrees with NN+3N predictions



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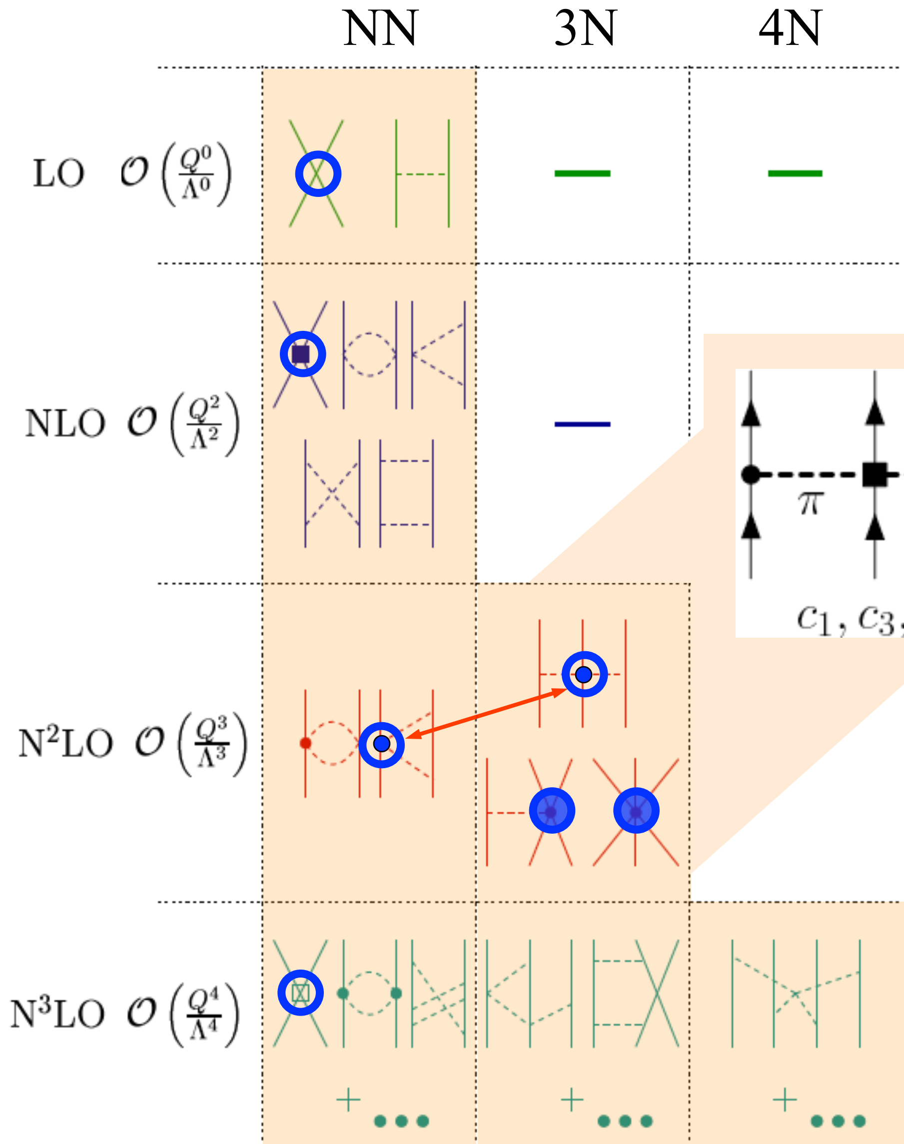
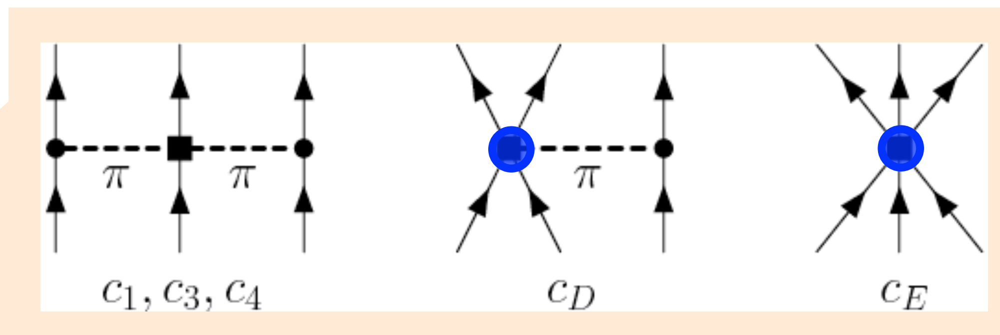


c_D, c_E don't contribute for neutrons because of Pauli principle and pion coupling to spin, also for c_4

Hebeler, AS (2010)



all 3- and 4-neutron forces are predicted to N^{3}LO!

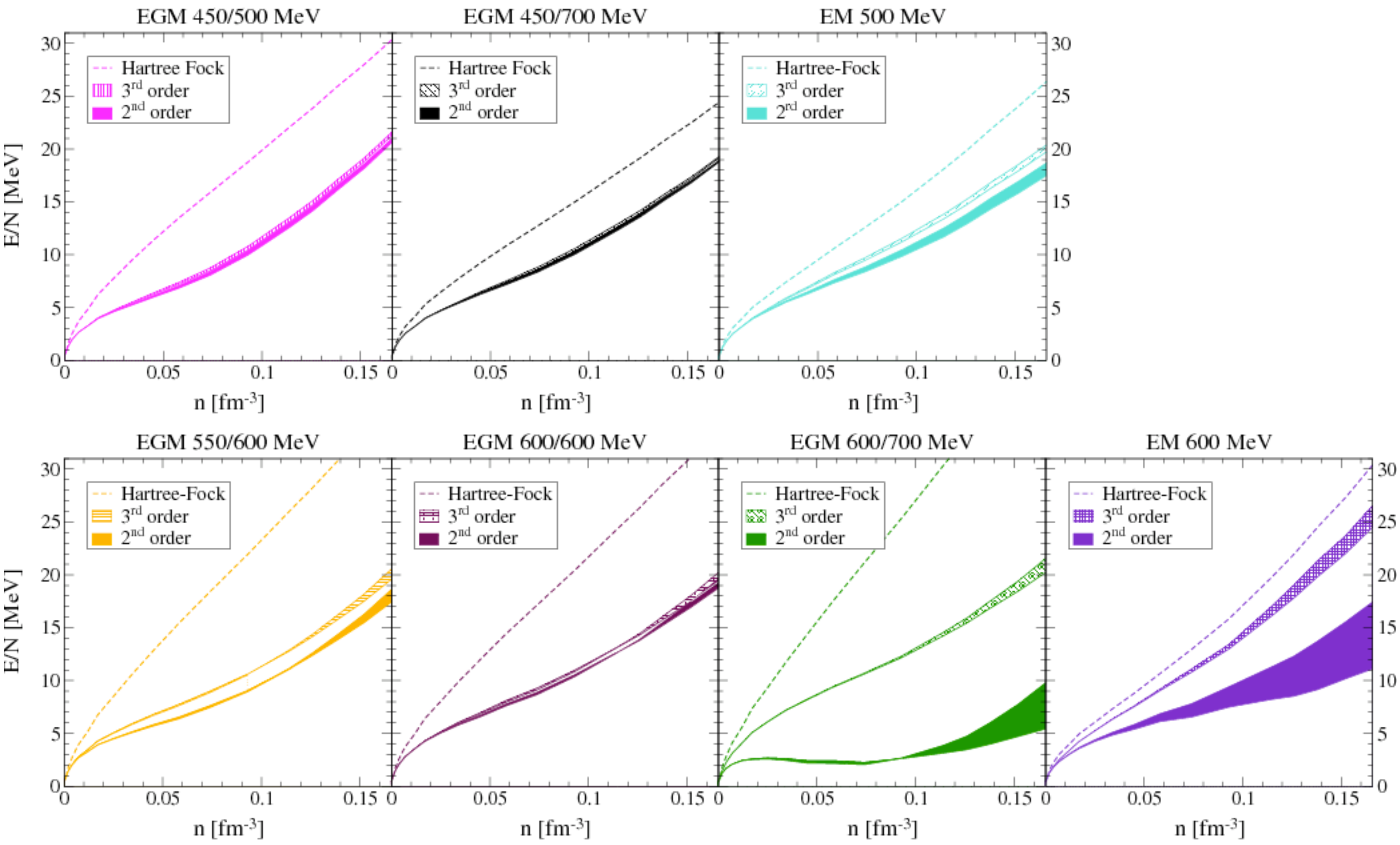
study 3N and 4N in neutron matter

Tews, Krüger, Hebeler, AS (2013) and in prep.

