MBPT calculations of infinite matter at zero temperature

Christian Drischler
with K. Hebeler, A. Schwenk, R. J. Furnstahl, J. Hoppe

MBPTs in Modern Quant. Chem and Nucl. Phys.
CEA Saclay, March 27, 2018

[Credit: ORNL]

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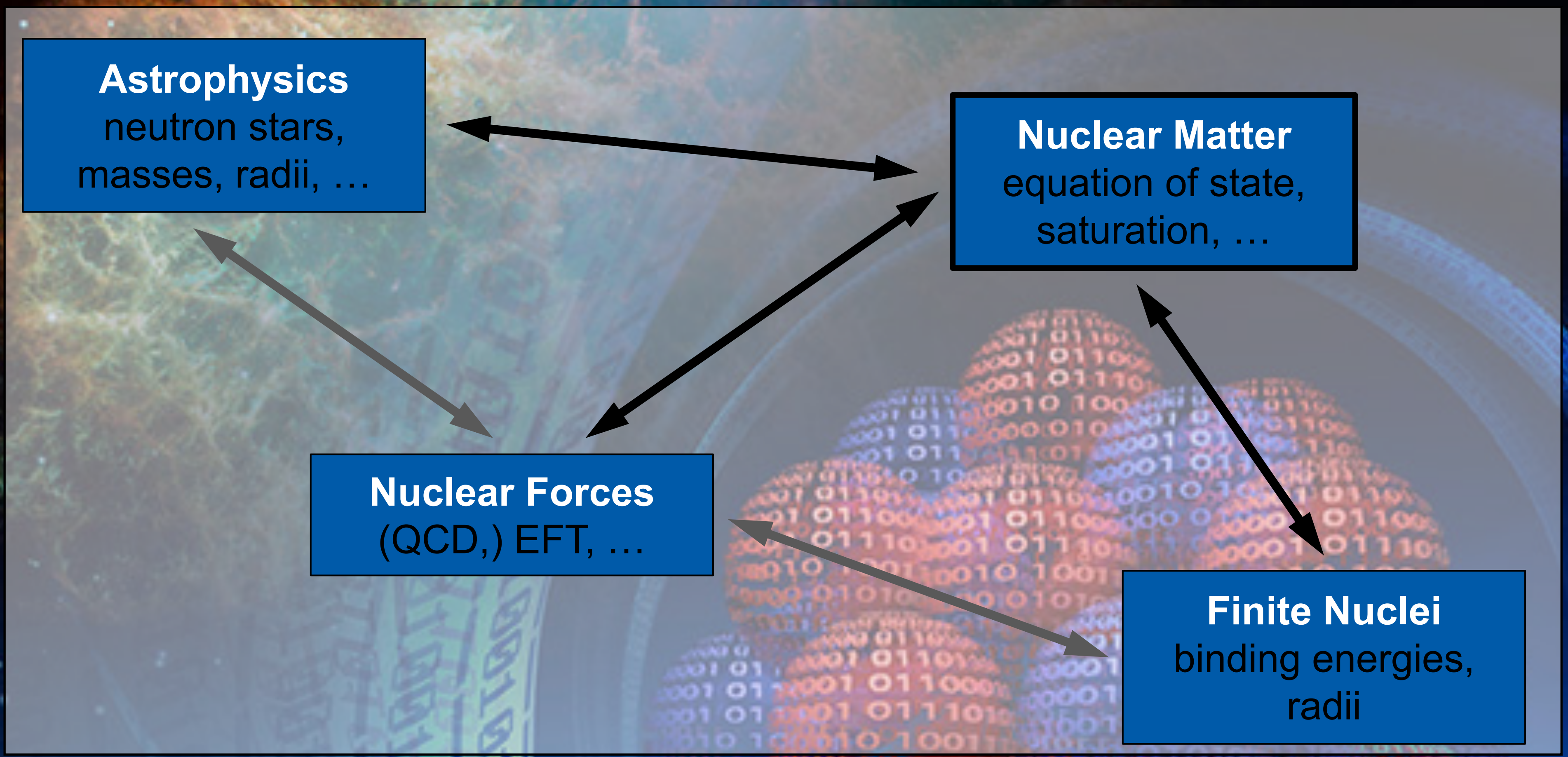
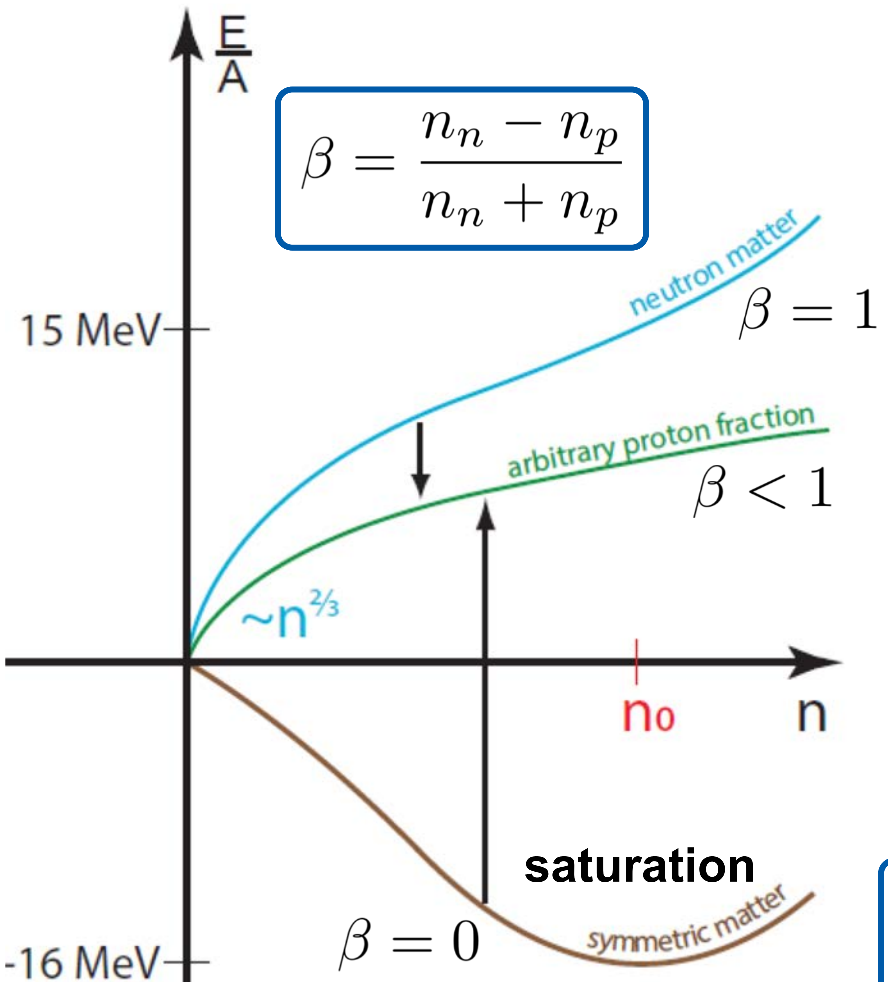


MBPT calculations of infinite matter at zero temperature

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.*, Ann. Rev. Nucl. Part. Sci. **65**, 457

Bethe–Weizsäcker formula

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

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Radius estimates for neutron stars

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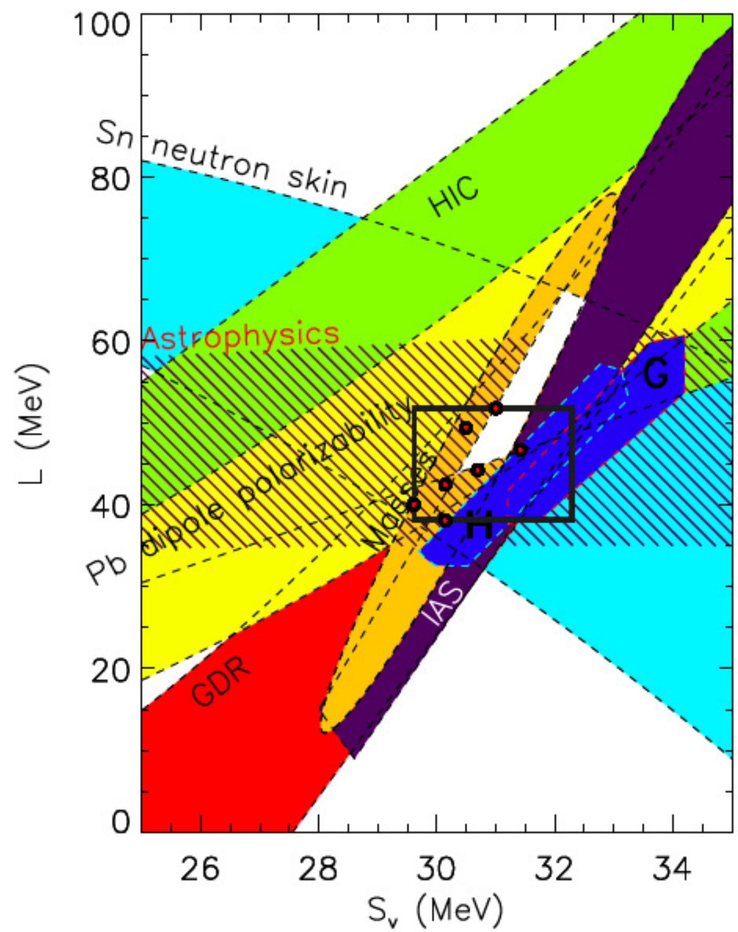
Hebeler *et al.*, Astrophys. J. **773**, 11

$$E_{\text{sym}}(n) = S_v + \frac{L}{3}\left(\frac{n-n_0}{n_0}\right) + \ldots$$

empirical relation by Lattimer, Prakash

$$P(\beta_{\text{eq}}, n_0) \simeq \frac{L}{3} n_0 \propto R^4_{1.4\,\text{M}_\odot}$$

pressure of neutron-star matter



Lattimer, Prakash, Astrophys. J. **550**, 426
Lattimer, Lim, Astrophys. J. **771**, 51

