

Many-Body Perturbation Theory for Nuclear Matter at High Orders



Christian Drischler

with K. Hebeler and A. Schwenk

New Ideas in Constraining Nuclear Forces
ECT* – Workshop, Trento, June 6, 2018



Astrophysics
neutron stars,
masses, radii, ...

Nuclear Matter
equation of state,
saturation, ...

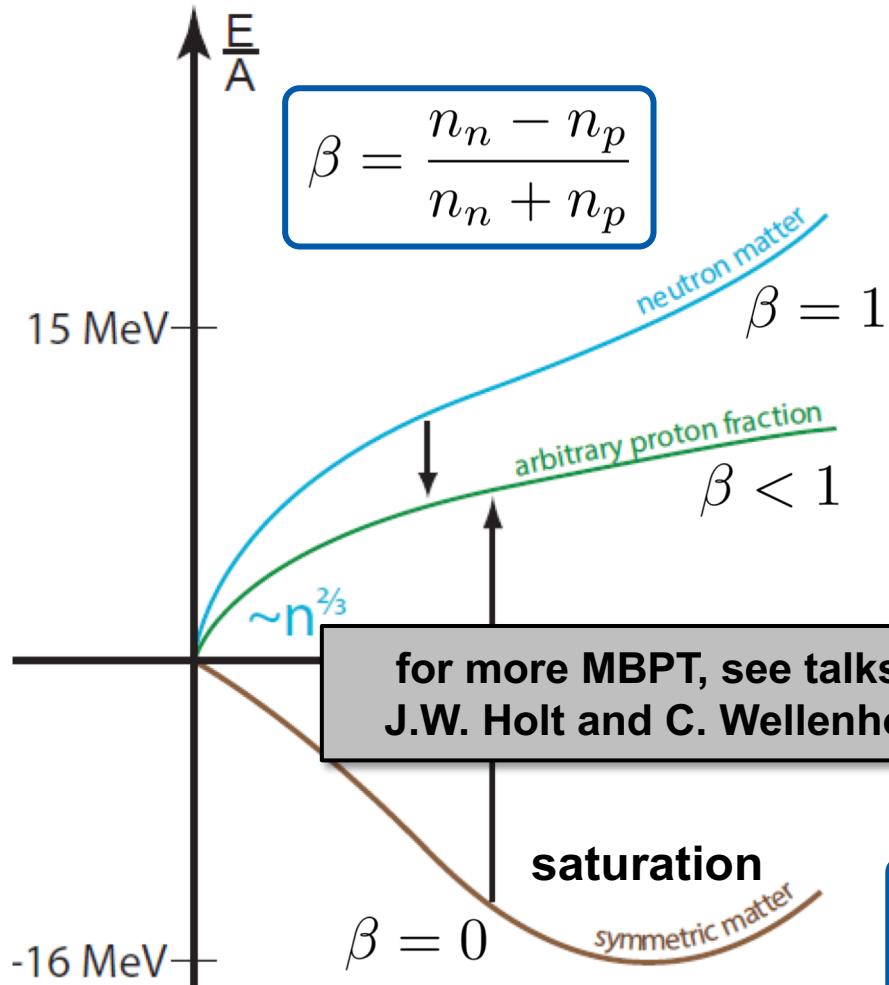
Nuclear Forces
(QCD,) EFT, ...

Finite Nuclei
binding energies,
radii

Many-Body Perturbation Theory for Nuclear Matter at High Orders

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Homogeneous nuclear matter



- theoretical **testbed** for benchmarking nuclear forces
 - saturation point (n_0, a_v)
 - incompressibility (K)
 - symmetry energy (S_v) and its slope (L) at saturation density
- **many-body perturbation theory**, but also in QMC, CC, SCGF, ...

for a recent review see:
Hebeler *et al.*, Annu. Rev. Nucl. Part. Sci. **65**, 457

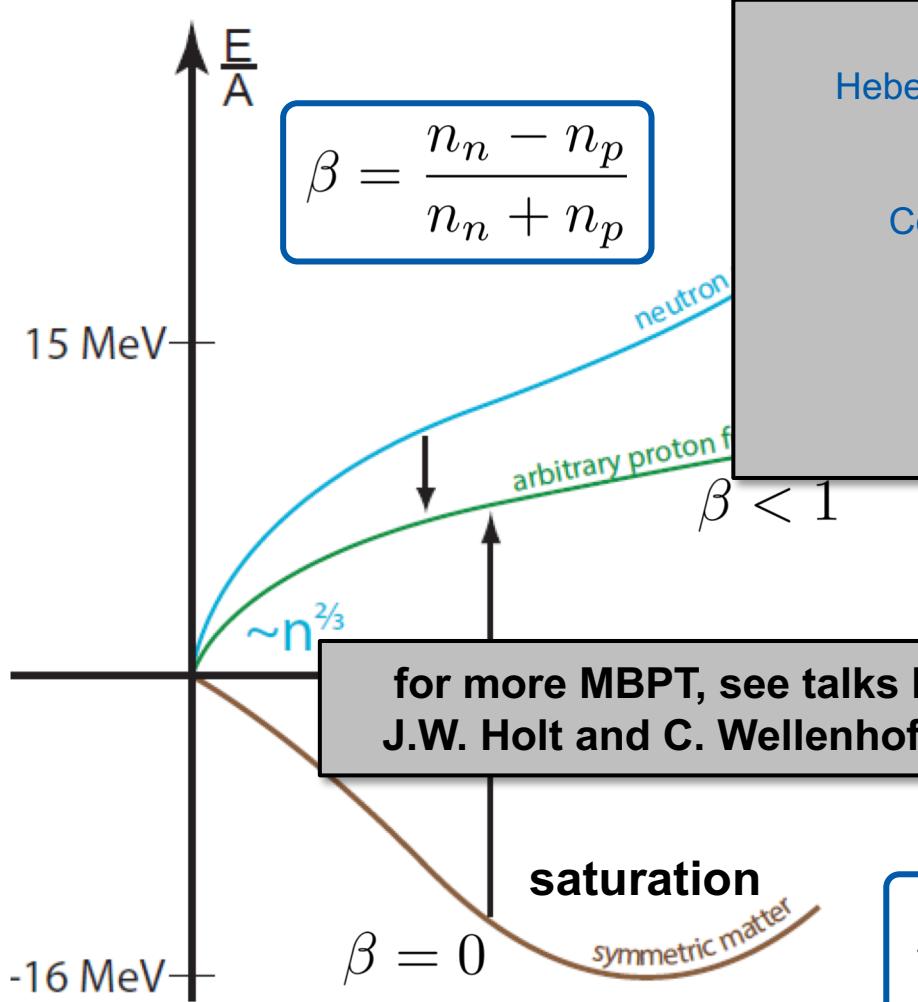
Bethe–Weizsäcker formula

$$\frac{E}{A}(\beta, n) = \frac{E}{A}(\beta = 0, n) + \beta^2 E_{\text{sym}}(n)$$

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Homogeneous nuclear matter



(Recent) MBPT calculations in MBPT

Hebeler, Bogner, Furnstahl, Nogga *et al.*, PRC **83**, 031301
Tews, Krüger, Hebeler, Schwenk, PRL **110**, 032504
Krüger, Tews, Hebeler, Schwenk, PRC **88**, 025802
Coraggio, Holt, Itaco, Machleidt *et al.*, PRC **89**, 044321
Wellenhofer, Holt, Kaiser, PRC **92**, 015801
CD, Carbone, Hebeler, Schwenk, PRC **94**, 054307
Holt, Kaiser, PRC **95**, 034326
Dyhdalo, Bogner, Furnstahl, PRC **96**, 054005
...

- many-body perturbation theory,
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Bethe–Weizsäcker formula

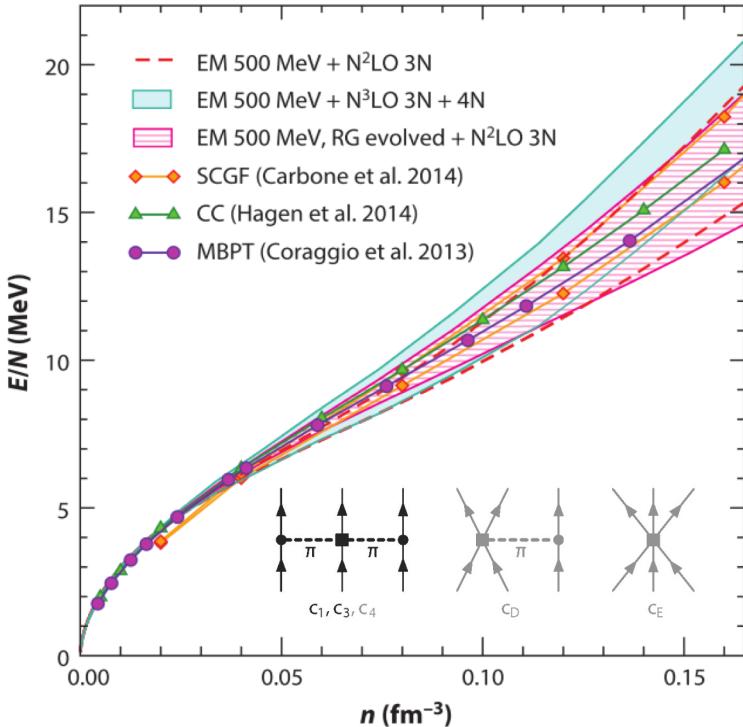
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Neutron-matter EOS

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Hebeler *et al.*, Annu. Rev. Nucl. Part. Sci. **65**, 457



for QMC see, e.g., Tews *et al.* PRC **93**, 024305

Remarkable agreement between
many-body frameworks and **different**
Hamiltonians

situation is different in **symmetric matter**

Improvements in MBPT needed:

- 1 Explore new ($N^3\text{LO+}$) potentials
- 2 Treatment of NN+3N & 4N forces
- 3 Computationally efficient tools



**Push state-of-the-art MBPT
calculations to higher orders**

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Progress in nuclear potentials

Semilocal momentum-space regularized chiral two-nucleon potentials up to fifth order

P. Reinert,^{1,*} H. Krebs,^{1,†} and E. Epelbaum^{1,‡}

¹*Institut für Theoretische Physik II, Ruhr-Universität Bochum, D-44780 Bochum, Germany*

High-quality two-nucleon potentials up to fifth order of the chiral expansion

D. R. Entem,^{1,*} R. Machleidt,^{2,†} and Y. Nosyk²

¹*Grupo de Física Nuclear, IUFFyM, Universidad de Salamanca, E-37008 Salamanca, Spain*

