# Chiral 3N interactions and asymmetric nuclear matter

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East Lansing, May 20, 2015

TECHNISCHE UNIVERSITÄT DARMSTADT

European Research Council
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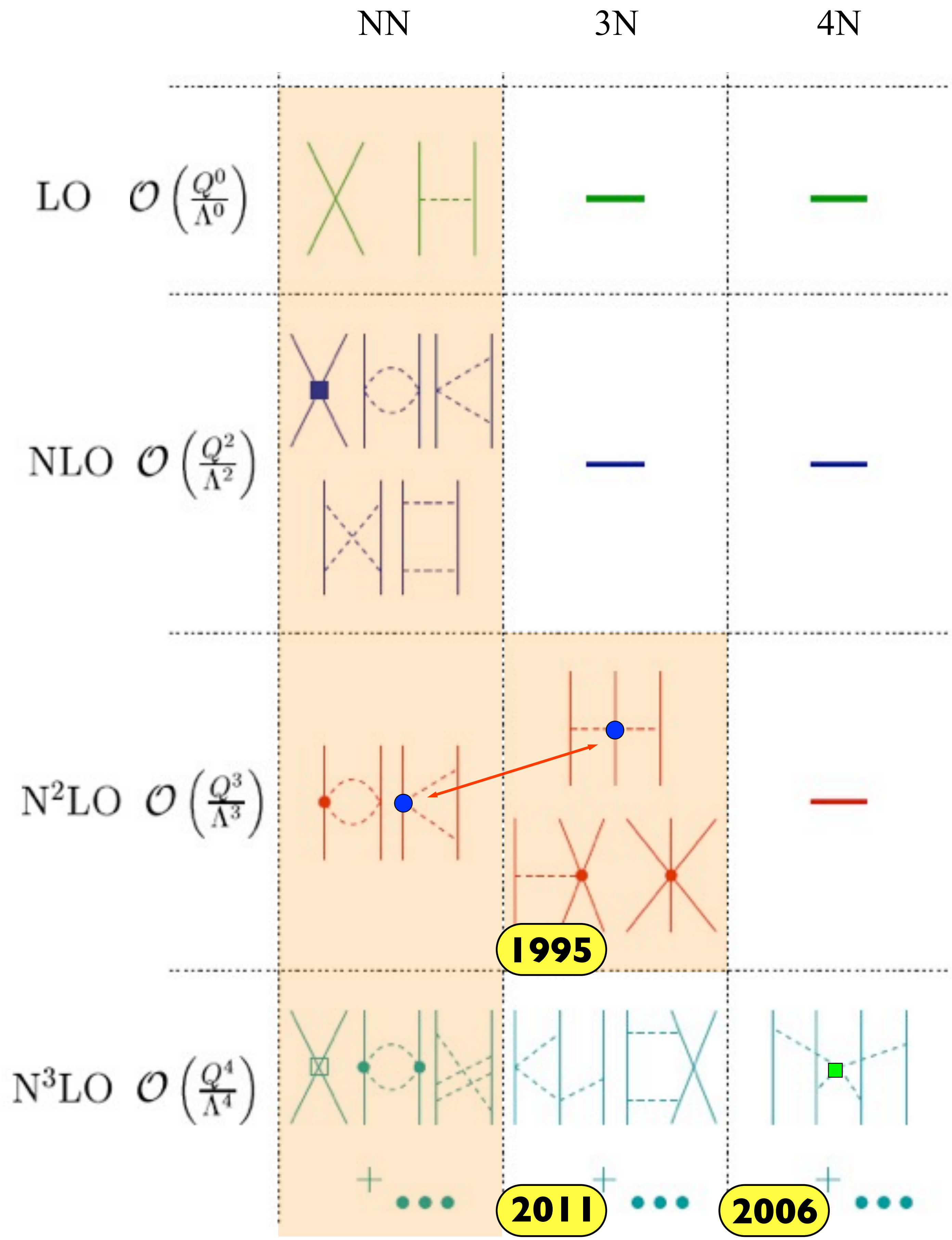
**MSU workshop**
**"Theory for open-shell nuclei near the limits of stability"**