MBPT calculations of infinite matter at zero temperature

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

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empirical relation by Lattimer, Prakash

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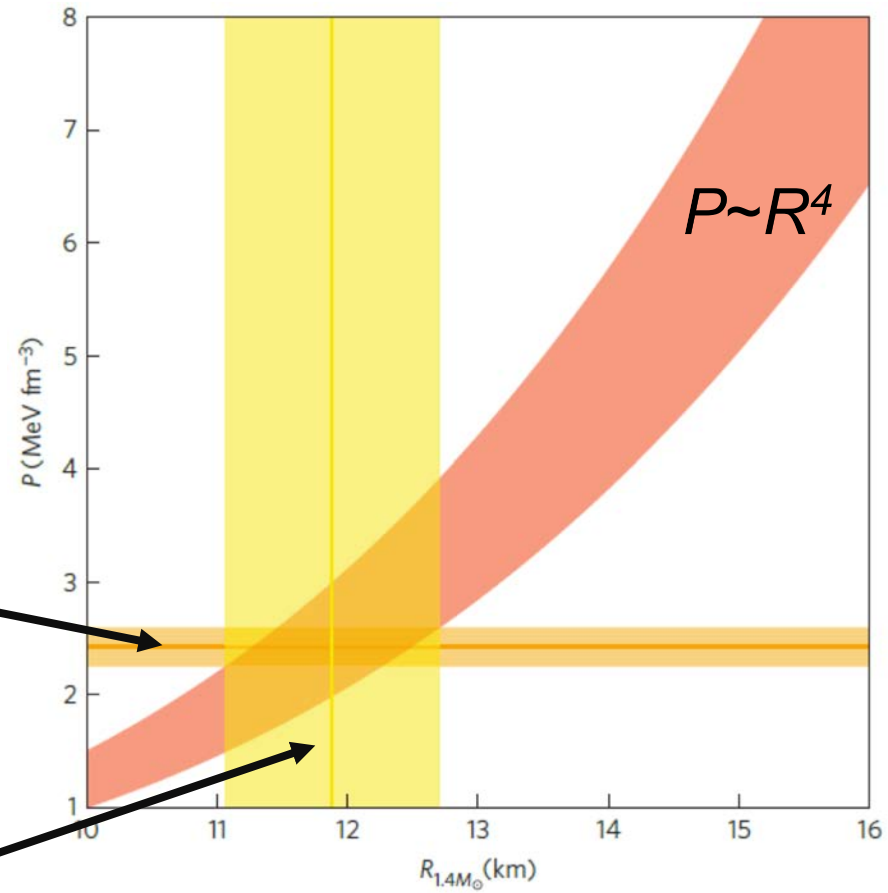
pressure of neutron-star matter

small uncertainties in pressure lead to **tight radius constraints**

» **pinning down *L* is important**

$$11.1\,\text{km} \leqslant R_{1.4\,\mathrm{M}_\odot} \leqslant 12.7\,\text{km}$$

Hagen *et al.*, Nat. Phys. **12**, 186



Lattimer, Prakash, Astrophys. J. **550**, 426
Lattimer, Lim, Astrophys. J. **771**, 51

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Guiding finite nuclei

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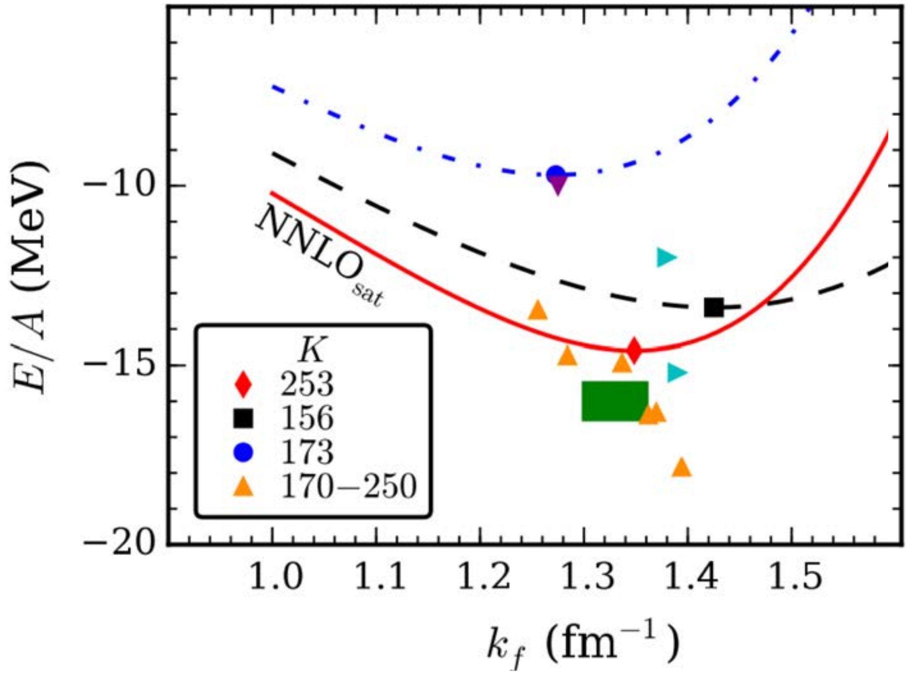
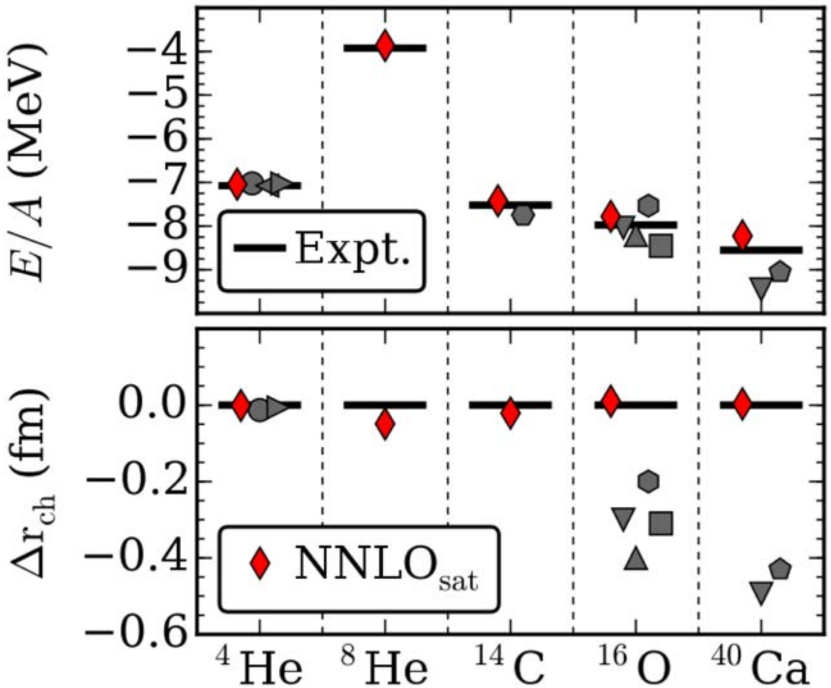
Ekström *et al.*, Phys. Rev. C **91**, 551301

Infinite Matter



$$\Delta r_{\mathrm{ch}} = r_{\mathrm{ch}}^{\mathrm{theo}} - r_{\mathrm{ch}}^{\mathrm{exp}}$$