Weinberg, van Kolck, Kaplan, Savage, Wise, Epelbaum, Kaiser, Machleidt, Meissner,…

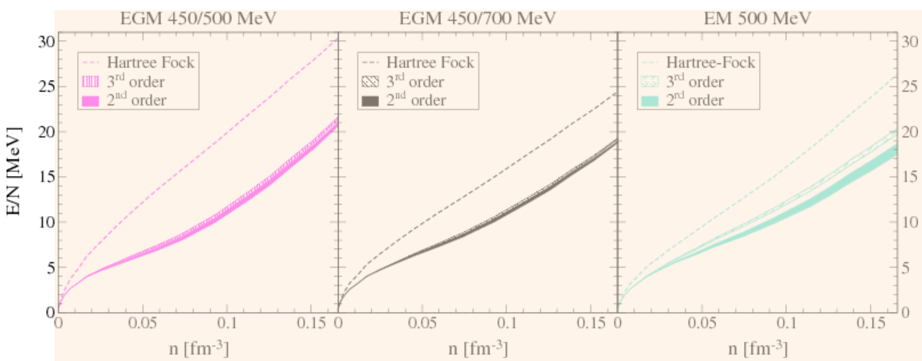
Neutron matter from chiral EFT interactions

direct calculations without RG/SRG evolution, 3N to N^2LO only

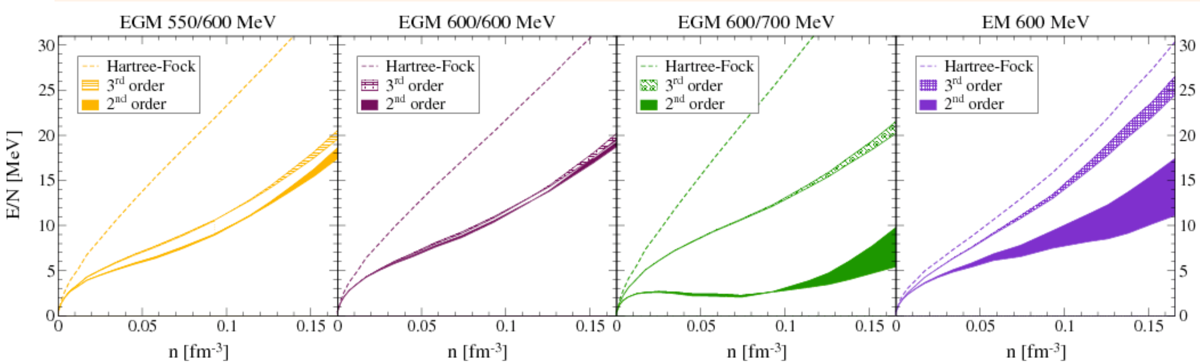


Measure of convergence and C_T values

N^3LO NN potential	$\vert\Delta E^{(2/3)}_{\text{NN-only}}\vert$	$\vert\Delta E^{(2/3)}_{\text{NN/3N}}\vert$	C_S [fm^2]	C_T [fm^2]
EGM 450/500 MeV	0.8 MeV	0.6 MeV	−4.19	−0.45
EGM 450/700 MeV	0.4 MeV	0.4 MeV	−4.71	−0.24
EM 500 MeV	1.1 MeV	1.7 MeV	−3.90	0.22
EGM 550/600 MeV	1.0 MeV	3.1 MeV	−1.24	0.36
EGM 600/600 MeV	0.2 MeV	1.5 MeV	3.45	2.07
EGM 600/700 MeV	11.4 MeV	16.1 MeV	1.31	1.00
EM 600 MeV	7.7 MeV	9.1 MeV	−3.88	0.28