²*Department of Physics, University of Idaho, Moscow, Idaho 83844, USA*

(Received 20 March 2017; revised manuscript received 30 May 2017; published 10 August 2017)

Δ isobars and nuclear saturation

A. Ekström,¹ G. Hagen,^{2,3} T. D. Morris,^{2,3} T. Papenbrock,^{2,3} and P. D. Schwartz^{2,3}

¹*Department of Physics, Chalmers University of Technology, SE-412 96 Göteborg, Sweden*

²*Physics Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, USA*

³*Department of Physics and Astronomy, University of Tennessee, Knoxville, Tennessee 37996, USA*

e.g., Carlsson, Ekström, Entem, Epelbaum, Forssén, Gezerlis, Krebs, Machleidt, Tews



Many-Body Perturbation Theory for Nuclear Matter at High Orders



Progress in nuclear potentials

Semilocal momentum-space regularized chiral two-nucleon potentials up to fifth order

Three-nucleon force in chiral EFT with explicit $\Delta(1232)$ degrees of freedom:
Longest-range contributions at fourth order

H. Krebs,^{1,*} A. M. Gasparyan,^{1,2,†} and E. Epelbaum^{1,‡}

¹*Institut für Theoretische Physik II, Ruhr-Universität Bochum, D-44780 Bochum, Germany*

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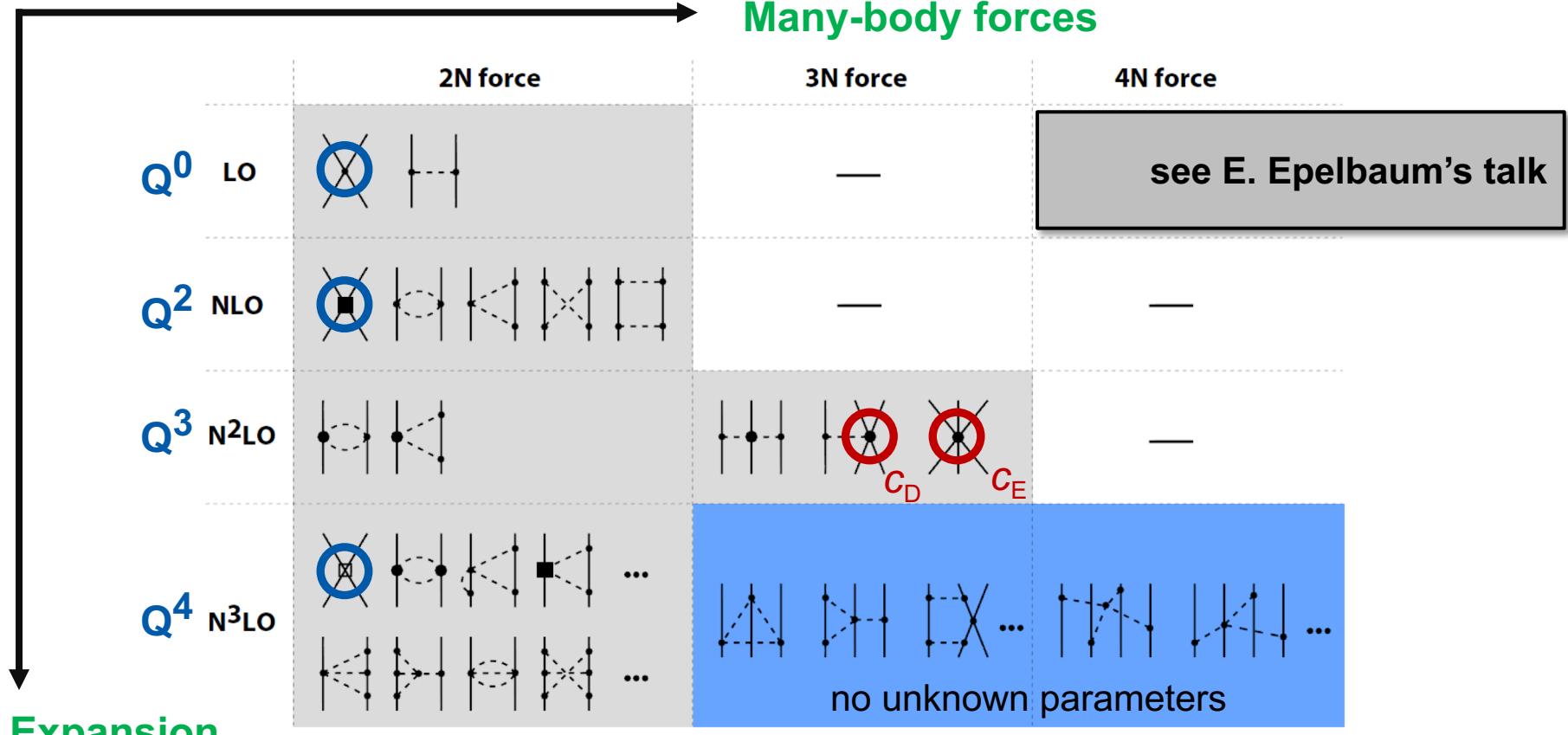


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Hierarchy of nuclear forces

e.g., Epelbaum, Hammer, Meißner, RMP 81, 1773



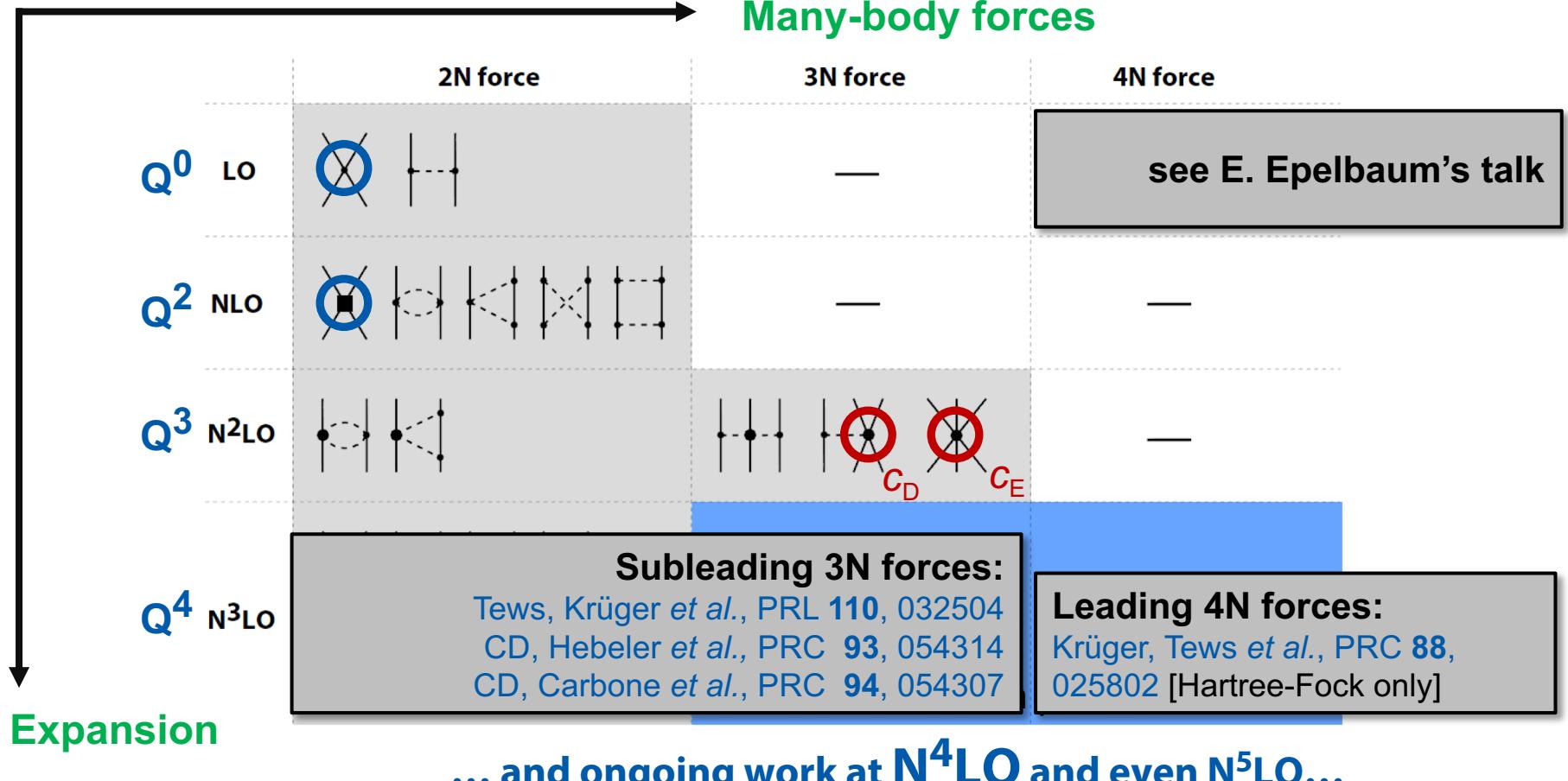
Weinberg, van Kolck, Kaplan, Savage, Wise, Bernard, Epelbaum, Kaiser, Krebs, Machleidt, Meißner, ...