Finite Nuclei



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

MBPT calculations of infinite matter at zero temperature

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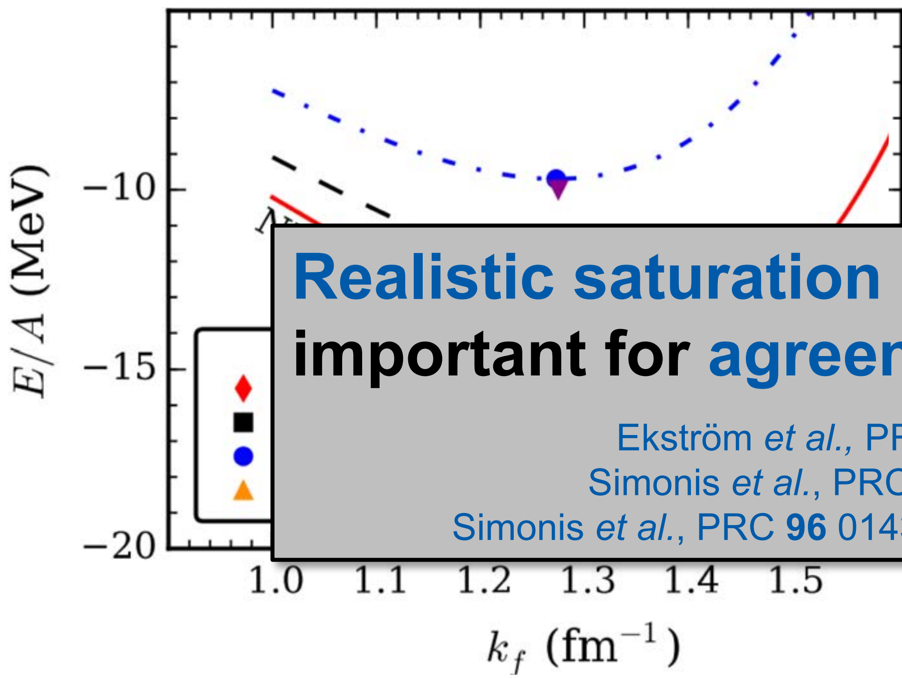
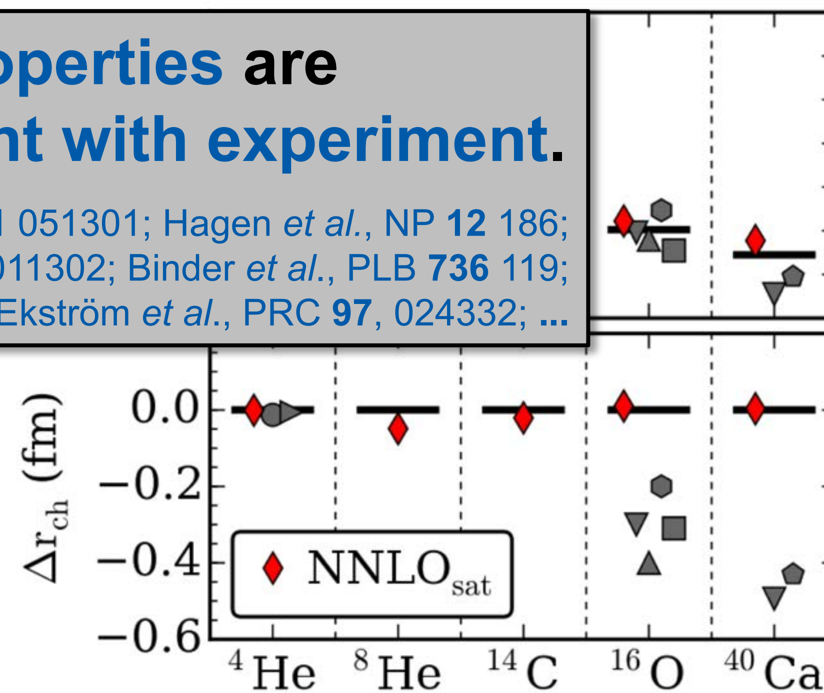
Ekström *et al.*, Phys. Rev. C **91**, 551301

Infinite Matter



$$\Delta r_{\mathrm{ch}} = r_{\mathrm{ch}}^{\mathrm{theo}} - r_{\mathrm{ch}}^{\mathrm{exp}}$$

Finite Nuclei



Realistic saturation properties are important for agreement with experiment.

Ekström *et al.*, PRC **91** 051301; Hagen *et al.*, NP **12** 186;
Simonis *et al.*, PRC **93** 011302; Binder *et al.*, PLB **736** 119;
Simonis *et al.*, PRC **96** 014303; Ekström *et al.*, PRC **97**, 024332; **...**

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

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Next-generation chiral potentials

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Is it feasible to **optimize chiral potentials** in terms of empirical **saturation properties** ?

No!

... so far, due to lack of (computational) efficiency.

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Chiral effective field theory

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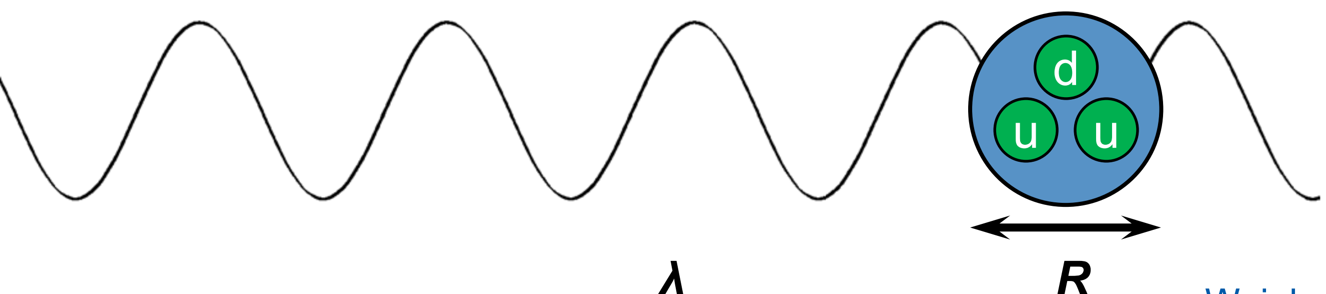
e.g., Epelbaum *et al.*, RMP **81**, 1773

Nuclear matter interacts via the strong interaction
(disregard Coulomb)

- QCD is non-perturbative at low energies of interest
- **modern approach**: **chiral EFT**
  - relevant degrees of freedom instead of quarks/gluons
  - use **nucleons** and **pions**



Steven Weinberg

Weinberg, Phys. Lett. B **251**, 288 (1990)
Weinberg, Nucl. Phys. B **363**, 3 (1991)
Weinberg, Phys. Lett. B **295**, 114 (1992)

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Chiral effective field theory

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e.g., Epelbaum *et al.*, RMP **81**, 1773

Nuclear matter interacts via the strong interaction (disregard Coulomb)

- QCD is non-perturbative at low energies of interest
- **modern approach**: **chiral EFT**
  - relevant degrees of freedom instead of quarks/gluons
  - use **nucleons** and **pions**
  - pion exchanges and short-range contact interactions
  - systematic expansion of nuclear forces:

$$Q = \max\left(\frac{p}{\Lambda_b}, \frac{m_\pi}{\Lambda_b}\right) \sim \frac{1}{3}$$

Steven Weinberg

Weinberg, Phys. Lett. B **251**, 288 (1990)
Weinberg, Nucl. Phys. B **363**, 3 (1991)
Weinberg, Phys. Lett. B **295**, 114 (1992)

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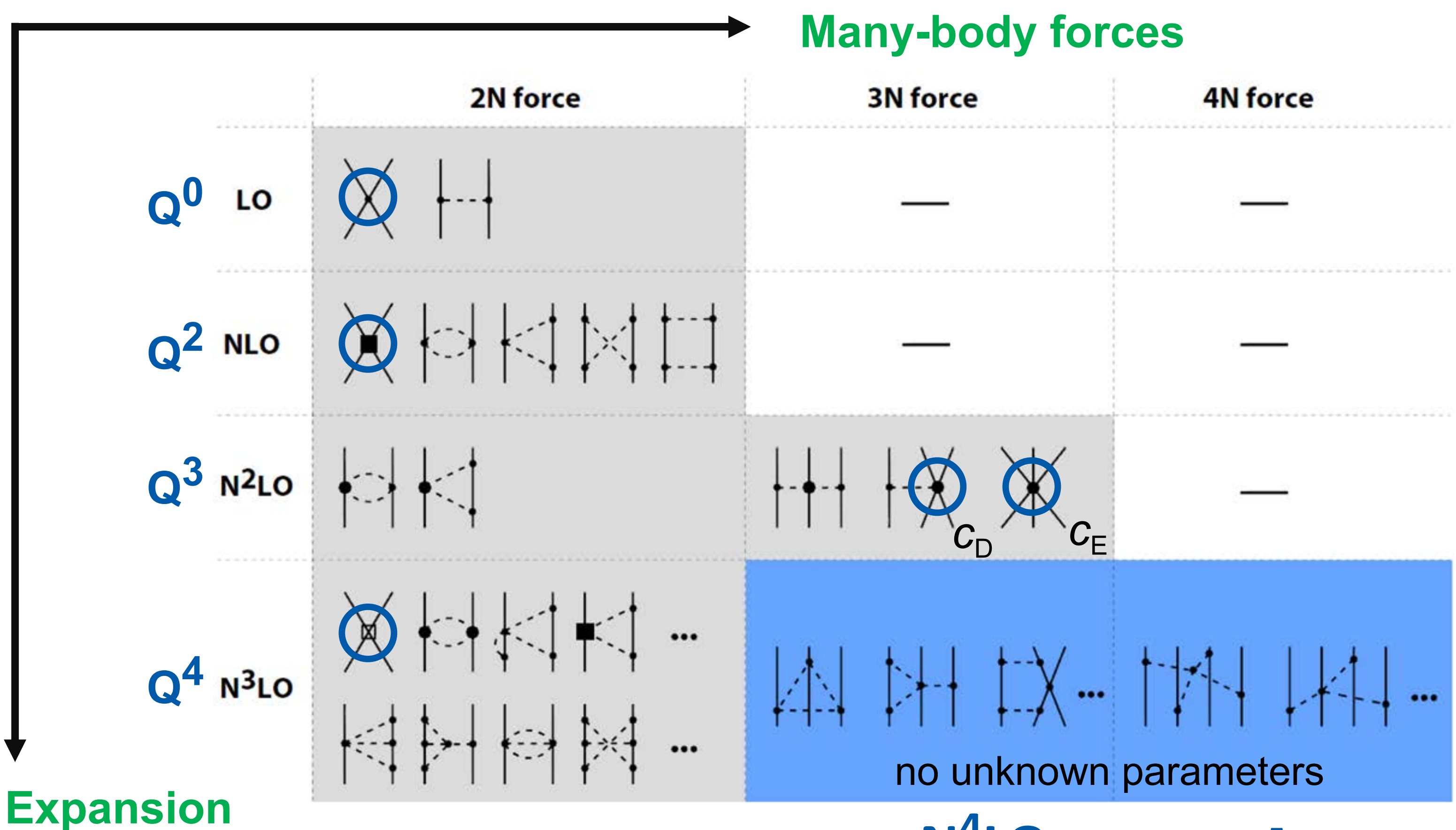
Hierarchy of nuclear forces in chiral EFT

e.g., Machleidt, Entem, Phys. Rep. **503**, 1



... and ongoing work at N^4LO and even N^5LO...