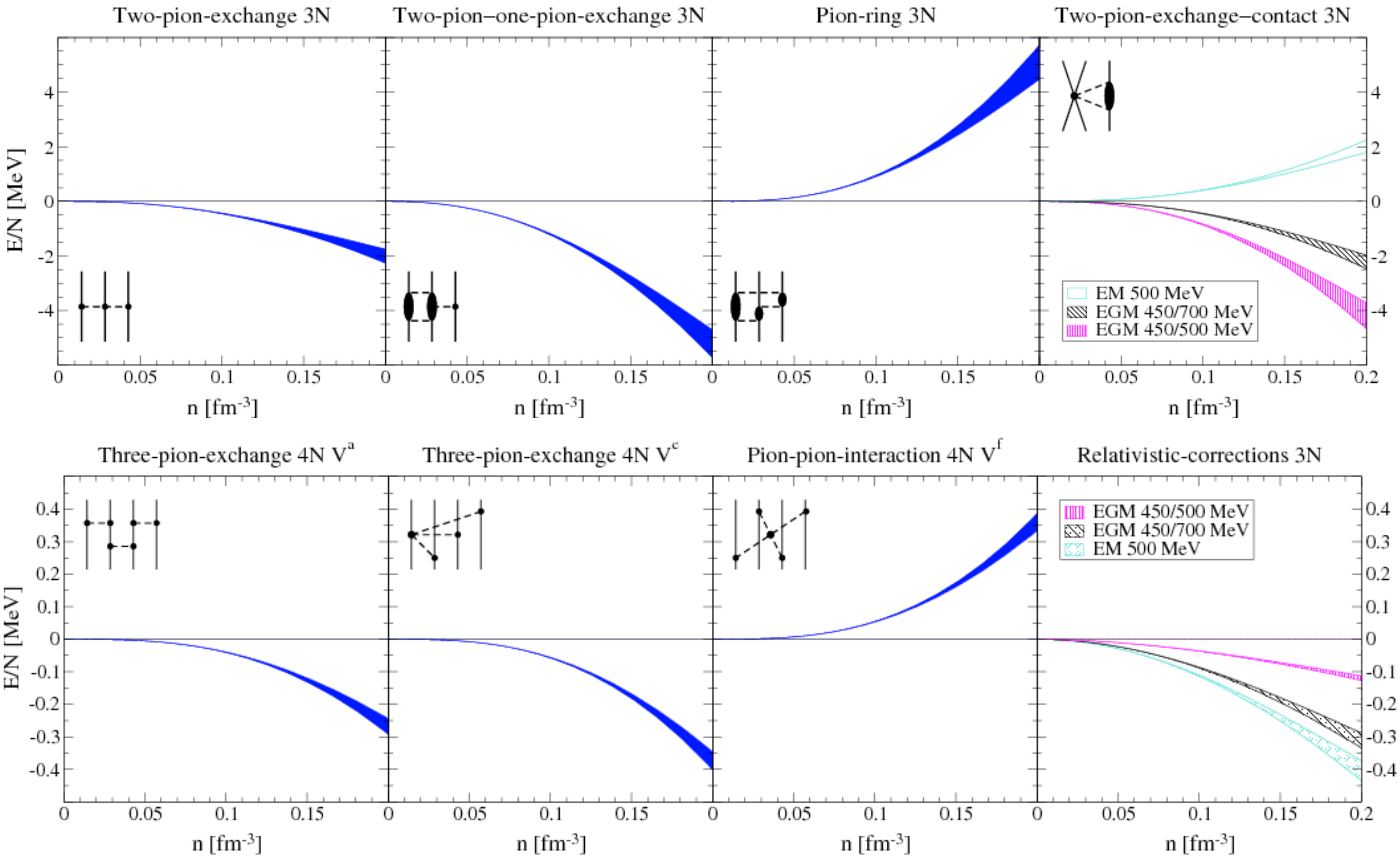


consider all NN interactions with good convergence pattern and small C_T



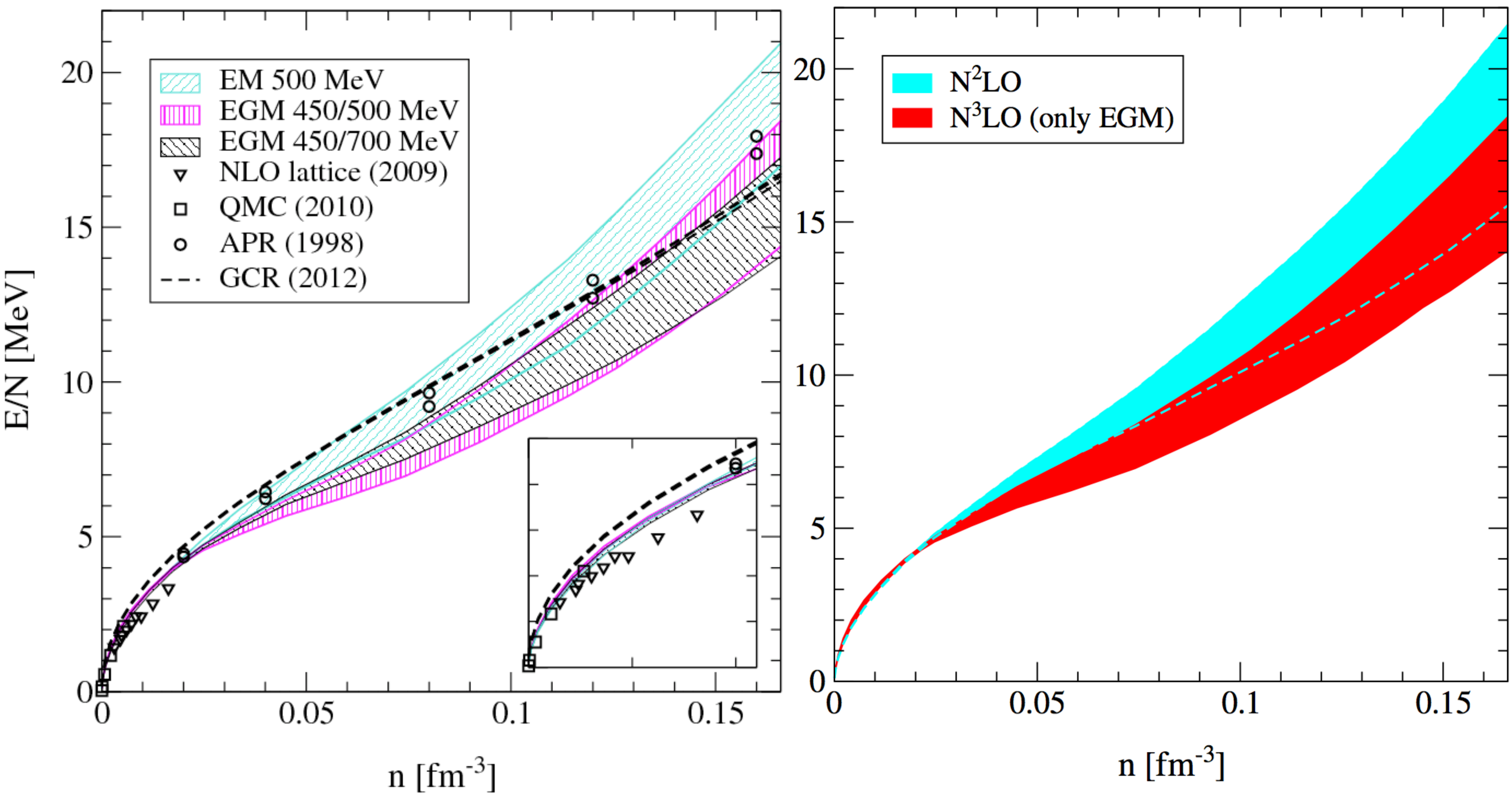
N^3LO 3N and 4N interactions in neutron matter