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Many-Body Perturbation Theory for Nuclear Matter at High Orders

Neutron star radii



Abbott *et al.* (LIGO/Virgo), arXiv:1805.11581

for QMC, see: Gandolfi *et al.*, Phys. Rev. C **85**, 032801

GW170817: Measurements of neutron star radii and equation of state

The LIGO Scientific Collaboration and The Virgo Collaboration
(compiled 30 May 2018)

On August 17, 2017, the LIGO and Virgo observatories made the first direct detection of gravitational waves from the coalescence of a neutron star binary system. The detection of this gravitational wave signal, GW170817, offers a novel opportunity to directly probe the properties of matter at the extreme conditions found in the interior of these stars. The initial, minimal-assumption analysis of the LIGO and Virgo data placed constraints on the tidal effects of the coalescing bodies, which were then translated to constraints on neutron star radii. Here, we expand upon previous analyses by working under the hypothesis that both bodies were neutron stars that are described by the same equation of state and have spins within the range observed in Galactic binary neutron stars. Our analysis employs two methods: the use of equation-of-state-insensitive relations between various macroscopic properties of the neutron stars and the use of an efficient parameterization of the defining function $p(\rho)$ of the equation of state itself. From the LIGO and Virgo data alone and the first method, we measure the two neutron star radii as $R_1 = 10.8_{-1.7}^{+2.0}$ km for the heavier star and $R_2 = 10.7_{-1.5}^{+2.1}$ km for the lighter star at the 90% credible level. If we additionally require that the equation of state supports neutron stars with masses larger than $1.97 M_\odot$ as required from electromagnetic observations and employ the equation of state parametrization, we further constrain $R_1 = 11.9_{-1.4}^{+1.4}$ km and $R_2 = 11.9_{-1.4}^{+1.4}$ km at the 90% credible level. Finally, we obtain constraints on $p(\rho)$ at supranuclear densities, with pressure at twice nuclear saturation density measured at $3.5_{-1.7}^{+2.7} \times 10^{34}$ dyn cm $^{-2}$ at the 90% level.

see talk by J.W. Holt

Hebeler *et al.*, Astrophys. J. **773**, 11

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Neutron star radii

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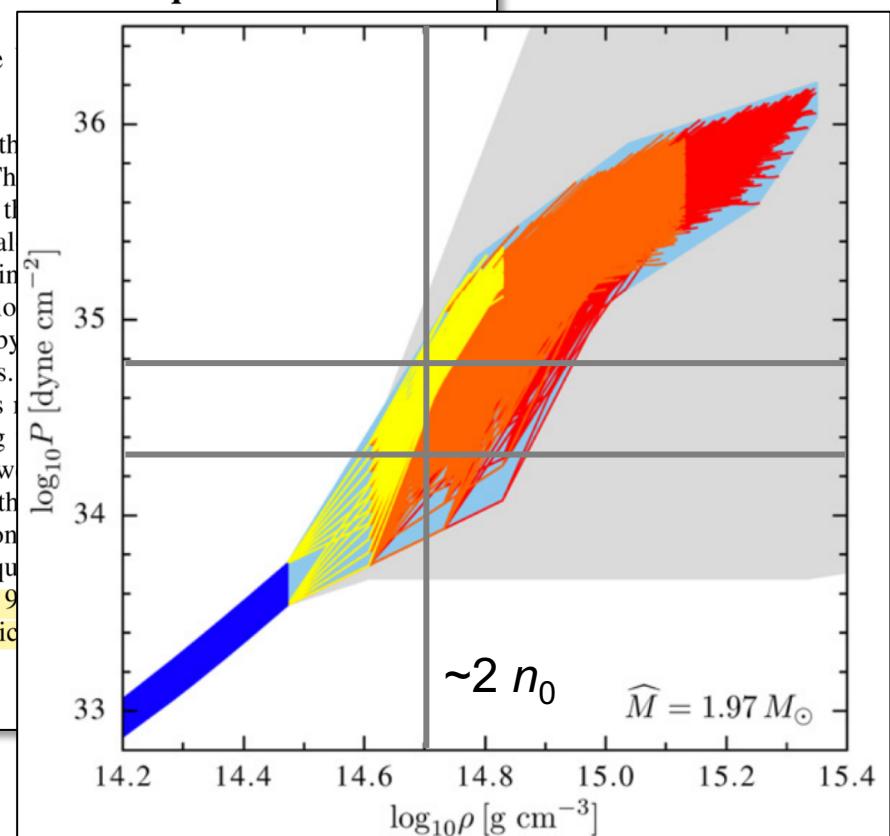
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see talk by J.W. Holt

Hebeler *et al.*, Astrophys. J. 773, 11

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3N contributions beyond Hartree-Fock

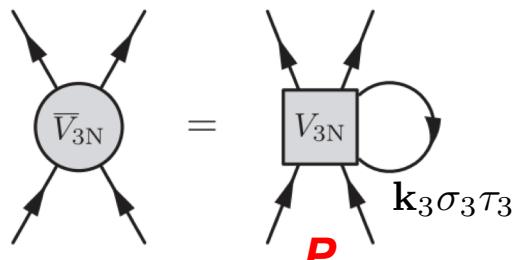
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CD, Hebeler, Schwenk, PRC **93**, 054314

Apply Wick's theorem:
normal-ordered NN level

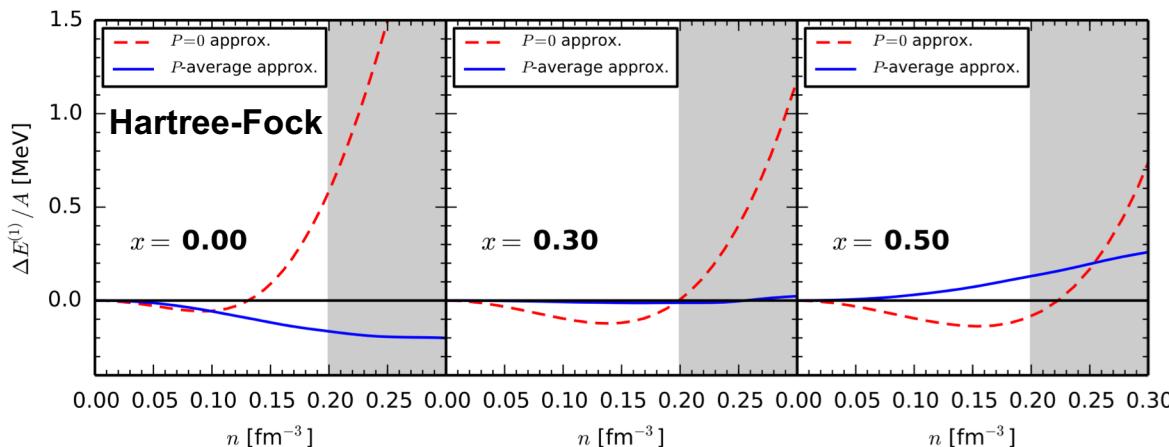
$$\overline{V}_{\text{as}} = V_{\text{NN}} + \xi \overline{V}_{3\text{N}}$$

initial NN potential
normal-ordered 3N forces
combinatorial factor



$$\overline{V}_{3\text{N}} = \text{Tr}_{\sigma_3} \text{Tr}_{\tau_3} \int \frac{d\mathbf{k}_3}{(2\pi)^3} n_{\mathbf{k}_3}^{\tau_3} \mathcal{A}_{123} V_{3\text{N}}$$

only approx. included: $P=0$ (operat., N²LO)
or P angle-averaged (PW basis, N²LO & N³LO)



Holt *et al.*, PRC **81**, 024002
Hebeler *et al.*, PRC **82**, 014314

N³LO 3N matrix elements:
Hebeler *et al.*, PRC **91**, 044001

Residual contributions
exact normal-ordering
4N forces

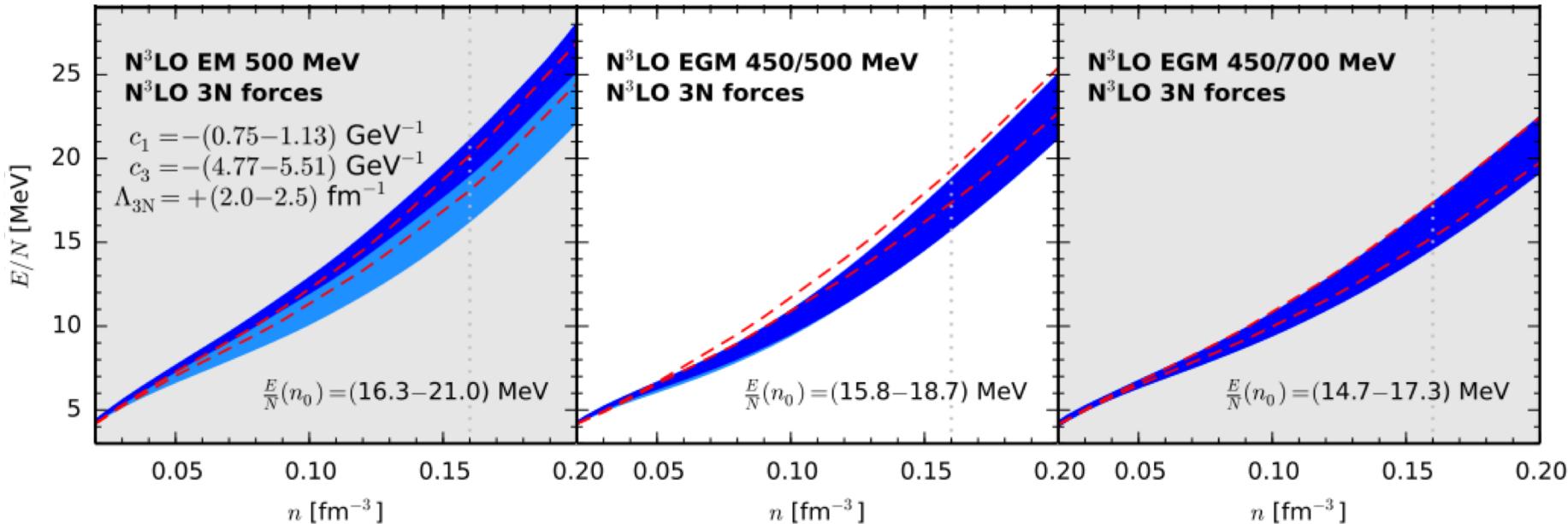


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Neutron matter: MB convergence

CD, Carbone, Hebeler, Schwenk, PRC **94**, 054307



Contributions from NN+3N forces up to 3rd order: (ladders only)

- based on N³LO NN potentials plus **leading/subleading** 3N forces
- MBPT **well converged** for EGM potentials
- 3rd-order contribution: important for EM 500 MeV (less perturbative)