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

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3N forces beyond Hartree-Fock?

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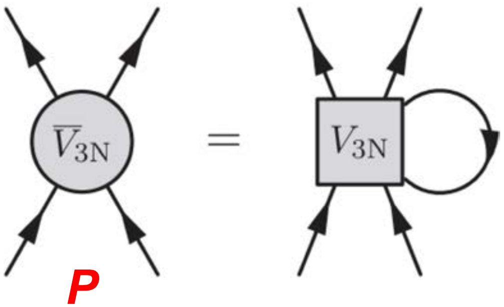
CD, Hebeler, Schwenk, Phys. Rev. C **93**, 054314

Effective NN potentials

by summing *one* particle over the occupied states of the Fermi sea

» dominant 3N contributions

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



some more applications:
Holt *et al.*, PPNP **73**, 35
Hebeler *et al.*, ARNPS **65**, 457
Wellenhofer *et al.*, PRC **92**, 015801
...

so far: only N^2LO 3N and ***P*** = 0

Improved method

- applicable to all nuclear forces
- N^3LO 3N forces due to recent partial-wave decomposition

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

» **towards *consistent* N^3LO calculations**

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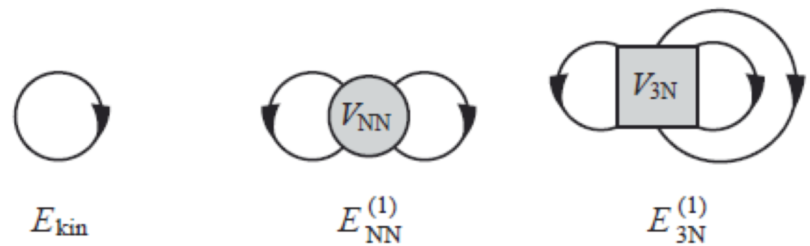
Normal ordering and MBPT diagrams

Hebeler *et al.*, Phys. Rev. C **82**, 014314

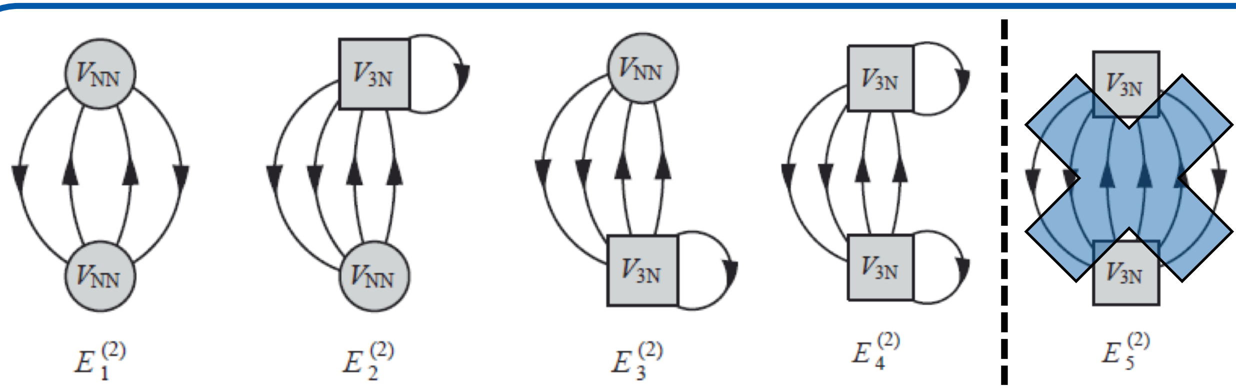
Apply Wick's theorem: normal-ordered NN level

$$\overline{V}_{\mathrm{as}} = V_{\mathrm{NN}} + \xi\, V_{\mathrm{eff}}$$

initial NN forces
normal-ordered 3N forces
combinatorial factor



Hartree-Fock



second order

+ higher orders

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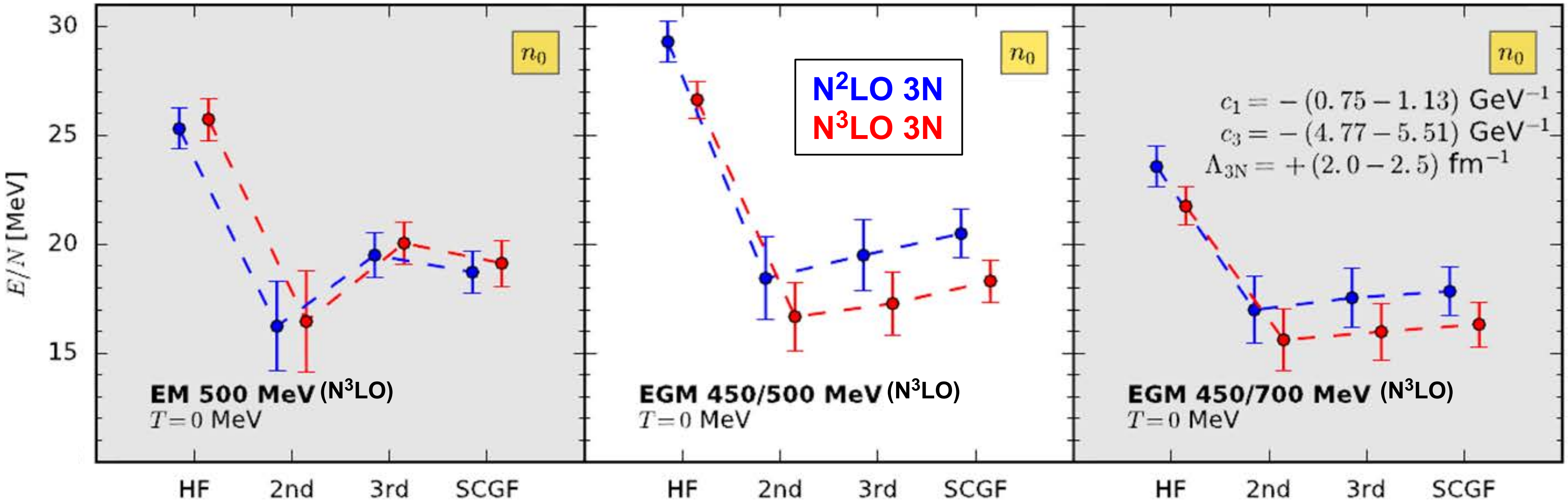
Neutron matter: MB convergence

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



State-of-the-art MBPT calculations up to 3rd order: (ladders only)

- based on N^{3}LO 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 at NN level

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P. D. Stevenson, Int. J. Mod. Phys. C **14**, 1135

The number of diagrams increases rapidly!

x 2^n

1, 3, 39, 840, 27 300, 1 232 280, …

***n* = 2 3 4 5 6 7**

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

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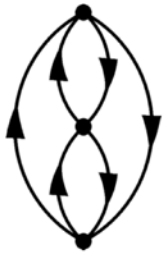
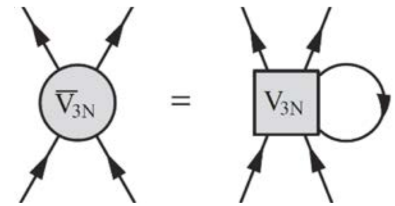
Significant challenges remain!

CD, Hebeler, Schwenk, arXiv:1710.08220



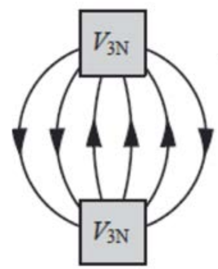
! Higher orders: particle-hole contributions

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



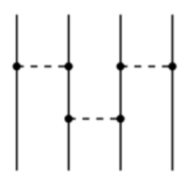
! Approximated normal-ordering

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

CD, Hebeler, Schwenk, arXiv:1710.08220

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

- based on analytic expressions, incl. **NN**, **3N**, and **4N** forces
- **no need for partial-wave decompositions**

$$\langle (\sigma_1' \tau_1') \ldots (\sigma_A' \tau_A') \,|\, \mathcal{A}_A V_{\mathrm{AN}} \left(\overline{\mathbf{p}}, \, \overline{\mathbf{p}}'\right) \,|\, (\sigma_1 \tau_1) \ldots (\sigma_A \tau_A) \rangle$$

analytic form of the forces & diagrams → **automatic code generation** → **optimized computation**

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Efficient Monte-Carlo framework

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CD, Hebeler, Schwenk, arXiv:1710.08220

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

- based on analytic expressions, incl. **NN**, **3N**, and **4N** forces
- **no need for partial-wave decompositions**

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
- rapid increase of number of diagrams: 3 (3^{rd}), **39 (4^{th})**, 840 (5^{th})

analytic form of the forces & diagrams → **automatic code generation** → **optimized computation**

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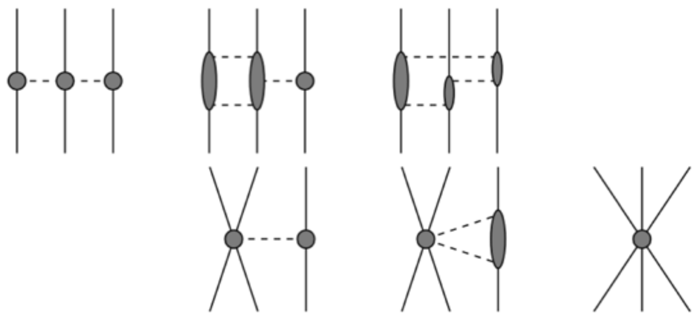
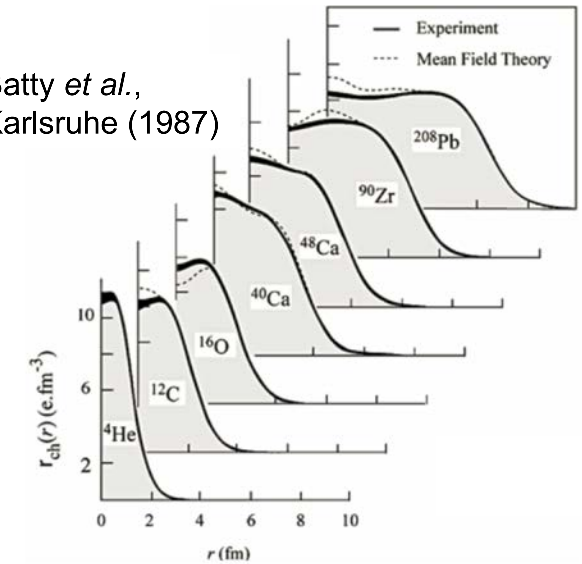


Batty *et al.*,
Karlsruhe (1987)



CD, Hebeler, Schwenk, arXiv:1710.08220.