evaluated at Hartree-Fock level

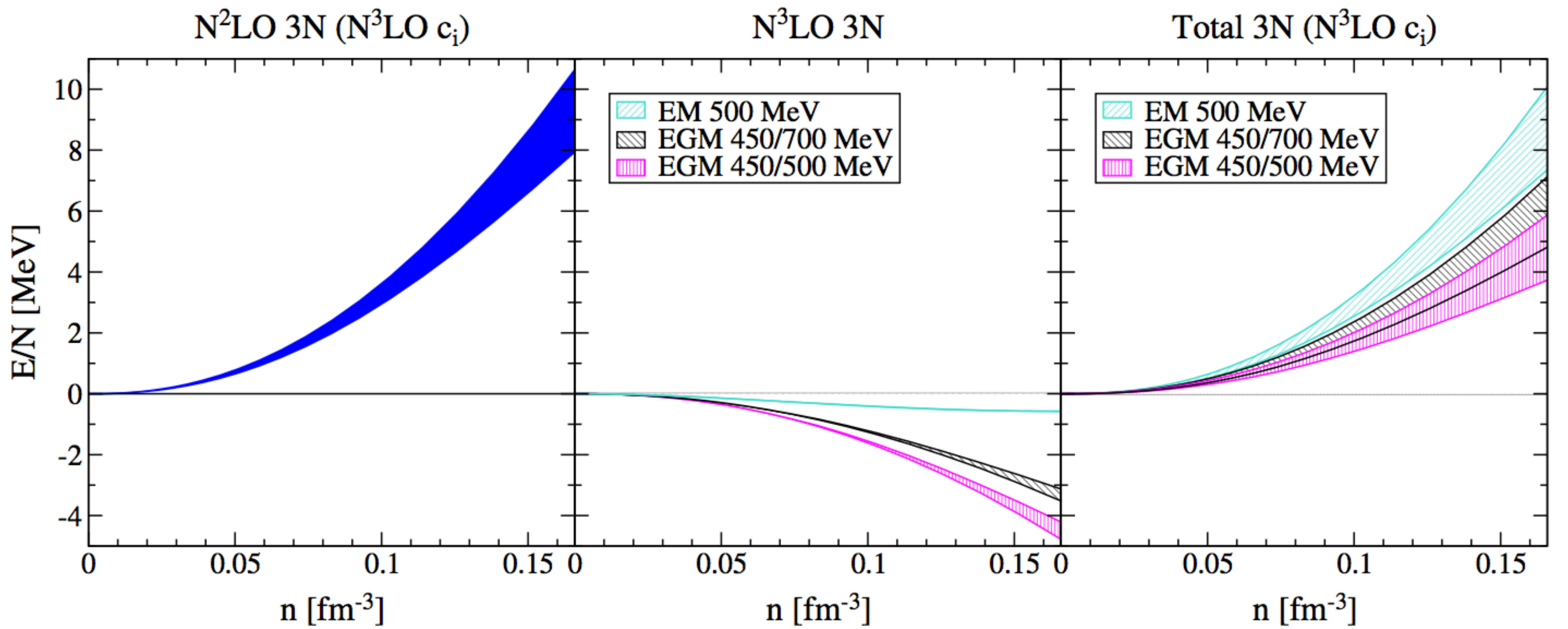


Complete N^3LO calculation of neutron matter

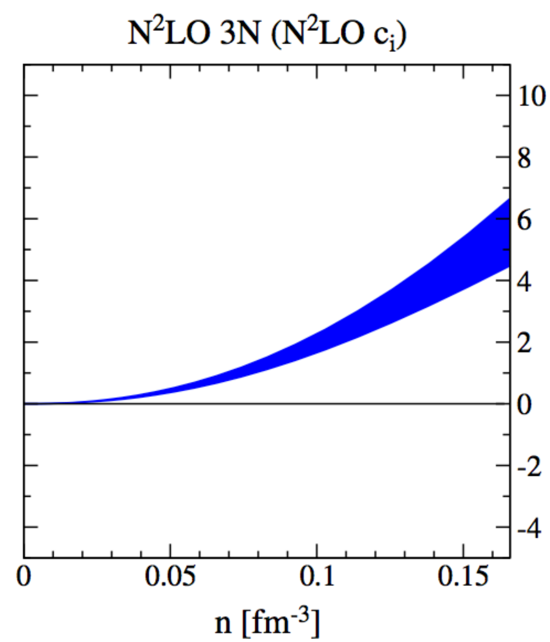
first complete N^3LO result, Hartree-Fock +2nd order +3rd order (pp+hh)
includes uncertainties from NN, 3N (dominates), 4N



N^2LO vs. N^3LO 3N

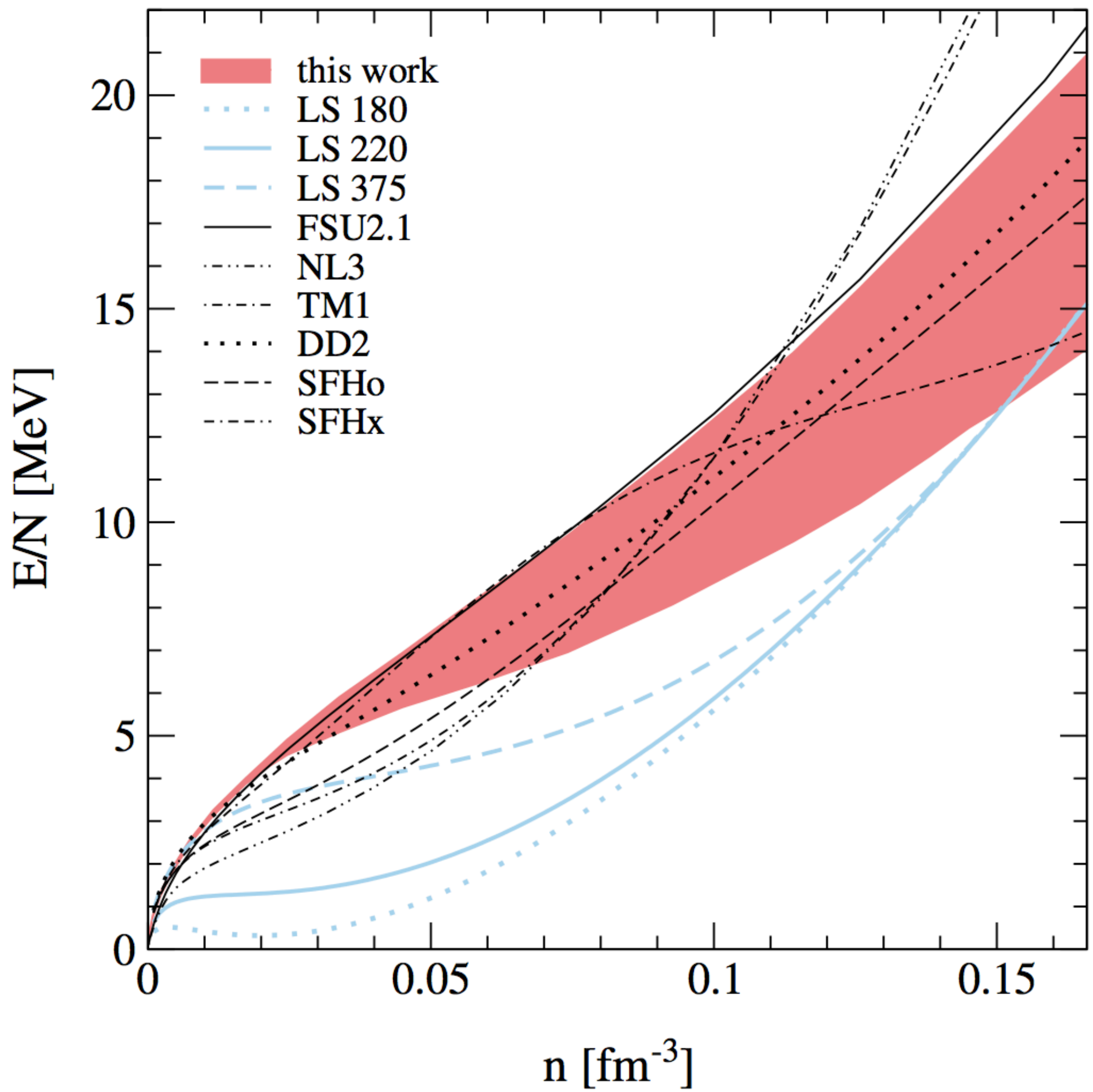


	c_1 [GeV^{-1}]	c_3 [GeV^{-1}]
N^2LO/N^3LO EGM NN [31, 32]	-0.81	-3.40
N^3LO EM NN [33, 34]	-0.81	-3.20
N^2LO KGE [39]	$-(0.26-0.58)$	$-(2.80-3.14)$
'N^2LO' KGE (recom.) [39]	$-(0.37-0.73)$	$-(2.71-3.38)$
N^3LO KGE [39]	$-(0.75-1.13)$	$-(4.77-5.51)$
N^2LO this work	$-(0.37-0.81)$	$-(2.71-3.40)$
N^3LO this work	$-(0.75-1.13)$	$-(4.77-5.51)$