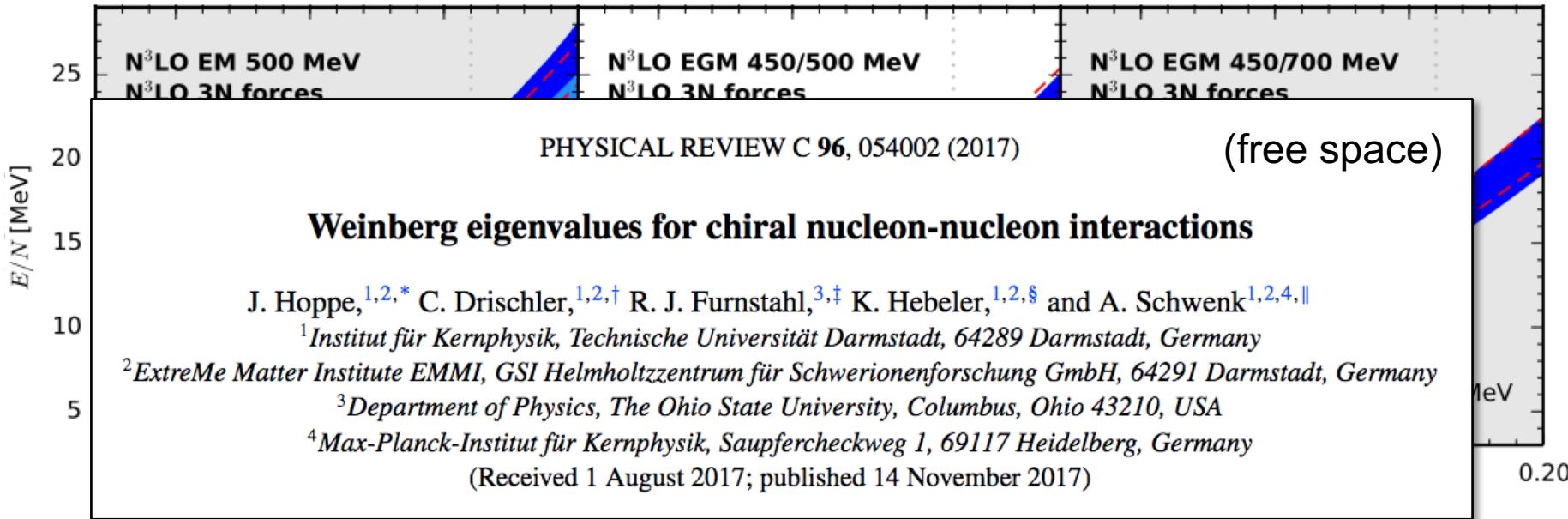
see also: Tews *et al.*, PRL **110**, 032504; Krüger *et al.*, PRC **88**, 025802

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Number of diagrams in MBPT



Stevenson, Int. J. Mod. Phys. C 14, 1135

The number of diagrams increases rapidly!

$\times 2^n$

1, 3, 39, 840, 27 300, 1 232 280, ...

$n = 2 \quad 3 \quad 4 \quad 5 \quad 6 \quad 7$

Integer sequence A064732:
Number of labeled Hugenholtz diagrams with n nodes.

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Significant challenges remain!

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CD, Hebeler, Schwenk, arXiv:1710.08220



Higher orders: particle-hole contributions

Coraggio *et al.*, PRC **89**, 044321; Holt, Kaiser, PRC **95**, 034326



Approximated normal-ordering

Holt *et al.*, PRC **81**, 024002; Hebeler, Schwenk, PRC **82**, 014314



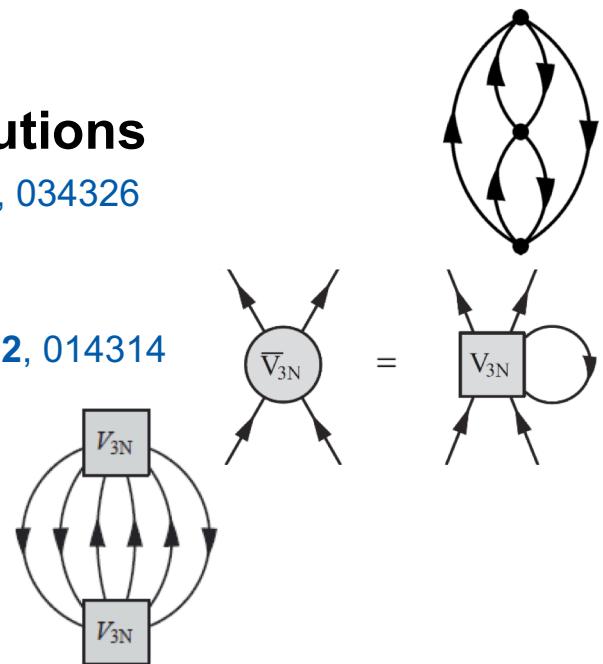
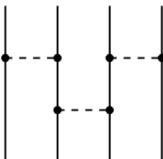
Neglected residual 3N diagrams

Hagen *et al.*, PRC **89**, 014319; Kaiser, EPJ A **48**, 58



Higher many-body forces

Hebeler *et al.*, PRC **91**, 044001



development of a novel
Monte-Carlo framework

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Efficient Monte-Carlo framework

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CD, Hebeler, Schwenk, arXiv:1710.08220

represent interactions as matrices **in spin-isospin space**

- using analytic expressions: **NN**, **3N**, **4N** forces (nonlocal) up to N³LO
- matrix elements: analytic functions of the single-particle momenta (in C⁺⁺)
- alternatively, **partial-wave summation** can be used

$$\langle (\sigma'_1 \tau'_1) \dots (\sigma'_A \tau'_A) | \mathcal{A}_A V_{\text{AN}} (\bar{\mathbf{p}}, \bar{\mathbf{p}}') | (\sigma_1 \tau_1) \dots (\sigma_A \tau_A) \rangle$$

analytic form of the
forces & diagrams

automatic code
generation

optimized
computation

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Efficient Monte-Carlo framework



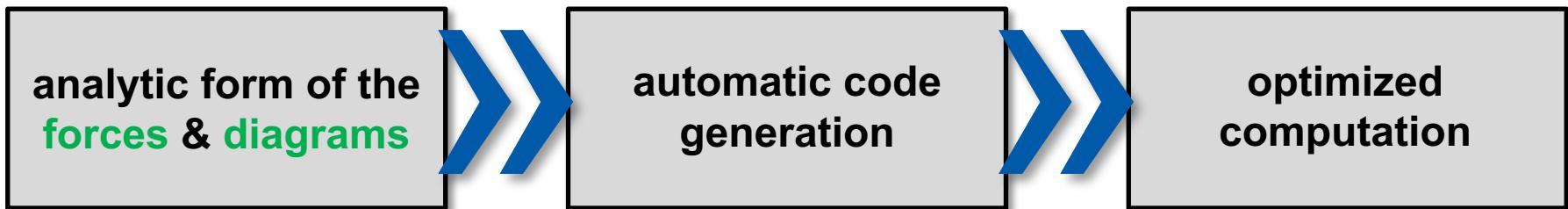
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efficient evaluation of diagrams in **MBPT** (single-particle basis)

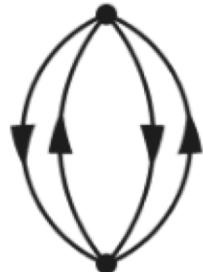
- **implementing diagrams** has become **straightforward** (also ph)
- spin-isospin traces are fully automated; multidim. momentum integrals
- developed **new VEGAS integrator**: openMP, MPI, and job management
- rapid increase of number of diagrams: 3 (3rd), 39 (4th), 840 (5th)



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Example: second-order contribution



$$\frac{E_{\text{NN}+3\bar{\text{N}}}^{(2)}}{V} = \frac{1}{4} \prod_{i=1}^4 \left[\text{Tr}_{\sigma_i} \text{Tr}_{\tau_i} \int \frac{d\mathbf{k}_i}{(2\pi)^3} \right] |\langle 12 | V_{as}^{(2)} | 34 \rangle|^2 \frac{n_{\mathbf{k}_1}^{\tau_1} n_{\mathbf{k}_2}^{\tau_2} (1 - n_{\mathbf{k}_3}^{\tau_3}) (1 - n_{\mathbf{k}_4}^{\tau_4})}{\varepsilon_{\mathbf{k}_1}^{\tau_1} + \varepsilon_{\mathbf{k}_2}^{\tau_2} - \varepsilon_{\mathbf{k}_3}^{\tau_3} - \varepsilon_{\mathbf{k}_4}^{\tau_4}} |i\rangle = |\mathbf{k}_i \sigma_i \tau_i\rangle$$

Partial-wave method (spin sums)

$$\begin{aligned} \sum_{S, M_S, M'_S} |\langle \mathbf{k} S M_S | V_{as}^{(2)} | \mathbf{k}' S M'_S \rangle|^2 &= \sum_L P_L(\cos \theta_{\mathbf{k}, \mathbf{k}'}) \\ &\times \sum_{J, l, l', S} \sum_{\tilde{J}, \tilde{l}, \tilde{l}'} (4\pi)^2 i^{(l-l'+\tilde{l}-\tilde{l}')} (-1)^{\tilde{l}+l'+L} C_{l\tilde{l}'0}^{L0} C_{l'\tilde{l}0}^{L0} \\ &\times \sqrt{(2l+1)(2l'+1)(2\tilde{l}+1)(2\tilde{l}'+1)} (2J+1)(2\tilde{J}+1) \\ &\times \left\{ \begin{array}{ccc} l & S & J \\ \tilde{J} & L & \tilde{l}' \end{array} \right\} \left\{ \begin{array}{ccc} J & S & l' \\ \tilde{l} & L & \tilde{J} \end{array} \right\} \langle k | V_{Sl'lJ}^{(2)} | k' \rangle \langle k' | V_{S\tilde{l}'\tilde{l}\tilde{J}}^{(2)} | k \rangle \\ &\times (1 - (-1)^{l+S+1}) (1 - (-1)^{\tilde{l}+S+1}), \end{aligned}$$

Tolos, Friman, Schwenk, NPA 806 105

- Needs an individual treatment of each diagram: **tedious**
- **inefficient**, esp. at higher orders

Single-particle basis

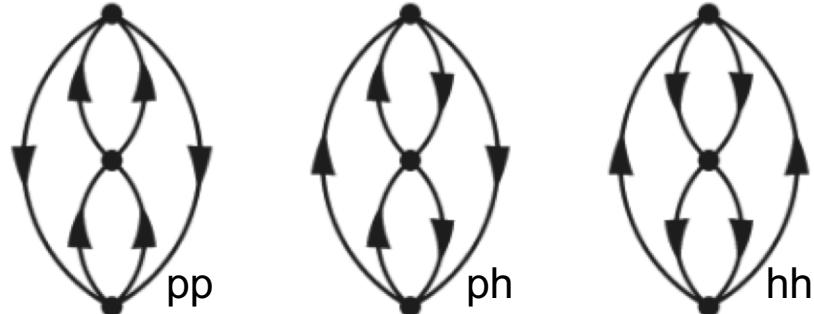
» $\frac{E_{\text{NN}}^{(2)}}{V} = \frac{1}{4} \sum_{\substack{ij \\ ab}} \frac{\langle ij | \mathcal{A}V_{\text{NN}} | ab \rangle \langle ab | \mathcal{A}V_{\text{NN}} | ij \rangle}{\varepsilon_i + \varepsilon_j - \varepsilon_a - \varepsilon_b}$

holes: i, j, k, \dots particles: a, b, c, \dots

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Example: third-order contributions