CHIRAL INTERACTIONS UP TO N^{3}LO AND NUCLEAR SATURATION

Objectives: MBPT calculations at fourth order
explore new N^{3}LO interactions

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Nuclear saturation

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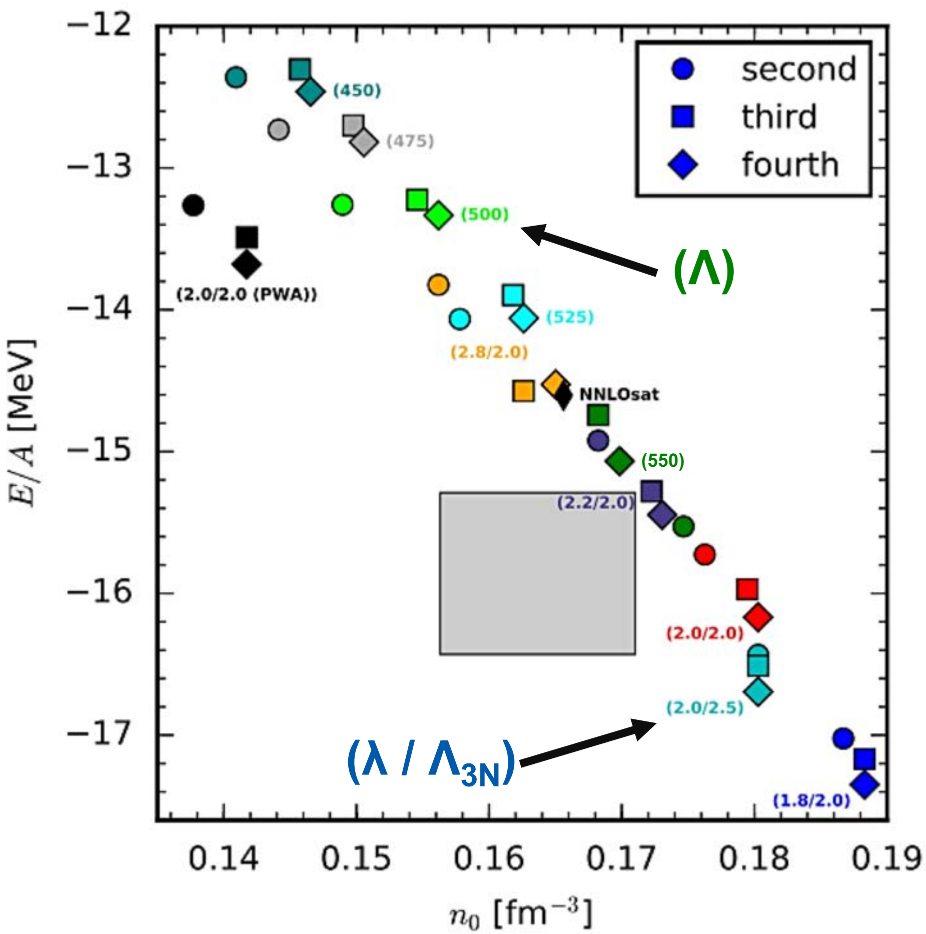
CD, Hebeler, Schwenk, arXiv:1710.08220



<u>**include contributions from up to**</u>

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

good many-body convergence

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

» **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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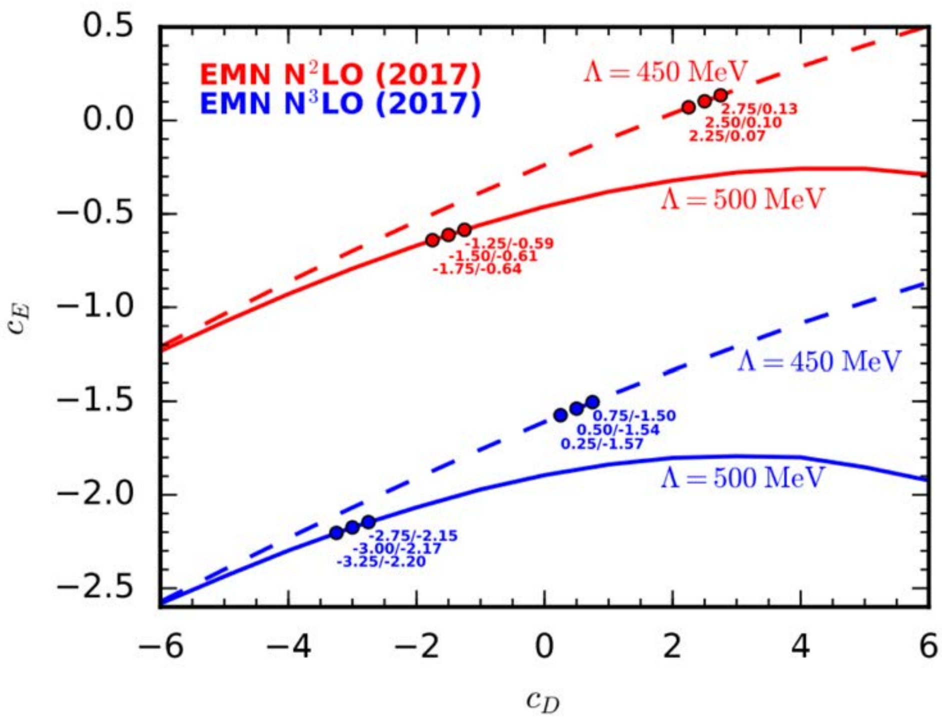
Fits to saturation region

CD, Hebeler, Schwenk, arXiv:1710.08220



use the Monte-Carlo framework to constrain 3N LECs

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

reasonable fits to saturation at N^2LO & N^3LO identified

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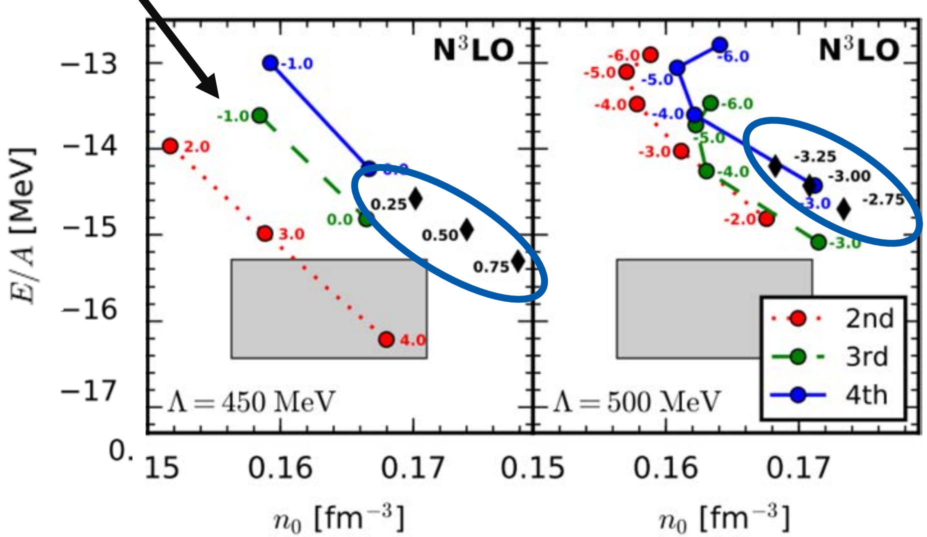
Fits to saturation region