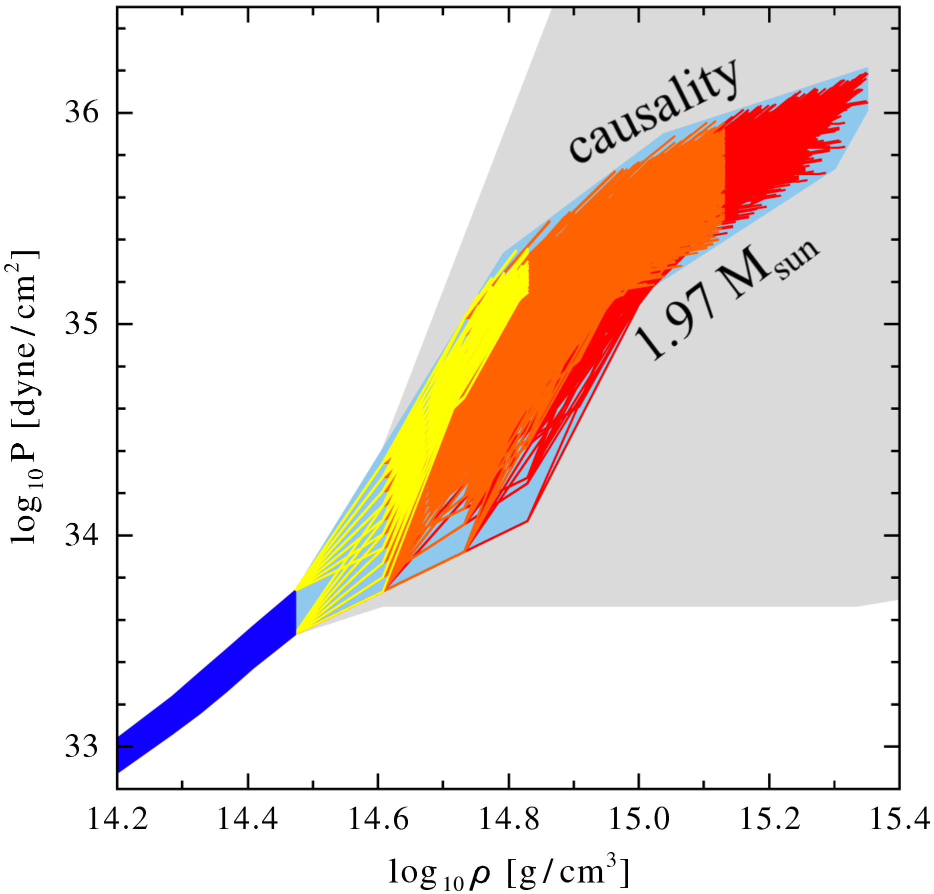
Comparisons to equations of state in astrophysics

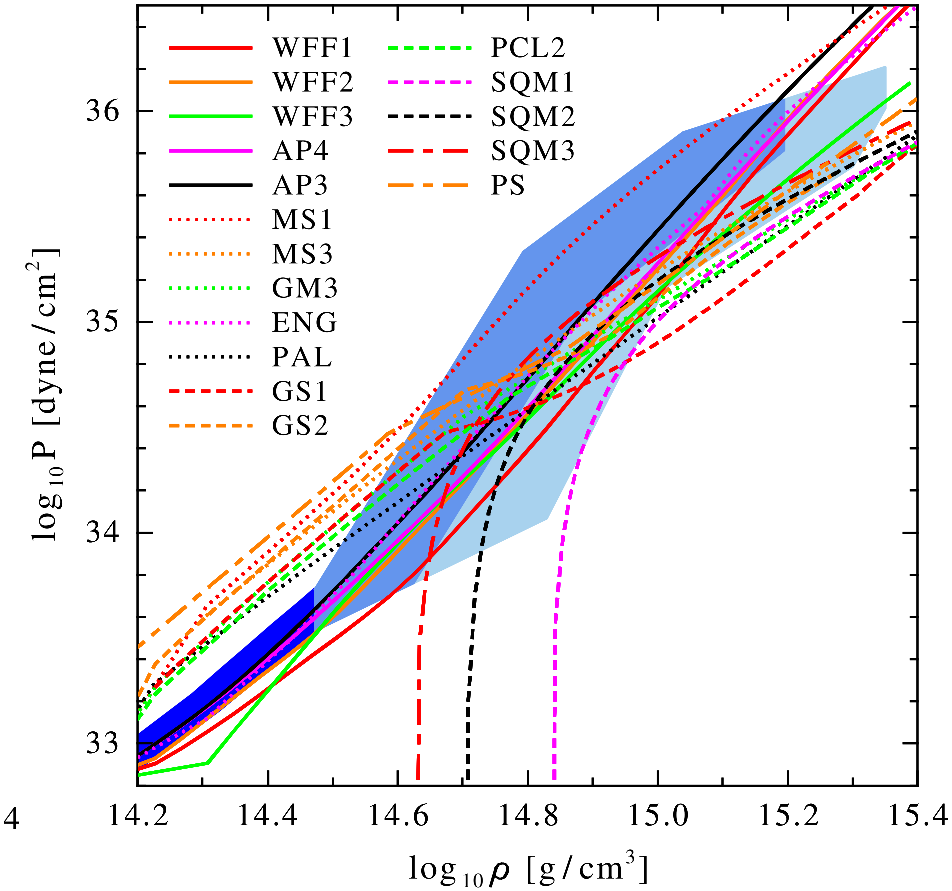
many equations of state used in supernova simulations not consistent with neutron matter results



Impact on neutron stars Hebeler, Lattimer, Pethick, AS (2010, 2013)

constrain high-density EOS by causality, require to support 1.97 M_{sun} star





low-density pressure sets scale, chiral EFT interactions provide strong constraints, ruling out many model equations of state

predicts neutron star radius: 9.7-13.9 km for M=1.4 M_{sun} (±18% !)

Neutron-star mergers and gravitational waves

explore sensitivity to neutron-rich matter in neutron-star merger and gw signal

Bauswein, Janka (2012), Bauswein, Janka, Hebeler, AS (2012).

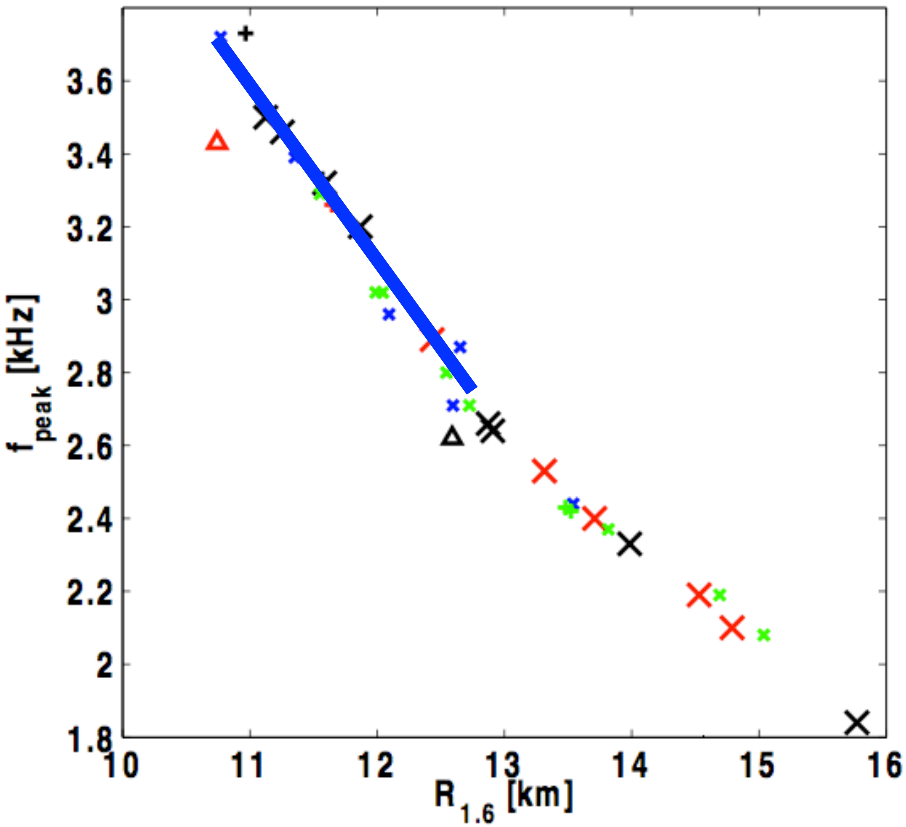


FIG. 10: Peak frequency of the postmerger GW emission versus the radius of a nonrotating NS with 1.6 $M_\odot$ for different EoSs. Symbols have the same meaning as in Fig. 8.