**Involved partial-wave
decomposition**

Coraggio, Holt *et al.*, PRC **89**, 044321
Holt, Kaiser, PRC **95**, 034326

Single-particle basis

$$\frac{E_1^{(3)}}{V} = +\frac{1}{8} \sum_{\substack{ijkl \\ ab}} \frac{\langle ij | \mathcal{A}_{12} V_{NN} | ab \rangle \langle kl | \mathcal{A}_{12} V_{NN} | ij \rangle \langle ab | \mathcal{A}_{12} V_{NN} | kl \rangle}{D_{ijab} D_{klab}}$$

$$\frac{E_2^{(3)}}{V} = + \sum_{\substack{ijk \\ abc}} \frac{\langle ij | \mathcal{A}_{12} V_{NN} | ab \rangle \langle ak | \mathcal{A}_{12} V_{NN} | ic \rangle \langle bc | \mathcal{A}_{12} V_{NN} | jk \rangle}{D_{ijab} D_{jkbc}}$$

$$\frac{E_3^{(3)}}{V} = +\frac{1}{8} \sum_{\substack{ij \\ abcd}} \frac{\langle ij | \mathcal{A}_{12} V_{NN} | ab \rangle \langle ab | \mathcal{A}_{12} V_{NN} | cd \rangle \langle cd | \mathcal{A}_{12} V_{NN} | ij \rangle}{D_{ijab} D_{ijcd}}$$

- **transparent & fast implementation**
- can be automated
- well-suited for massive **parallel computation**
- requires high level of optimization

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Energy expressions

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Stevenson, Int. J. Mod. Phys. C 14, 1135

How to obtain the n^{th} -order energy expressions



1, 3, 39, 840, 27 300, 1 232 280, ...

$n =$ 2 3 4 5 6 7



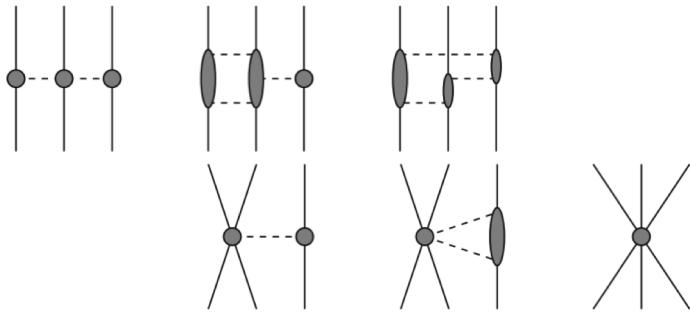
Automatic diagram generation

- remarkably simple set of rules (matrix representation)
- conversion to expressions: developed for B-MBPT

Arthuis, Duguet, Tichai *et al.*, in prep.

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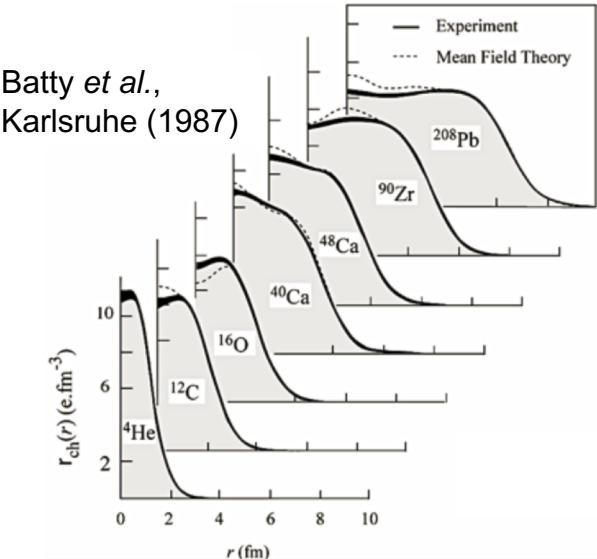
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CD, Hebeler, Schwenk, arXiv:1710.08220.

CHIRAL INTERACTIONS UP TO N³LO AND NUCLEAR SATURATION

Objectives: MBPT calculations at fourth order
explore new N³LO interactions

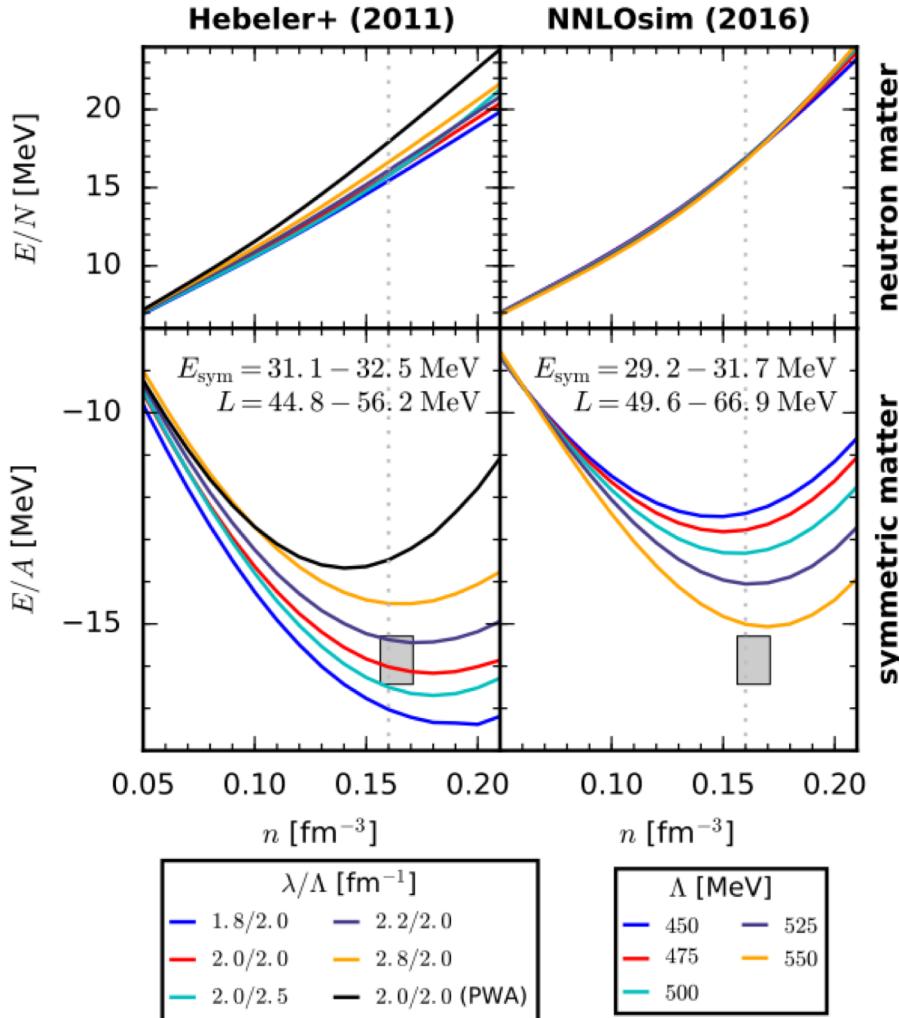


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Nuclear saturation

CD, Hebeler, Schwenk, arXiv:1710.08220



include contributions from up to

- **NN (4th), NN plus 3N (3rd),**
- **residual 3N–3N term (2nd)**

Hebeler *et al.*, PRC 83, 031301
Carlsson *et al.*, PRX 6, 011019

good many-body convergence

» **interactions are perturbative**
for these densities

Coester-like linear correlation

Coester *et al.*, PRC 1, 769

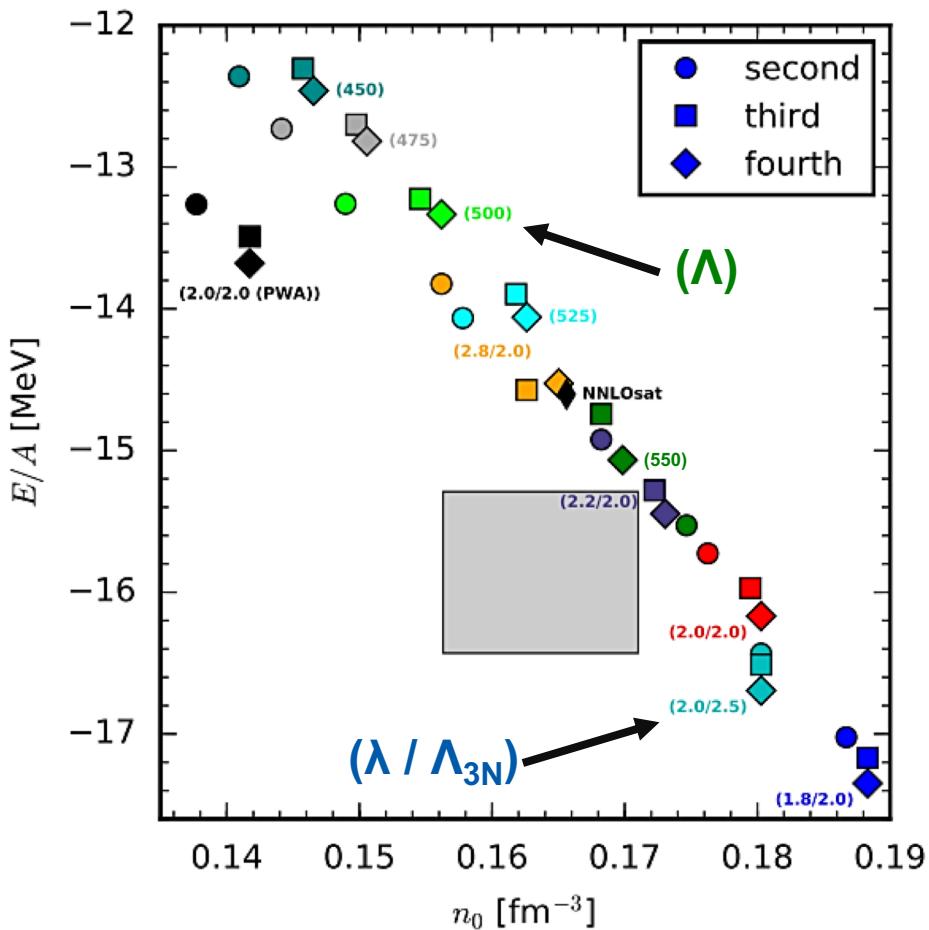
$$E_{\text{sym}} = 31.1 - 32.5 \text{ MeV}$$
$$L = 44.8 - 56.2 \text{ MeV}$$