CD, Hebeler, Schwenk, arXiv:1710.08220

(c_D) **NN** plus **3N forces** at **N^{3}LO**



Λ = 450 MeV **Λ = 500 MeV**

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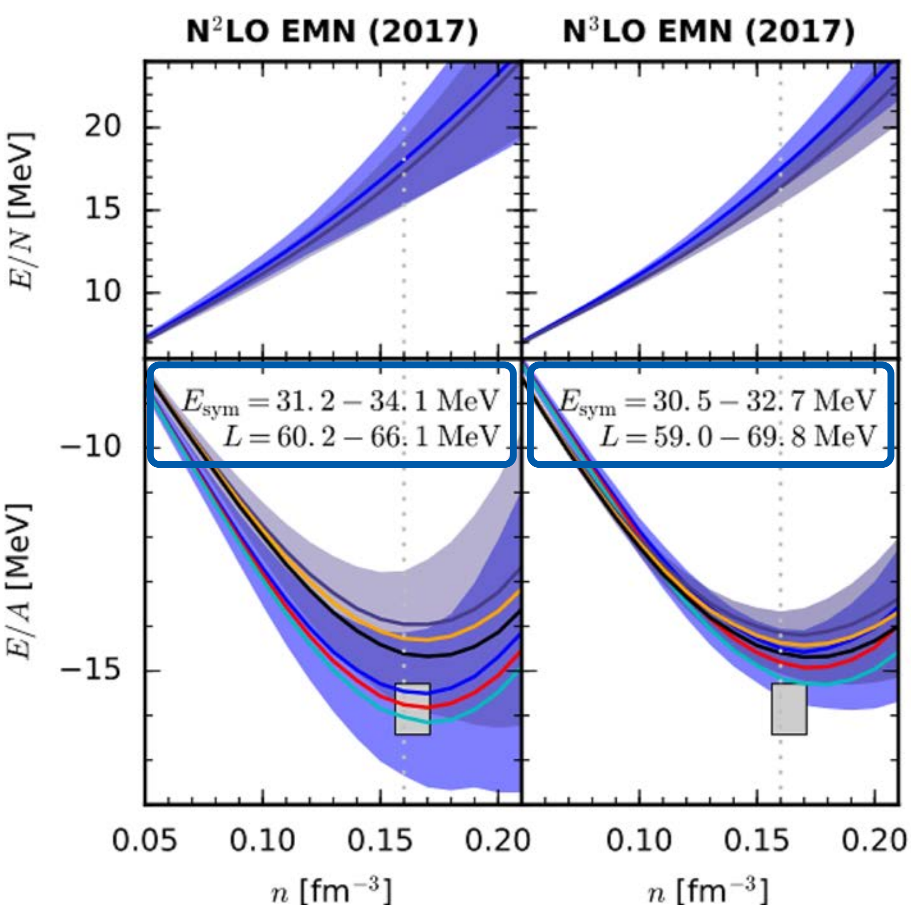


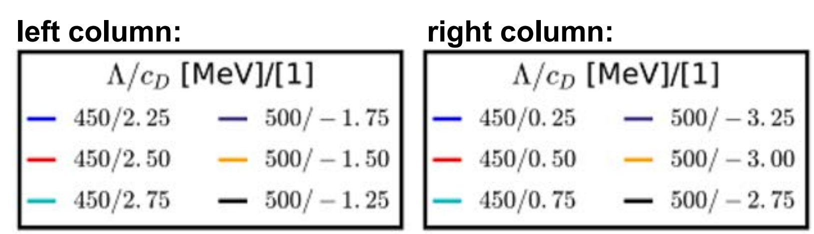
Neutron and symmetric matter with consistent NN + 3N forces

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

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

Symmetric matter @ N^{3}LO:

- **reduced cutoff dependence**
- **reduced theo. uncertainties**



see also:
Bogner, Schwenk, Furnstahl, Nogga, NPA **763**, 59
Srinivas, Ramanan, PRC **94**, 064303
Dyhdalo, Bogner, Furnstahl, PRC **96**, 054005
Reinert, Krebs, Epelbaum, arXiv:1711.08821

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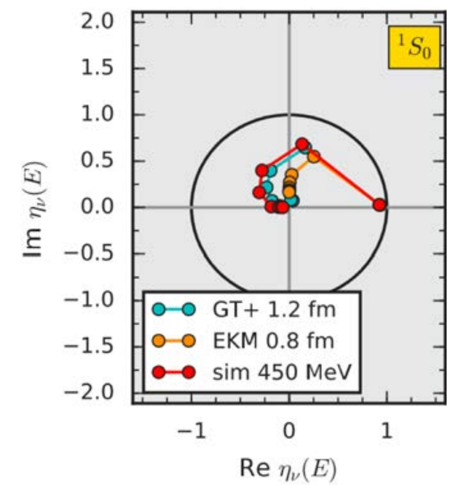
Weinberg, Phys. Rev. **131**, 440

Quasiparticles and the Born Series*

STEVEN WEINBERG†
Department of Physics, University of California, Berkeley, California
(Received 14 February 1963)



Hoppe, CD, Furnstahl, Hebeler, Schwenk, PRC **96**, 054002.

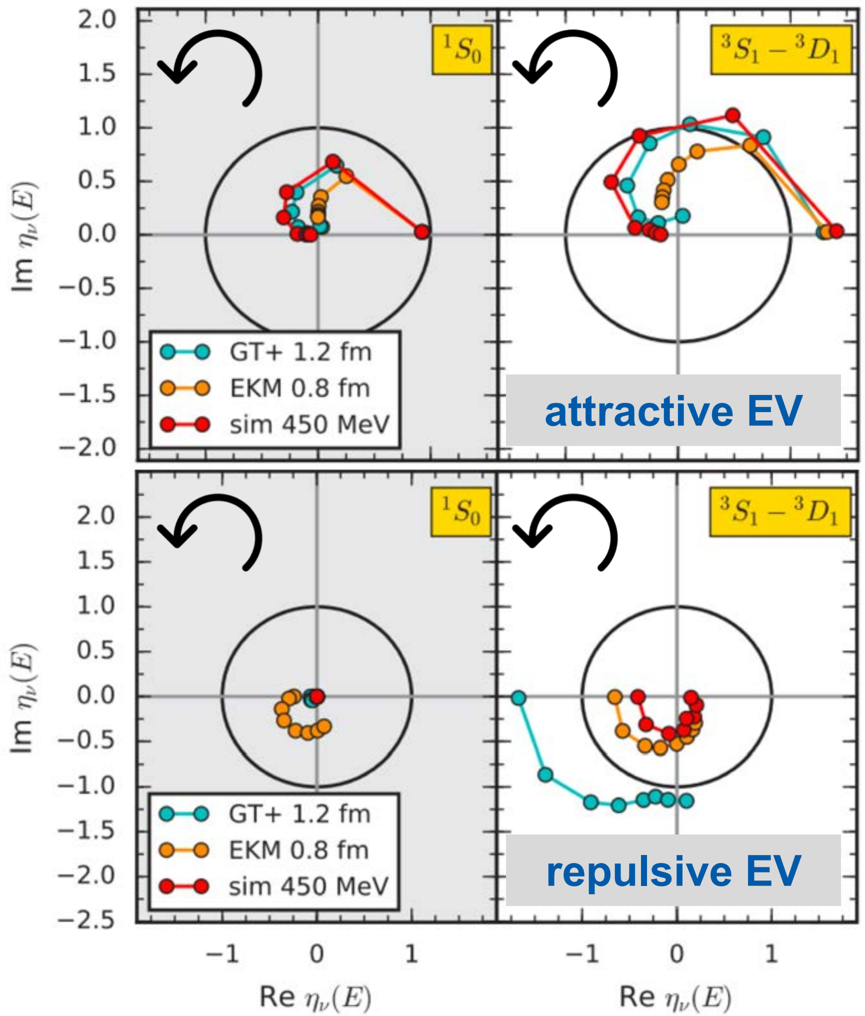
WEINBERG EIGENVALUES FOR CHIRAL NN INTERACTIONS

Objectives: quantify perturbativeness of recent NN potentials
insights into different regularization schemes

MBPT calculations of infinite matter at zero temperature

Basic concept

Weinberg, Phys. Rev. **131**, 440



Lippmann-Schwinger equation

$$T(W) = V + V G_0(W) T(W)$$

$$= V \sum_{n=0}^{\infty} (G_0(W) V)^n$$

Born series

e.g., in free space $G_0(W) = \frac{1}{W - H_0}$

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Basic concept

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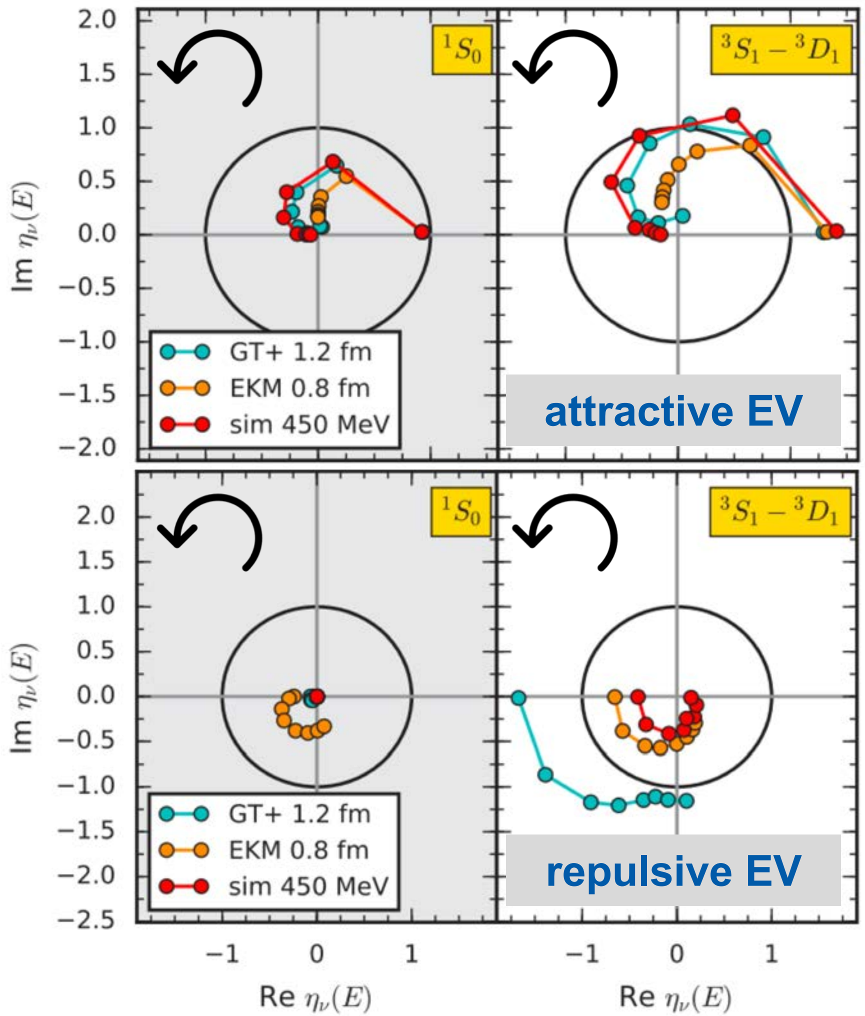
Weinberg, Phys. Rev. **131**, 440