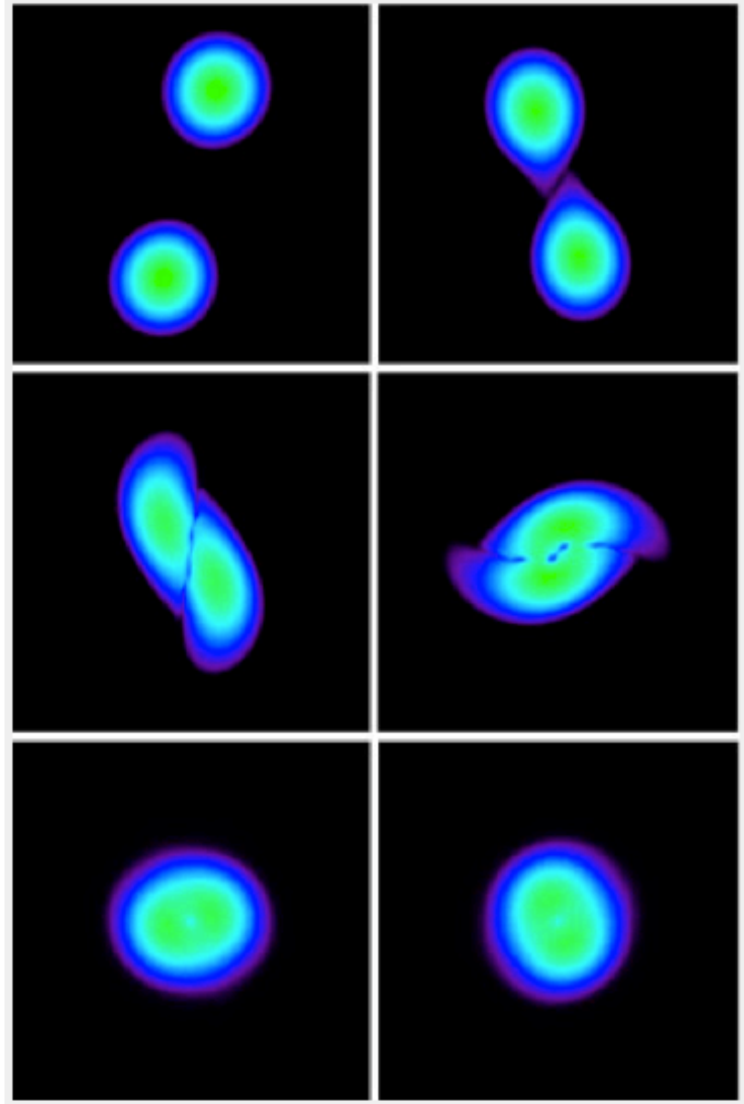


Fig. 1: Various snapshots of the collision of two neutron stars initially revolving around each other. The sequence simulated by the computer covers only 0.03 seconds. The two stars orbit each other counterclockwise (top left) and quickly come closer (top right). Finally they collide (centre left), merge (centre right), and form a dense, superheavy neutron star (bottom). Strong vibrations of the collision remnant are noticeable as deformations in east-west direction and in north-south direction (bottom panels). (Simulation: Andreas Bauswein and H.-Thomas Janka/MPA)

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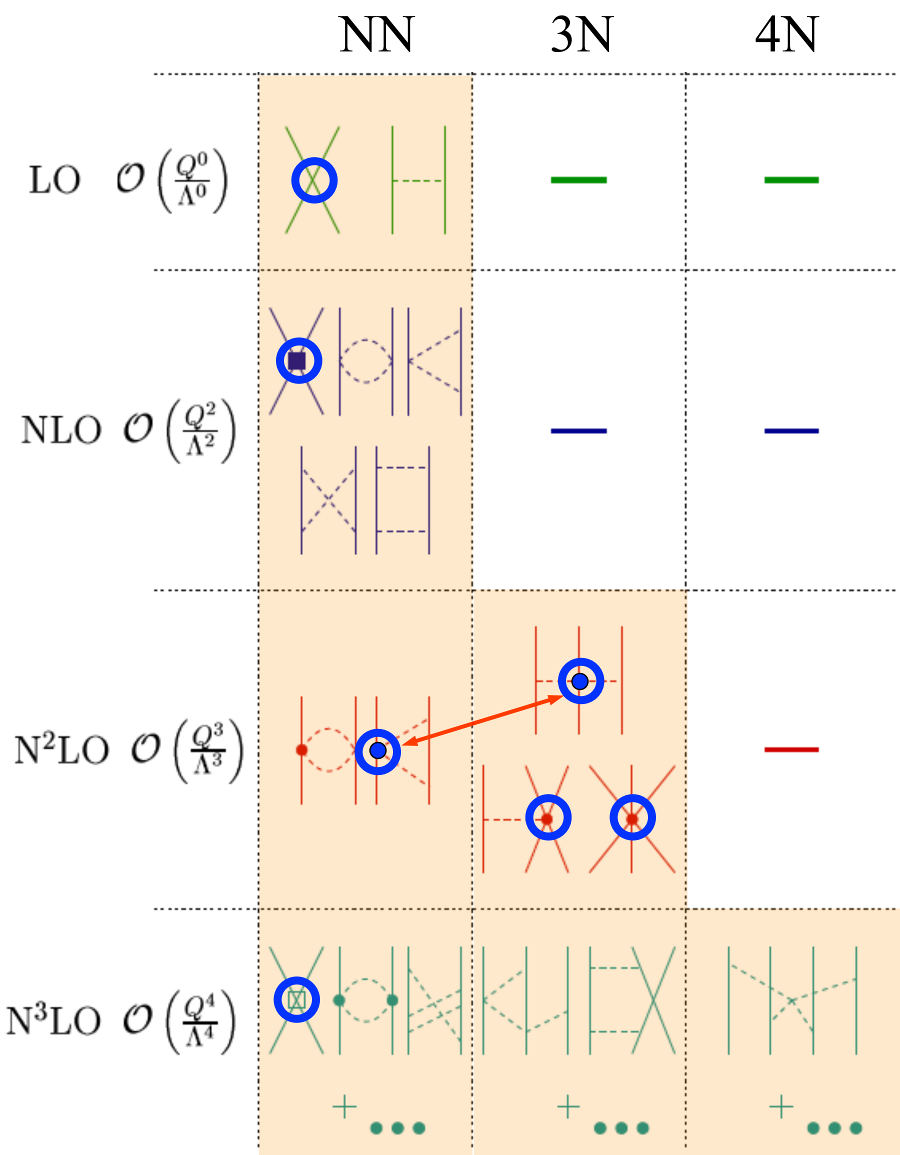
A. Gezerlis, I. Tews, E. Epelbaum, K. Hebeler, S. Gandolfi, A. Nogga, AS, arXiv:1303.6243

QMC with chiral EFT interactions - challenges



EFT includes nonlocal interactions

caused by usual regulator
on relative momenta

and k-dependent contact interactions
k=mom. transfer in exchange channel

pion exchanges to N^2LO local
except for regulator

strategies so far:
try directly in QMC
Schmidt et al.

separate local + nonlocal parts
and treat nonlocal perturbatively
Furnstahl, Wendt,…