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Nuclear saturation

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CD, Hebeler, Schwenk, arXiv:1710.08220



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Hebeler *et al.*, PRC 83, 031301

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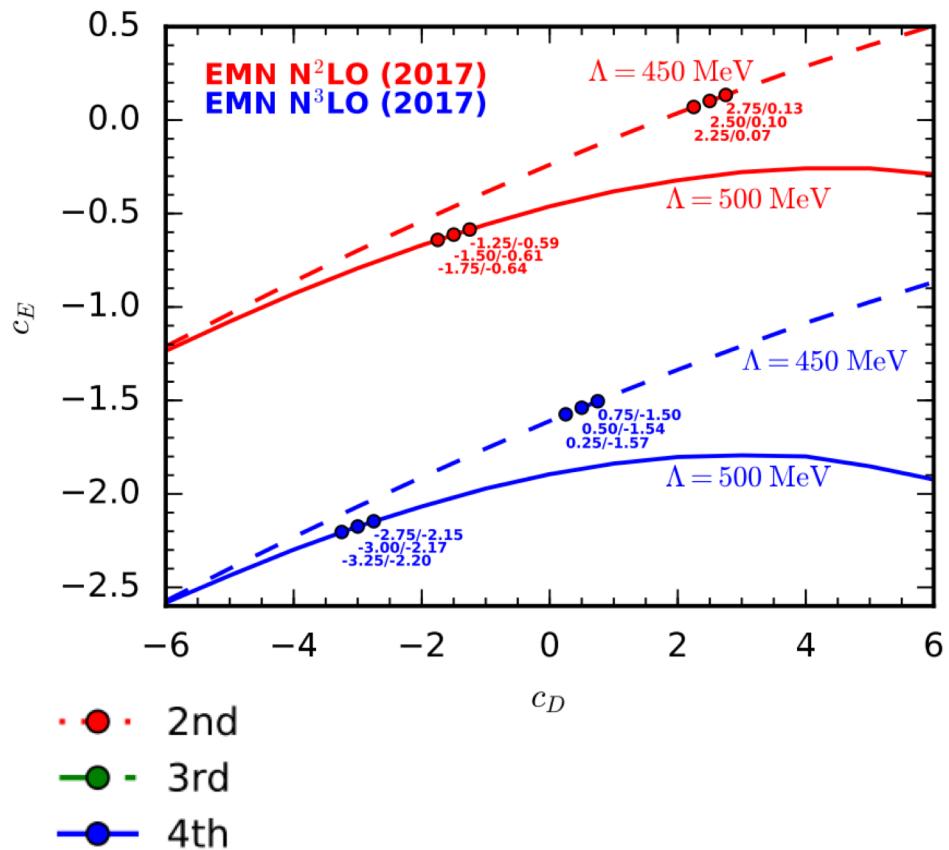
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Fits to saturation region

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CD, Hebeler, Schwenk, arXiv:1710.08220

use the Monte-Carlo framework to
constrain 3N LECs



- $N^2\text{LO} / N^3\text{LO}$ EMN potentials**
with $\Lambda = 450 \text{ MeV}$ & $\Lambda = 500 \text{ MeV}$
Entem, Machleidt, Nosyk, PRC **96**, 024004
- fit to ${}^3\text{H}$ binding energy:** $c_E(c_D)$
consistently at $N^2\text{LO} / N^3\text{LO}$
- study saturation properties:**
 ${}^3\text{H}$ binding energy important !

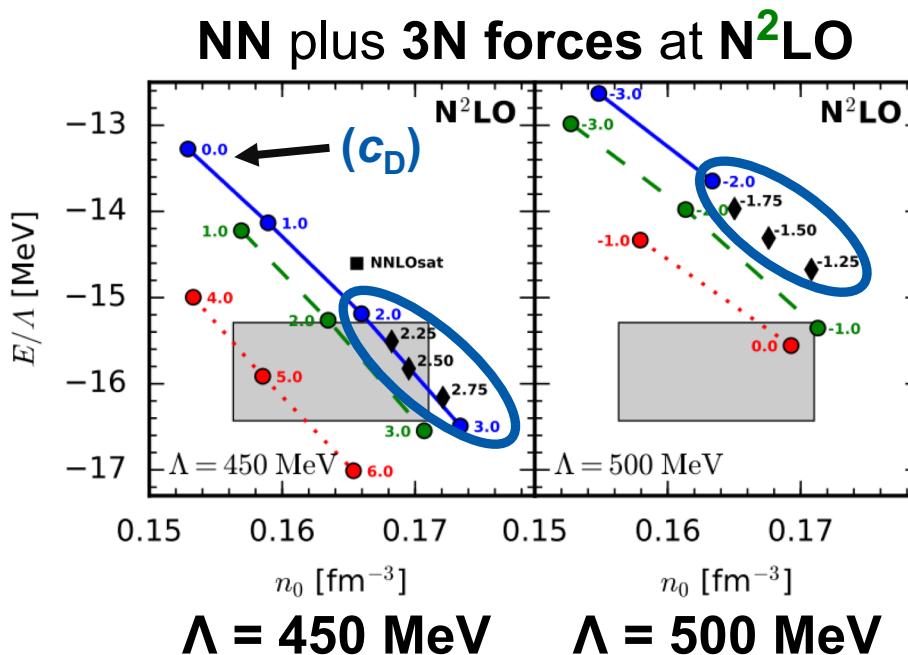
fits close to saturation point
at $N^2\text{LO}$ & $N^3\text{LO}$ identified

Many-Body Perturbation Theory for Nuclear Matter at High Orders

Fits to saturation region

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CD, Hebeler, Schwenk, arXiv:1710.08220



- 2nd
- 3rd
- 4th

use the Monte-Carlo framework to constrain 3N LECs

- **N²LO / N³LO EMN potentials** with $\Lambda = 450 \text{ MeV}$ & $\Lambda = 500 \text{ MeV}$
Entem, Machleidt, Nosyk, PRC **96**, 024004
- **fit to ³H binding energy:** $c_E(c_D)$ consistently at N²LO / N³LO
- **study saturation properties:** 3rd order contribution important !

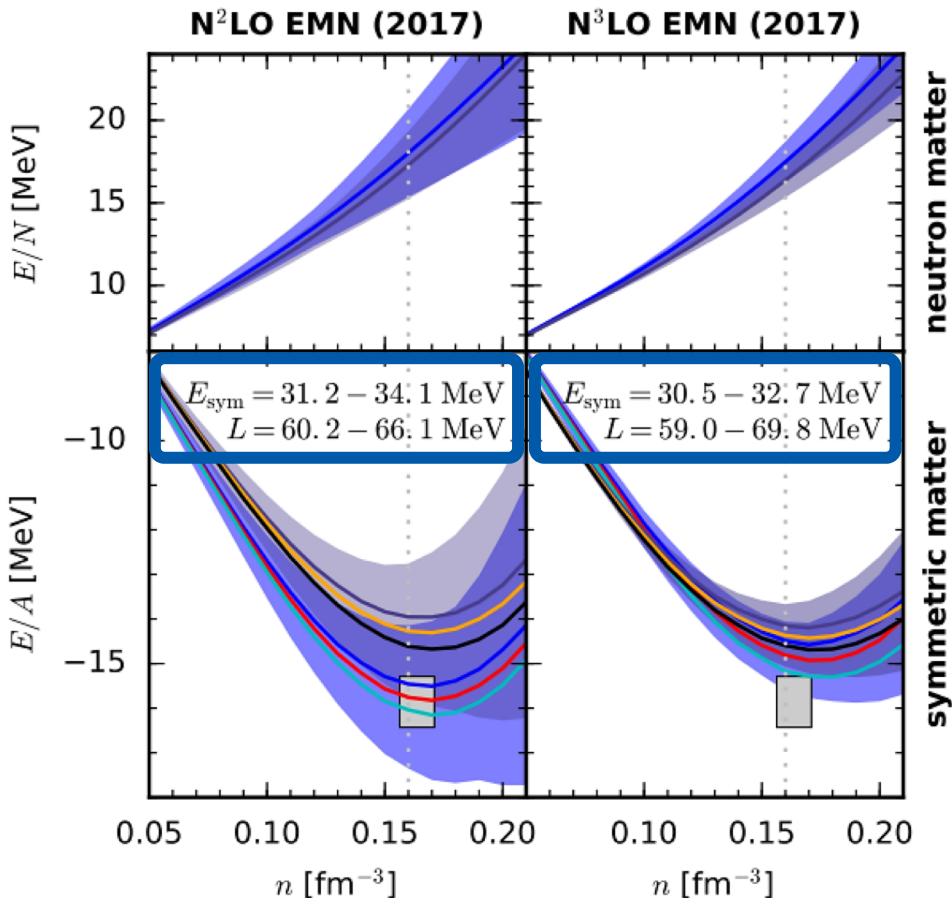
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Neutron and symmetric matter with consistent NN + 3N forces

- 4N HF energy ~ 150 keV @ n_0
- narrow ranges for E_{sym} and L
- uncertainties from chiral EFT

Epelbaum *et al.*, EPJ A 51, 53

Symmetric matter @ N³LO:

- reduced cutoff dependence
- reduced theo. uncertainties

left column:

Λ/c_D [MeV]/[1]	
450/2.25	500/-1.75
450/2.50	500/-1.50
450/2.75	500/-1.25

right column:

Λ/c_D [MeV]/[1]	
450/0.25	500/-3.25
450/0.50	500/-3.00
450/0.75	500/-2.75

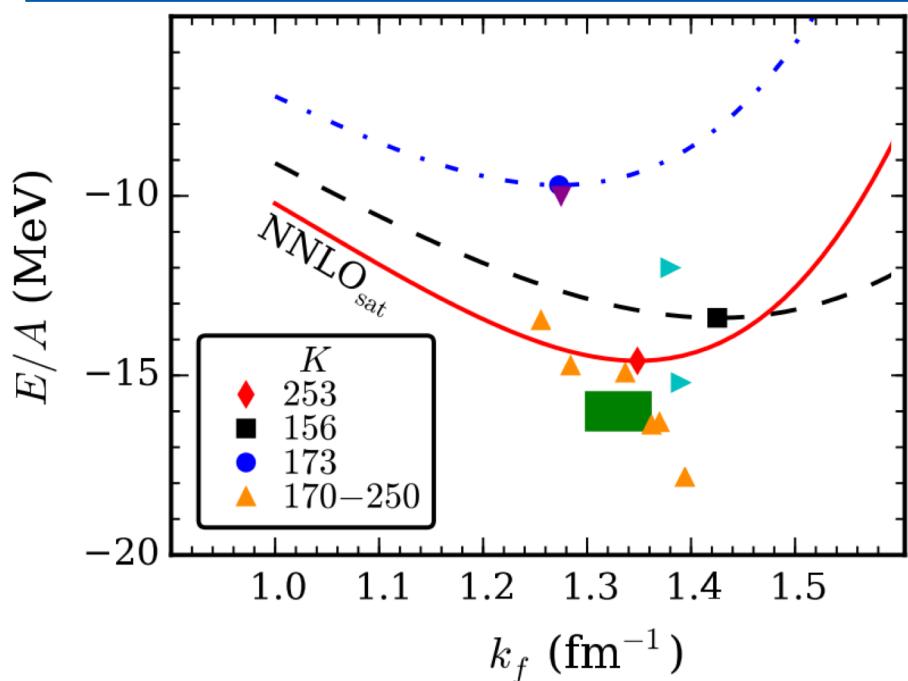
Many-Body Perturbation Theory for Nuclear Matter at High Orders

Guiding finite nuclei

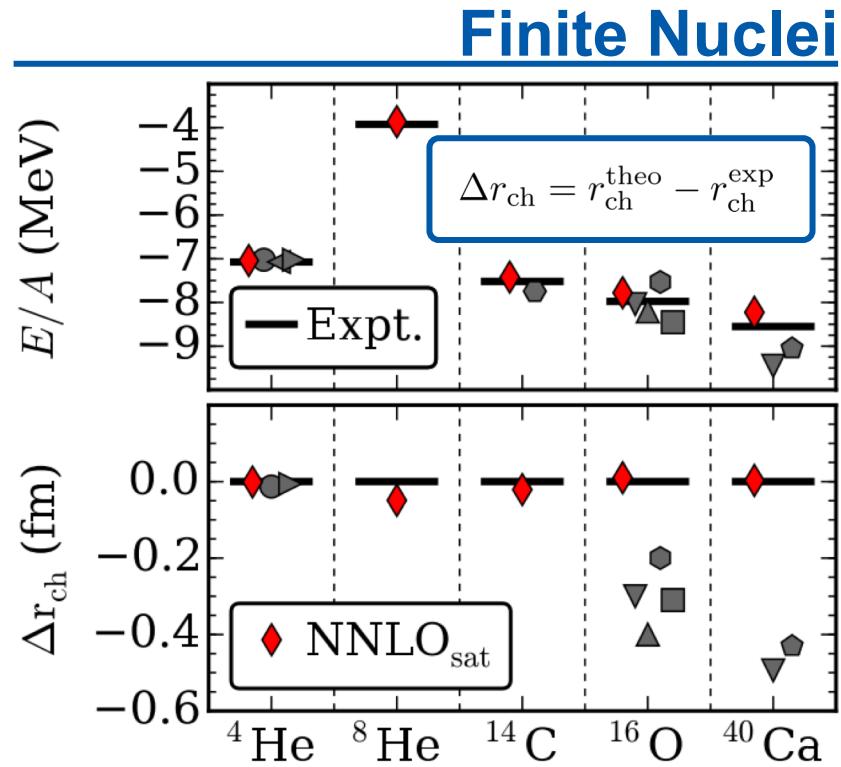
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Ekström *et al.*, Phys. Rev. C **91**, 551301

Infinite Matter



***Ab initio* calculations overbind
medium-mass and heavy nuclei,
underestimate charge radii**



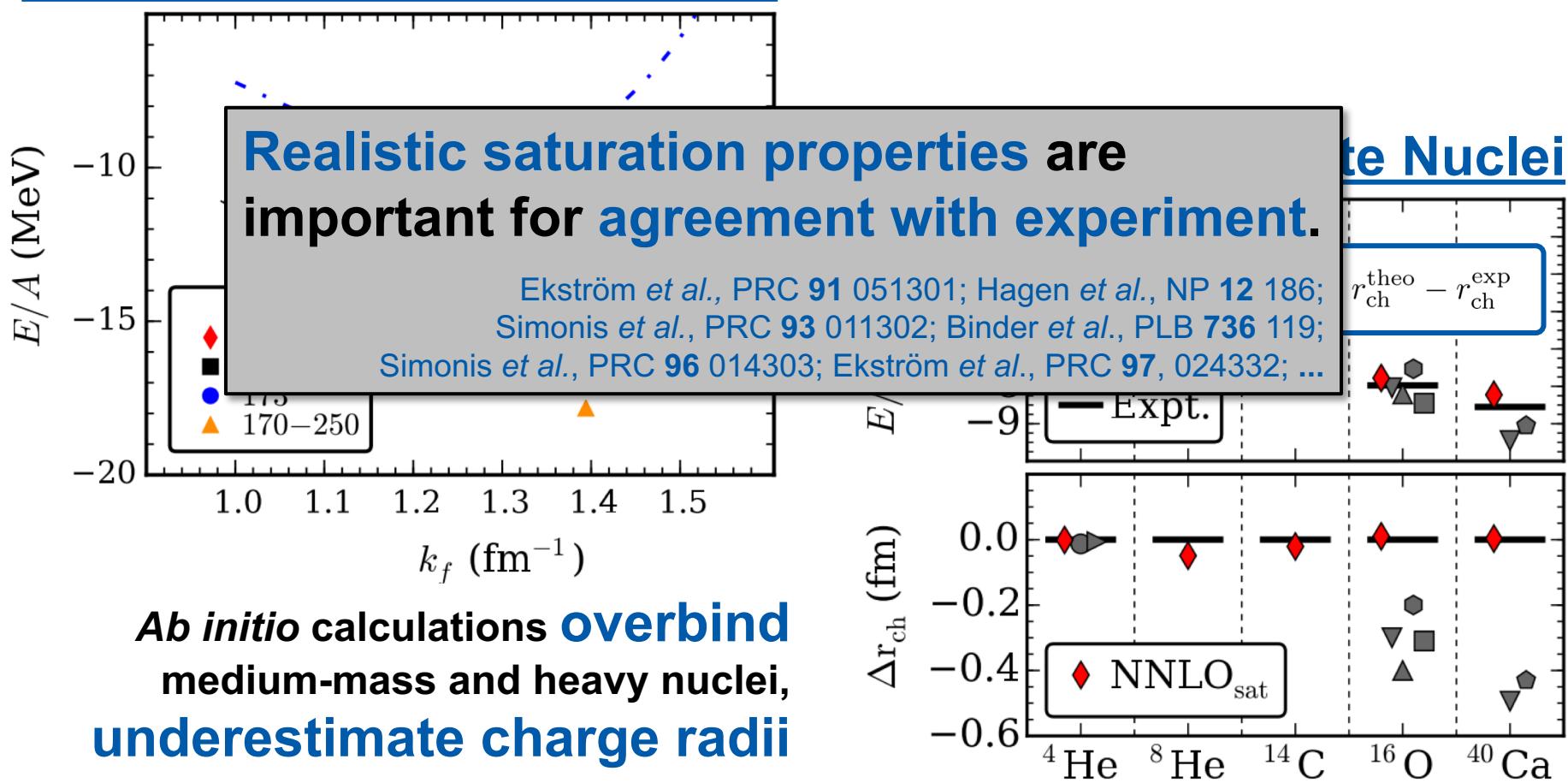
Many-Body Perturbation Theory for Nuclear Matter at High Orders

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Guiding finite nuclei

Ekström *et al.*, Phys. Rev. C **91**, 551301

Infinite Matter

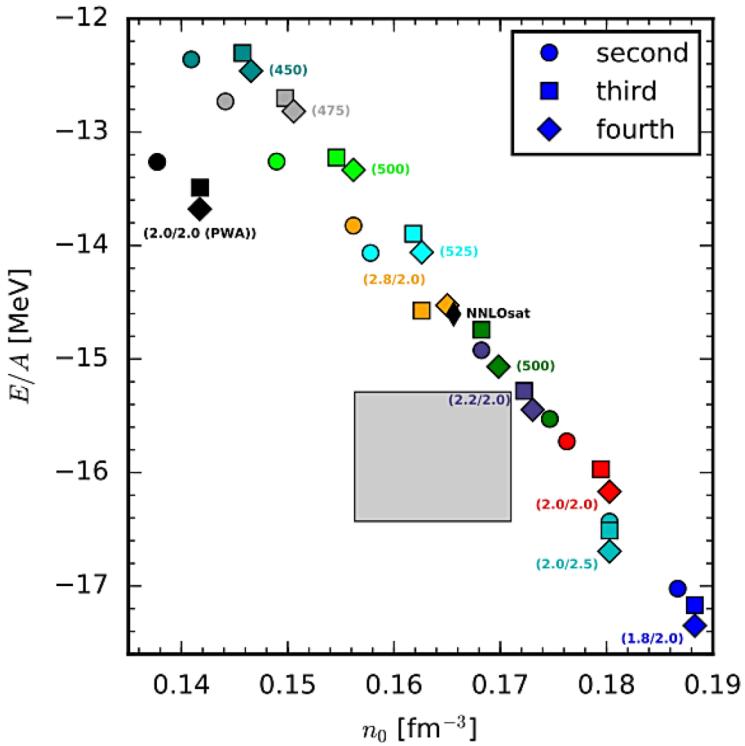


Many-Body Perturbation Theory for Nuclear Matter at High Orders

Guiding finite nuclei

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Simonis, Stroberg *et al.*, Phys. Rev. C **96**, 014303