Lippmann-Schwinger equation

$$T(W) = V + V G_0(W) T(W)$$

$$= V \sum_{n=0}^{\infty} \eta_\nu(W)^n$$

Born series

e.g., in free space $G_0(W) = \frac{1}{W - H_0}$

Weinberg eigenvalue problem

$$G_0(W) V \left|\Psi_\nu(W)\right\rangle = \eta_\nu(W) \left|\Psi_\nu(W)\right\rangle$$

series converges iff: all $|\eta_\nu(W)| < 1$

modified Schrödinger equation

$$\left(H_0 + \frac{V}{\eta_\nu(W)} \right) \left|\Psi_\nu(W)\right\rangle = W \left|\Psi_\nu(W)\right\rangle$$

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Regularization

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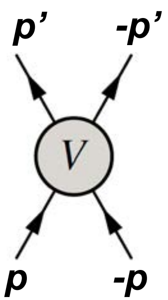
Hoppe, CD, Furnstahl *et al.*, PRC **96**, 054002



	regulator functions		chiral order/ cutoff range
	short range (contact)	**long range** (pion exchanges)	
local (GT+)	$\alpha e^{-\tilde{r}^n}$	$1 - e^{-\tilde{r}^n}$	**up to N^{2}LO** R_0 = 0.9–1.2 fm
nonlocal (EMN)	$e^{-\tilde{p}^{2n}} e^{-\tilde{p}'^{2n}}$		**up to N^{4}LO** Λ = 450–550 MeV
semilocal (EKM)	$e^{-\tilde{p}^{n_1}} e^{-\tilde{p}'^{n_1}}$	$\left(1 - e^{-\tilde{r}^2}\right)^{n_2}$	**up to N^{4}LO** R_0 = 0.8–1.2 fm Λ ~ 493–329 MeV

$\tilde{r} = \frac{r}{R_0}$ $\tilde{p} = \frac{p}{\Lambda}$ $n > 0$

see recent Reinert, Krebs, Epelbaum, arXiv: 1711.08821

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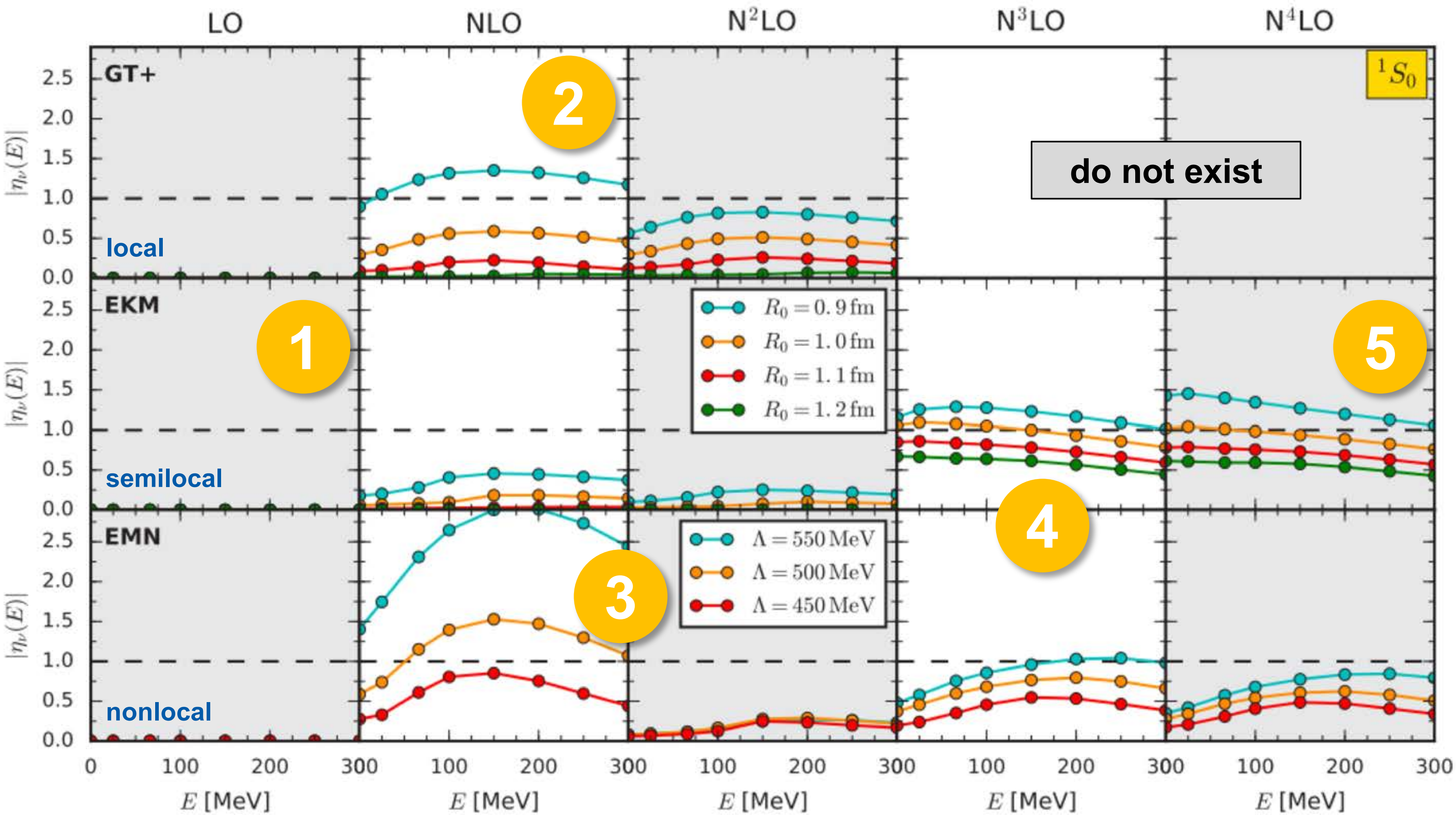
Largest repulsive eigenvalues I

Hoppe, CD, Furnstahl *et al.*, PRC **96**, 054002



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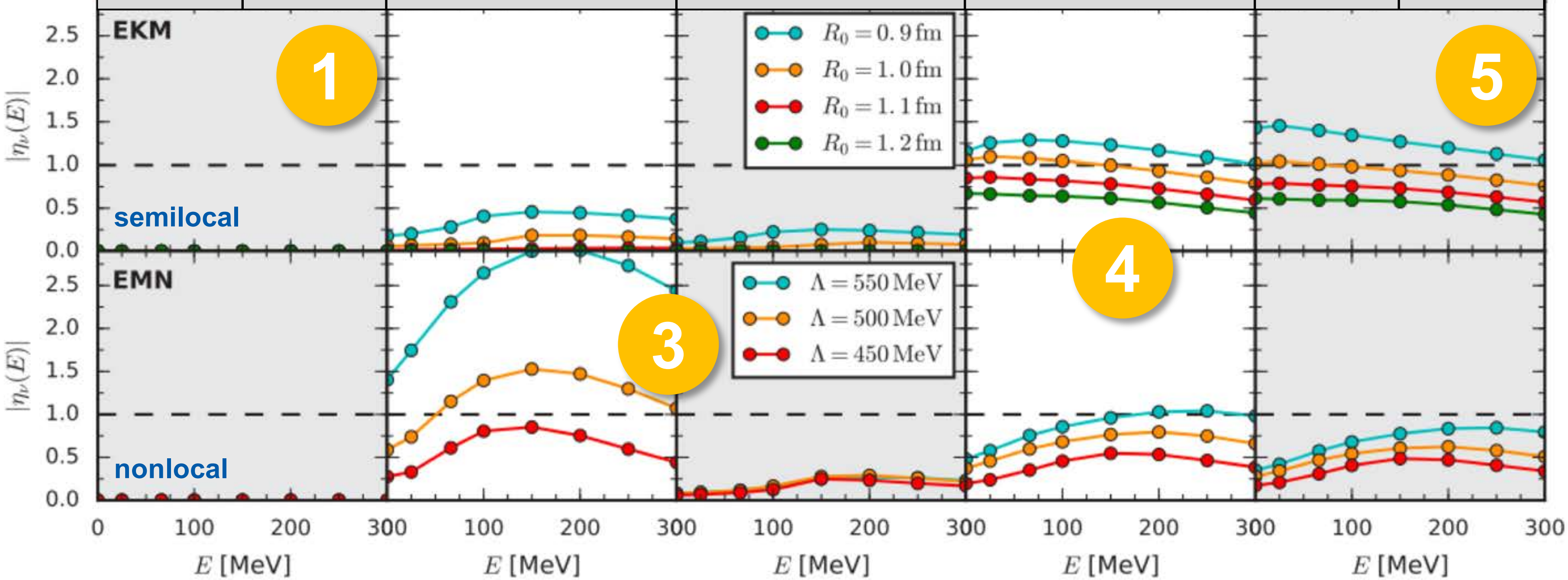
Largest repulsive eigenvalues I