Local chiral EFT interactions

keep pion exchanges to N^2LO local

regulate in coordinate space $f_{\text{long}}(r) = 1 - e^{-(r/R_0)^4}$

construct local contact interactions $C_S + C_T\, \boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2$

with regulator on momentum transfer $\int \frac{d\mathbf{q}}{(2\pi)^3}\, C_{S,T}\, f_{\text{local}}(q^2)\, e^{i\mathbf{q}\cdot\mathbf{r}} = C_{S,T}\, \frac{e^{-(r/R_0)^4}}{\pi\Gamma\left(\frac{3}{4}\right) R_0^3}$

at NLO use freedom to treat k^2 operators for isospin dependence

$$
\begin{aligned}
V_{\text{short}}^{\text{NLO}} &= C_1\, q^2 + C_2\, q^2\, \boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2 \\
&+ \left(C_3\, q^2 + C_4\, q^2\, \boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2\right) \boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2 \\
&+ i\, \frac{C_5}{2}\, (\boldsymbol{\sigma}_1 + \boldsymbol{\sigma}_2) \cdot \mathbf{q} \times \mathbf{k} \\
&+ C_6\, (\boldsymbol{\sigma}_1 \cdot \mathbf{q})(\boldsymbol{\sigma}_2 \cdot \mathbf{q}) \\
&+ C_7\, (\boldsymbol{\sigma}_1 \cdot \mathbf{q})(\boldsymbol{\sigma}_2 \cdot \mathbf{q})\, \boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2\,,
\end{aligned}
$$

TABLE I. Short-range couplings for $R_0 = 1.2\,\text{fm}$ at LO, NLO, and N^2LO (with a spectral-function cutoff $\widetilde{\Lambda} = 800\,\text{MeV}$) [30]. The couplings C_{1-7} are given in fm^4 while the rest are in fm^2.

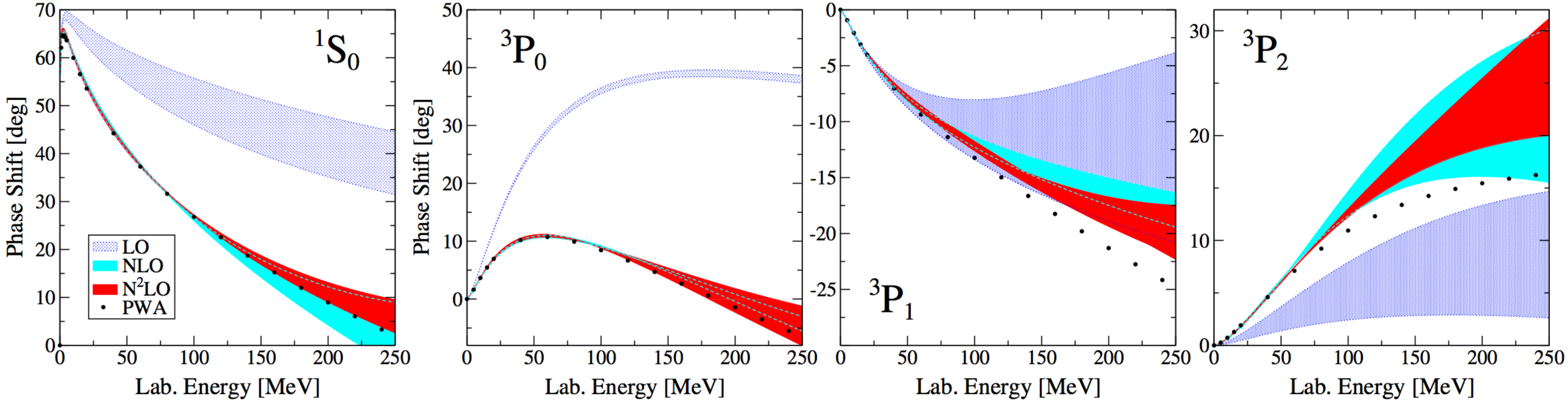
	LO	NLO	N^2LO
C_S	−1.83406	−0.64687	1.09225
C_T	0.15766	0.58128	0.24388
C_1		0.18389	−0.13784
C_2		0.15591	0.07001
C_3		−0.13768	−0.13017
C_4		0.02811	0.02089
C_5		−1.99301	−1.82601
C_6		0.26774	0.18700
C_7		−0.25784	−0.24740
C_{nn}			0.05009

M. Freunek, Diploma Thesis (2007)

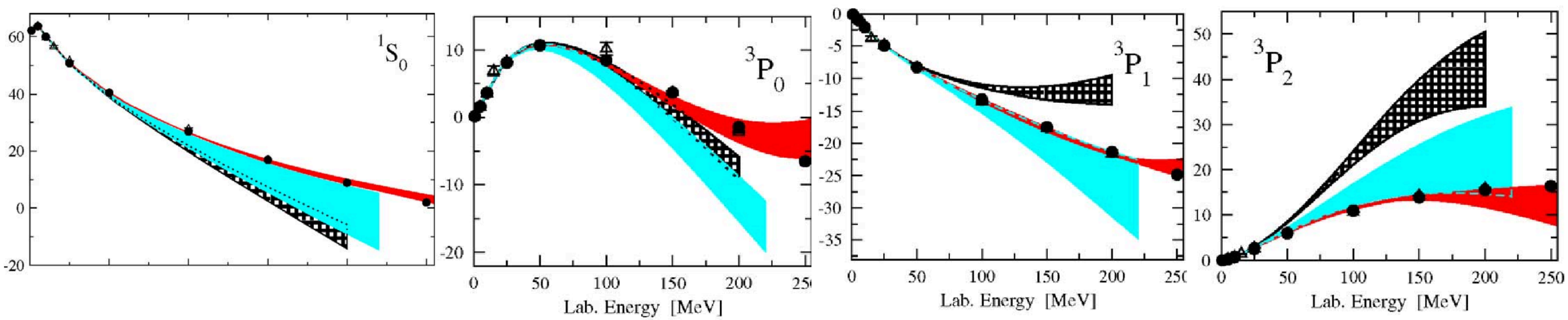
Phase shift fits

fit to E_{lab}=1, 5, 10, 25, 50, 100 MeV, SF cutoff = 800 MeV

vary R_0 from 0.8-1.2 fm, corresponds to ~600-400 MeV



considerably better than EGM N^2LO potentials



Auxiliary Field Diffusion Monte Carlo

A. Gezerlis, S. Gandolfi

AFDMC: Hubbard-Stratonovich transformation using auxiliary fields to change quadratic spin-isospin operator dependences to linear

include full interaction at LO, NLO, and N^2LO in propagator
NN interactions only, next:3N