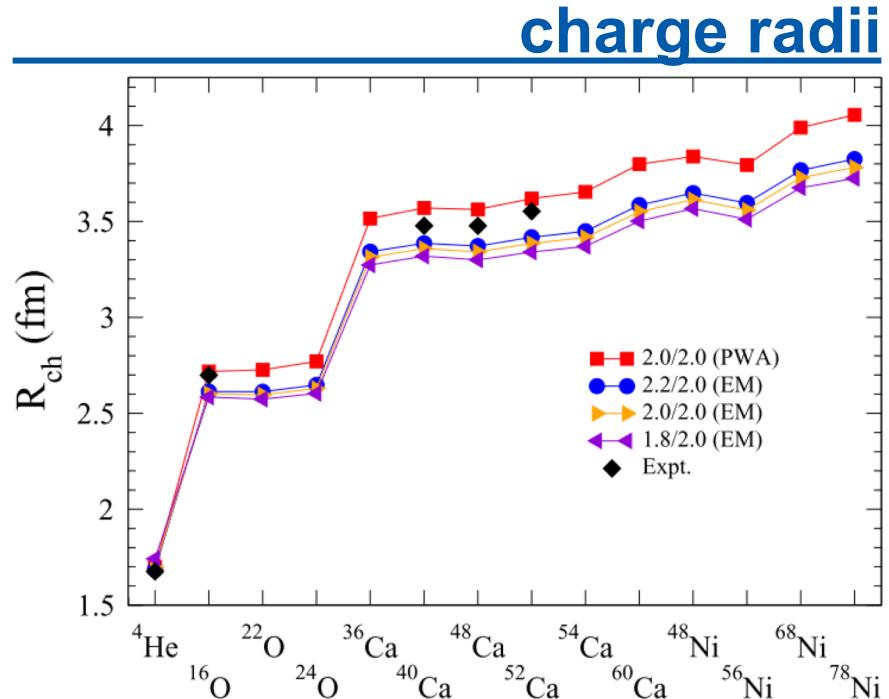


$\lambda / \Lambda_{3N} = 1.8 / 2.0$ (EM) exhibits
good agreement with experiment

potentials fit in Hebeler *et al.*, PRC **83**, 031301

“Hebeler *et al.*” interactions:

- N^3 LO NN (SRG) + N^2 LO 3N forces
- c_D, c_E only fit to few-body data



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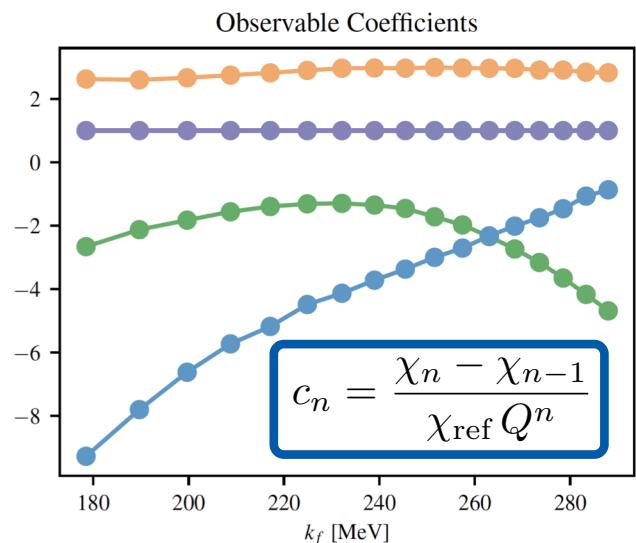
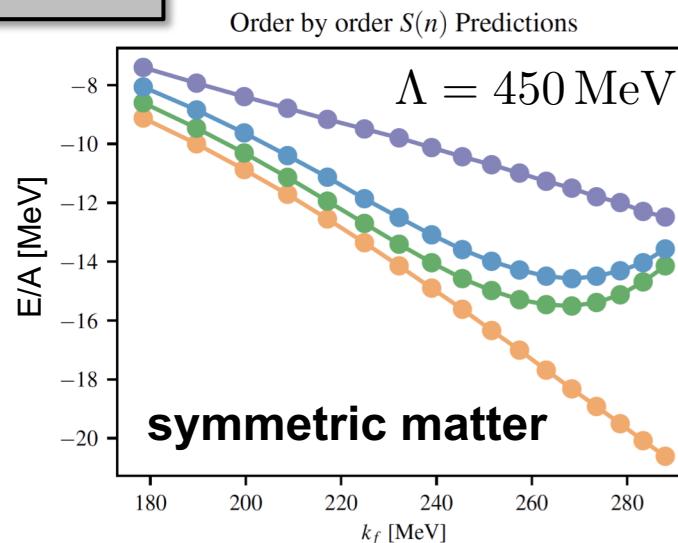
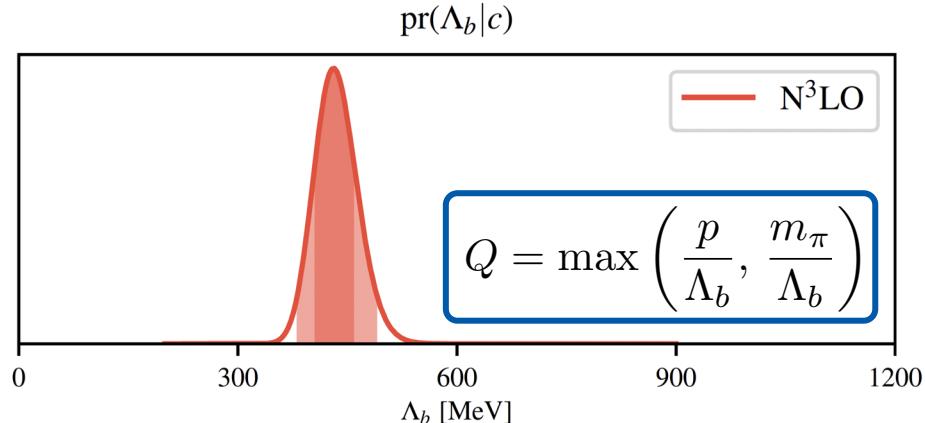
Bayesian analysis: uncertainty estimates

together with Melendez, Furnstahl, Phillips

$$\chi_k = \chi_{\text{ref}} \sum_{n=0}^k c_n Q^n$$

see talk by S. Wesolowski

- LO
- NLO
- N²LO
- N³LO



e.g., Melendez, Wesolowski, Furnstahl, PRC 96, 024003; Furnstahl, Klco, Phillips et al., PRC 92, 024005

Many-Body Perturbation Theory for Nuclear Matter at High Orders

Bayesian analysis: uncertainty estimates

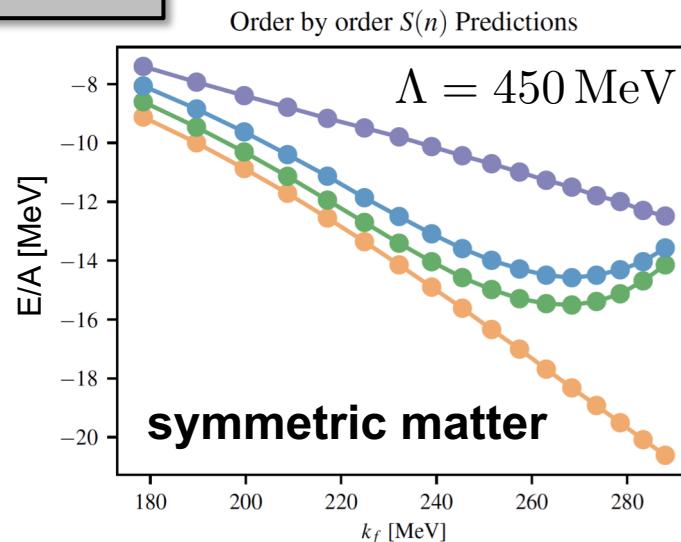
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together with Melendez, Furnstahl, Phillips

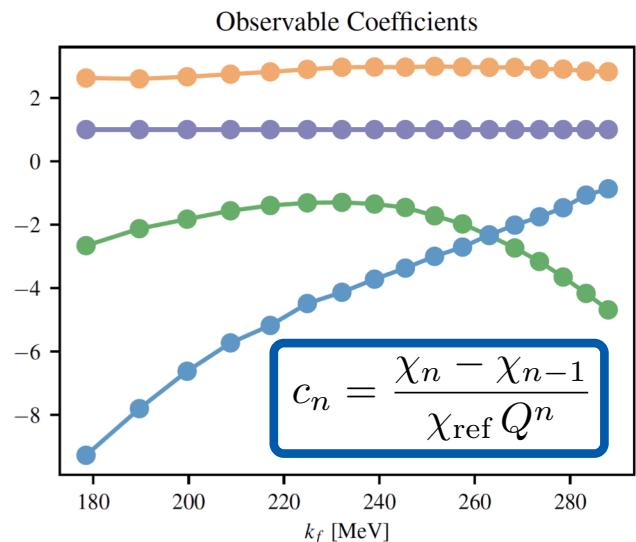
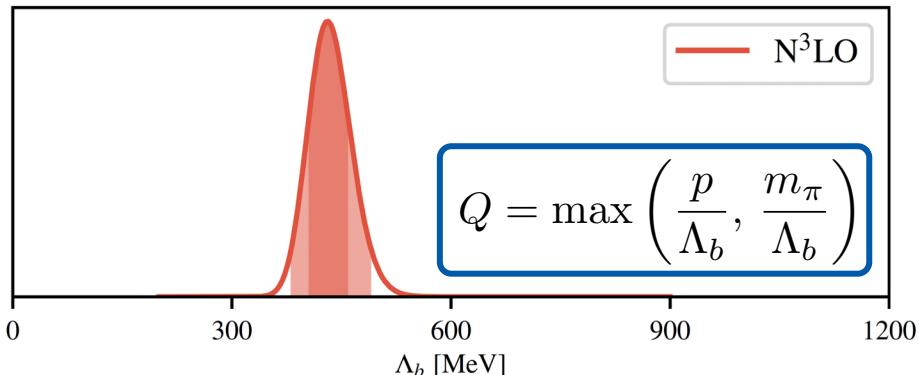
$$\chi_k = \chi_{\text{ref}} \sum_{n=0}^k c_n Q^n$$

see talk by S. Wesolowski

- LO
- NLO
- N²LO
- N³LO



$$\text{pr}(\Lambda_b | c)$$



e.g., Melendez, Wesolowski, Furnstahl, PRC 96, 024003; Furnstahl, Klco, Phillips et al., PRC 92, 024005

Many-Body Perturbation Theory for Nuclear Matter at High Orders

Outlook



1

Apply the new Hamiltonians to finite nuclei
calculations will provide additional insights ...

2

Extend framework to asymmetry/temperature
single-particle energies, mass-radius relations, ...

3

Quantify theoretical uncertainties
Bayesian truncation errors: naturalness, breakdown scale, ...

4

Constrain fits of next-gen. chiral potentials
in terms of saturation, perturbativeness, ...

Collaborators:

R.J. Furnstahl

K. Hebeler

K. McElvain

J. Melendez

D. Phillips

A. Schwenk

C. Wellenhofer

**Thank you
for your attention!**



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