Hoppe, CD, Furnstahl *et al.*, PRC **96**, 054002

B (^{3}H)	LO	NLO	N^{2}LO	N^{3}LO	N^{4}LO	emp.
EKM	11.30	8.36	8.26	7.53	7.63	8.48
EMN	11.02	8.31	8.21	8.09	8.08	



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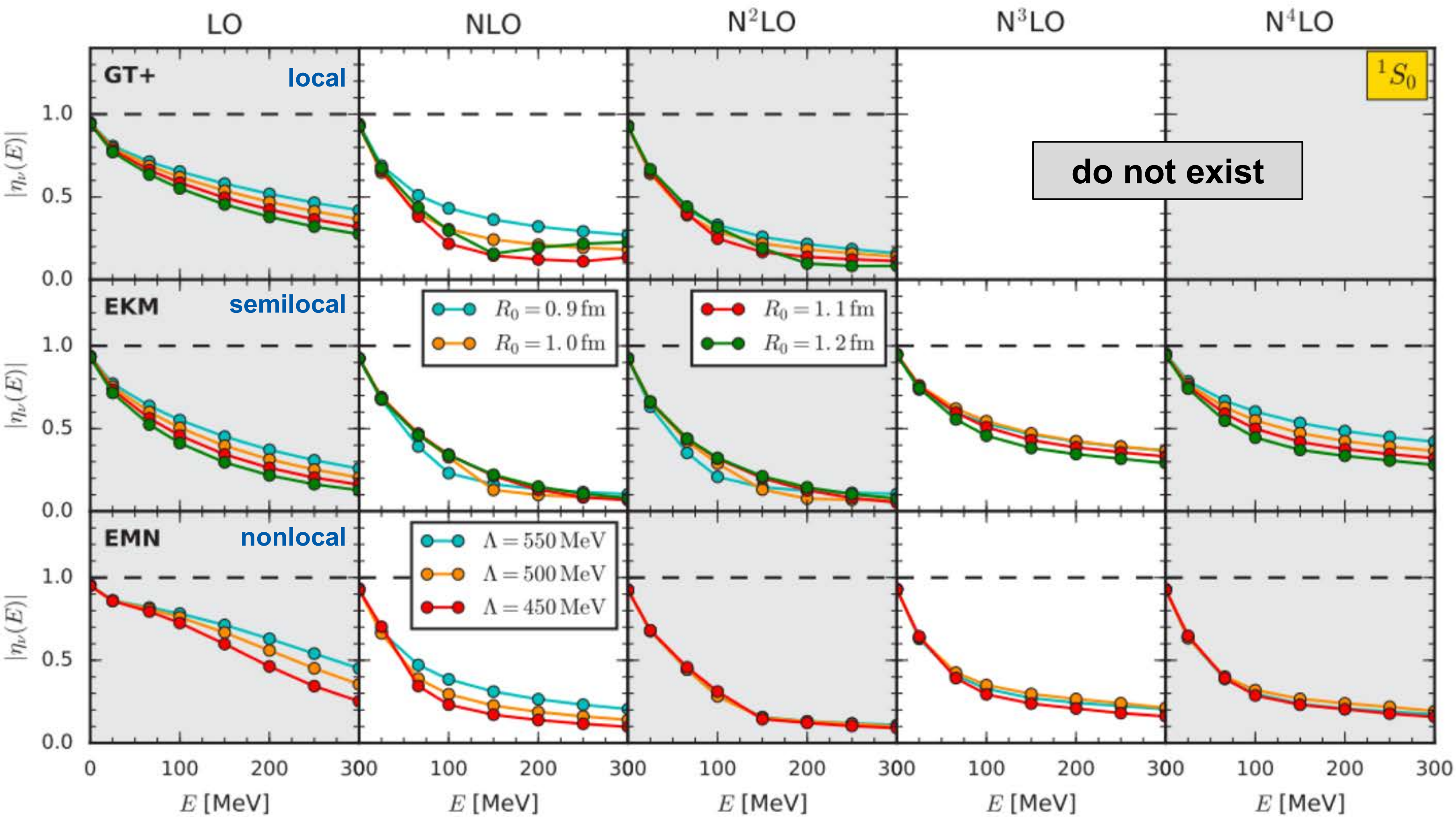
Largest attractive eigenvalues

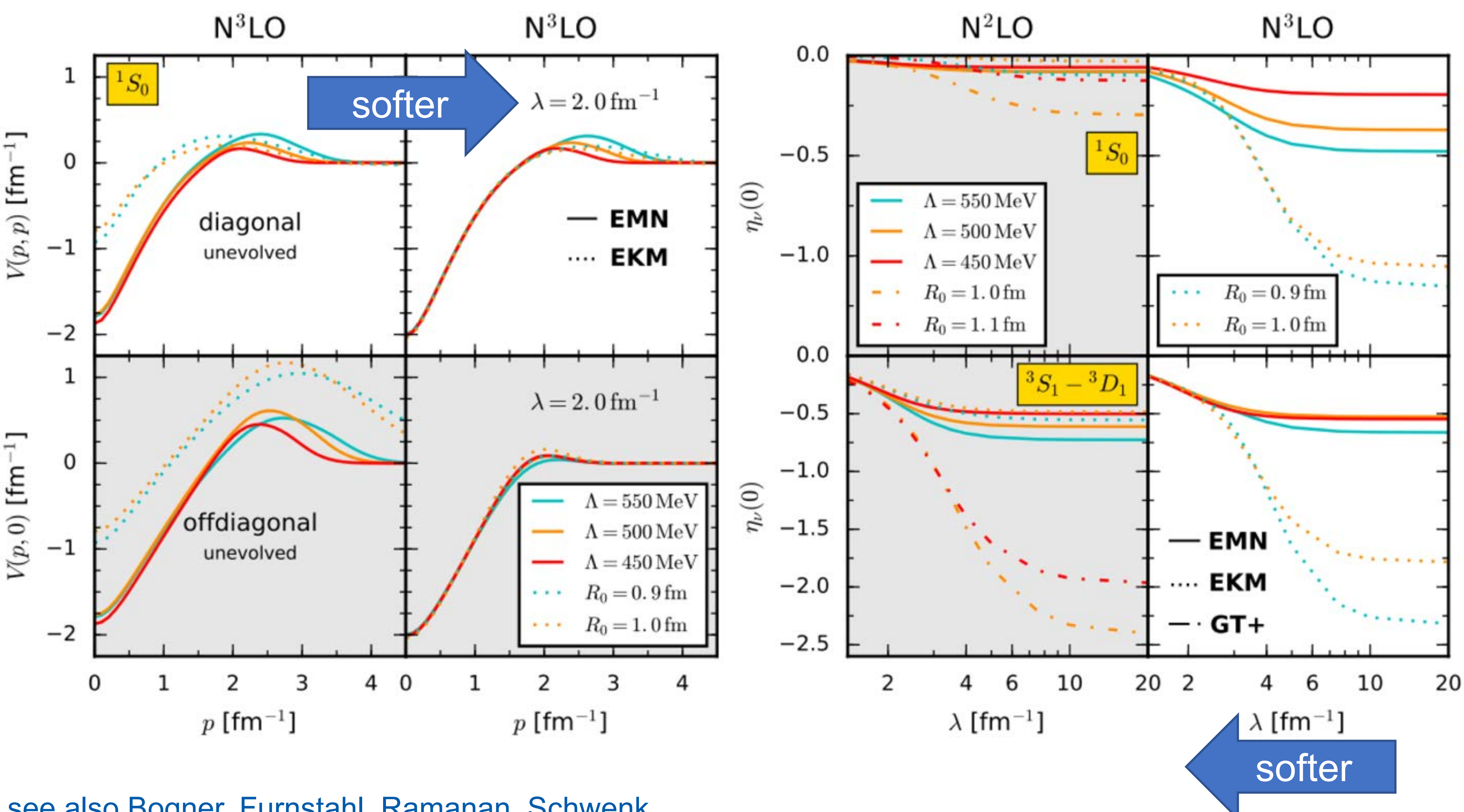
Hoppe, CD, Furnstahl *et al.*, PRC **96**, 054002



MBPT calculations of infinite matter at zero temperature

Softening the potentials via SRG

Hoppe, CD, Furnstahl *et al.*, PRC **96**, 054002



see also Bogner, Furnstahl, Ramanan, Schwenk, …

MBPT calculations of infinite matter at zero temperature

Summary

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1 Full N^{3}LO calculations

- **novel normal-ordering method:** include general 3N interactions

Phys. Rev. C **93**, 054314

- improved predictions: neutron matter
- MBPT vs. SCGF: MB convergence

Phys. Rev. C **94**, 054307

2 Monte-Carlo Framework

- **push the limits of MBPT to higher orders**
- *state-of-the-art* calculations
- explore new chiral interactions up to N^{3}LO

arXiv:1710.08220

3 Weinberg eigenvalue analysis

- **study** of large set of NN potentials with **new regularization schemes**
- insights into their idiosyncrasies at different orders and partial waves
- monitor fits of new chiral potentials

Phys. Rev. C **96**, 054002

MBPT calculations of infinite matter at zero temperature

Outlook

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1. **Apply the new Hamiltonians to finite nuclei**
   calculations will provide additional insights …
2. **Perform calculations in asymmetric matter**
   extract astrophysical quantities, mass-radius relations, …
3. **Extend framework to finite temperatures**
   study thermal properties, tabulate equation of state, …
4. **Constrain fits of next-gen. chiral potentials**
   in terms of saturation, uncertainty quantification, …

Thank you for your attention!

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