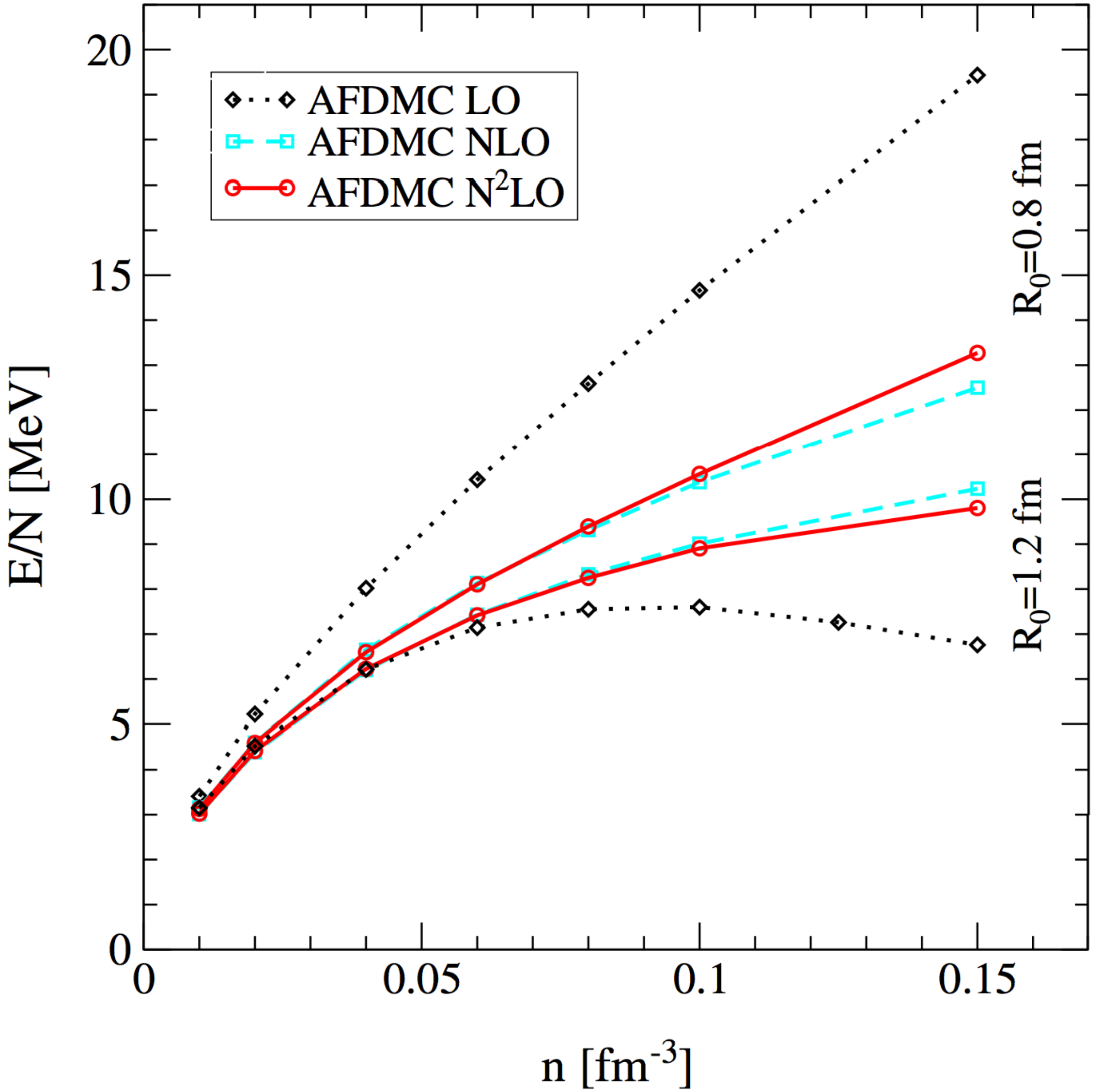
next: test which parts of chiral EFT interactions are perturbative
(N^3LO contributions will have nonlocal parts)

optimal number of 66 particles,
include contributions from 26 neighboring cells of simulation box

statistical uncertainty smaller than points
no to full Jastrow: 0.1-0.5 MeV (1-5%) for R_0=1.2-0.8 fm

AFDMC results for neutron matter

order-by-order convergence up to saturation density

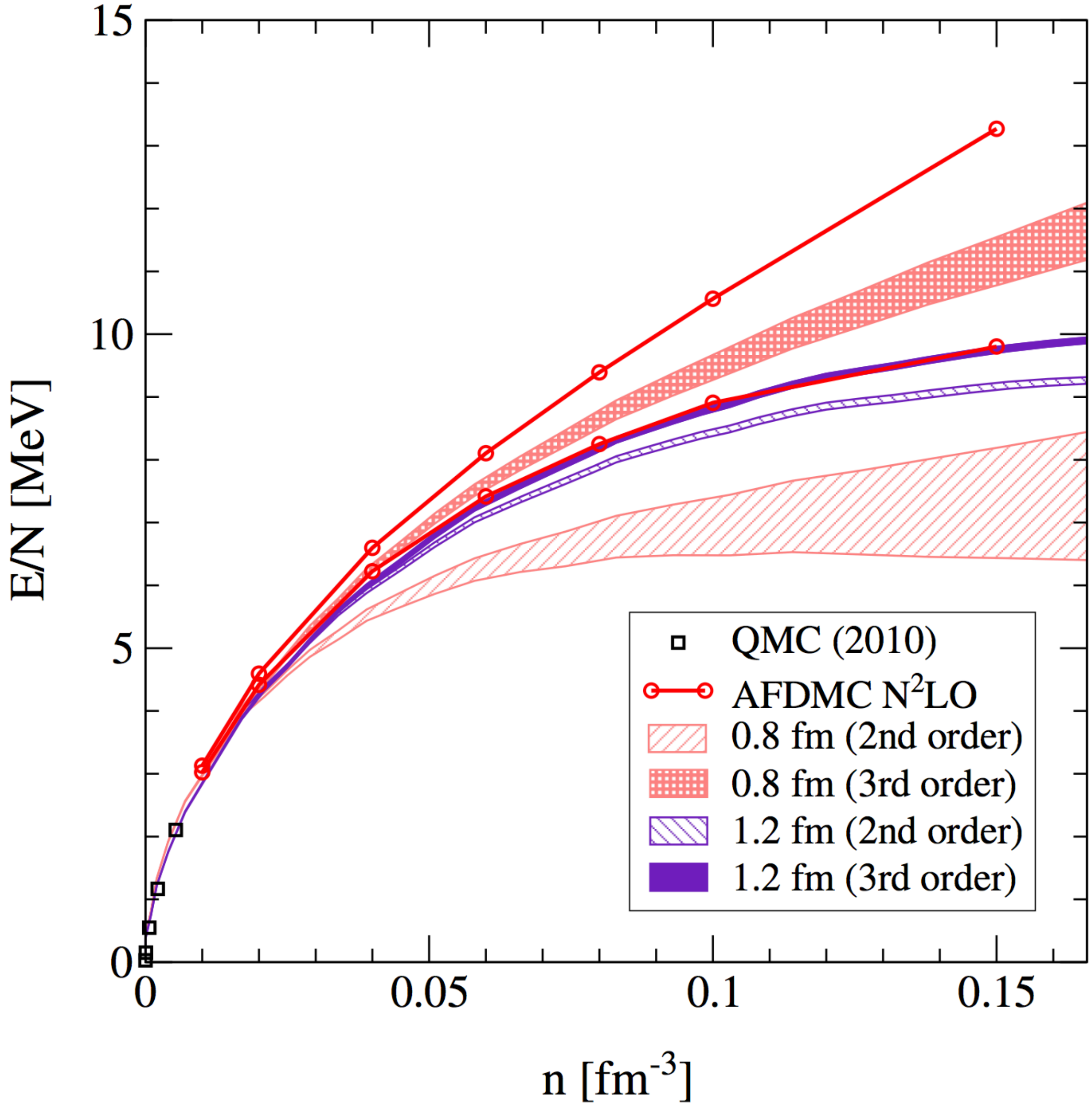


bands similar to phase shift bands

NLO ~ N^2LO due to large c_i

Comparison to perturbative calculations at N^2LO

Hartree-Fock +2nd order +3rd order (pp+hh), same as for N^3LO calcs.



band at each order from free to HF spectrum

low cutoffs (400 MeV)
3rd order corr. small,
excellent agreement
with AFDMC

Summary

3N forces key for neutron-rich nuclei
J.D. Holt, J. Menendez, T. Otsuka, J. Simonis, T. Suzuki

Neutron matter constrains neutron stars and astrophysics,
first complete N^3LO calculation
I. Tews, T. Krüger, K. Hebeler, J.M. Lattimer, C.J. Pethick

First QMC calculations with chiral EFT interactions for neutron matter
validates perturbative calculations for low cutoffs
A. Gezerlis, I. Tews, E. Epelbaum, K. Hebeler, S. Gandolfi, A. Nogga