# Chiral effective field theory for nuclear forces

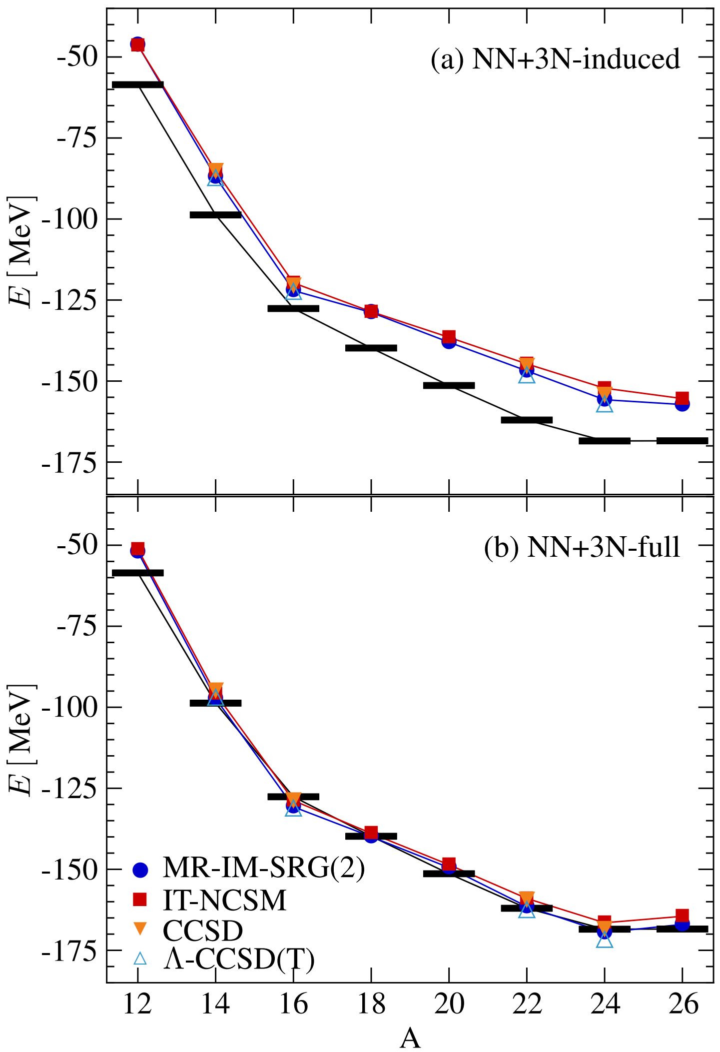
- choose relevant degrees of freedom: here nucleons and pions
- operators constrained by symmetries of QCD
- short-range physics captured in few short-range couplings
- separation of scales: Q << $\Lambda_b$, breakdown scale $\Lambda_b$~500 MeV
- power-counting: expand in powers Q/$\Lambda_b$
- systematic: work to desired accuracy, obtain error estimates

treatment of NN and 3N forces not consistent in present ab initio calculations



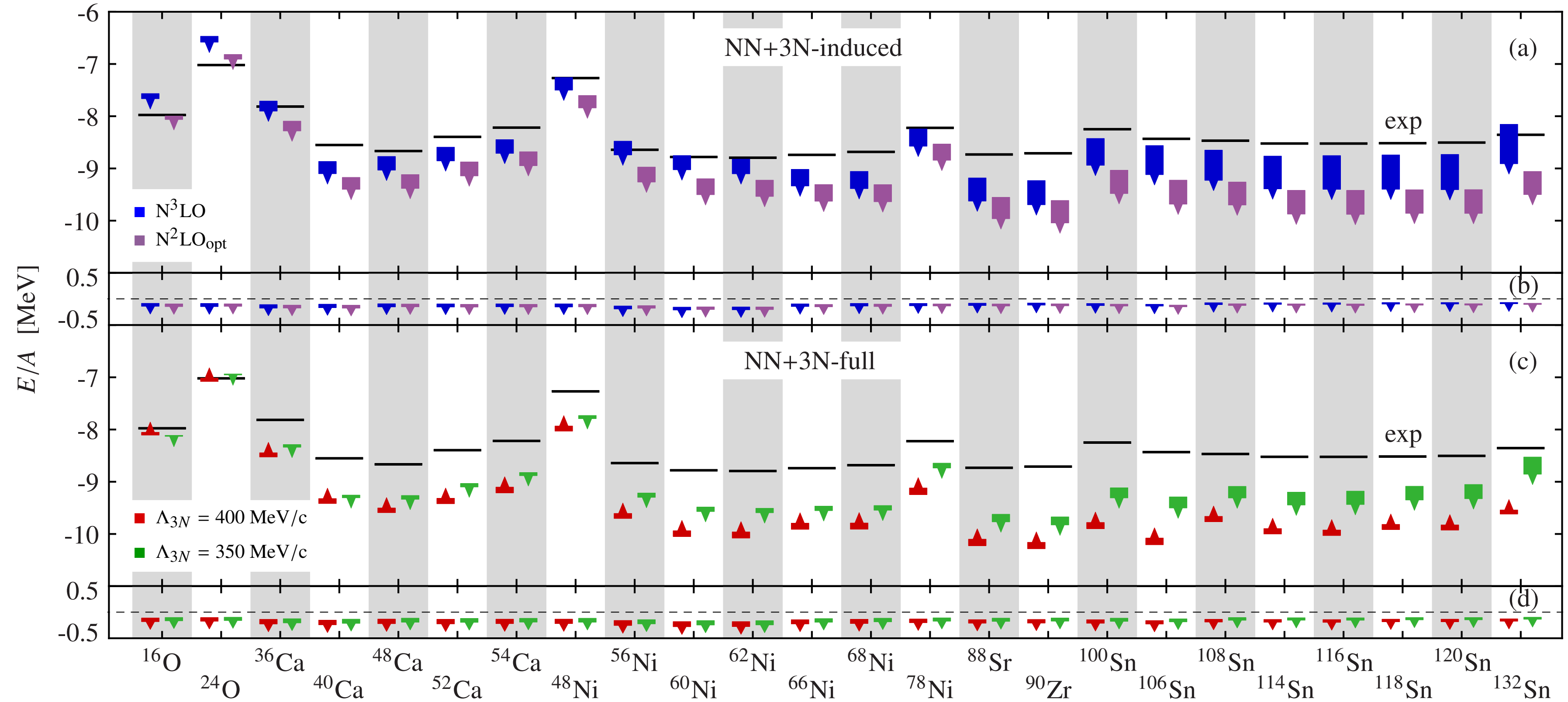
# Open issues in nuclear interactions

oxygen chain




Hergert et al.,
PRL 110, 242501 (2013)

heavy nuclei




Binder et al., Phys. Lett B 736, 119 (2014)

- remarkable agreement between different many-body frameworks
- significant overbinding in heavy nuclei

# Open issues in nuclear interactions

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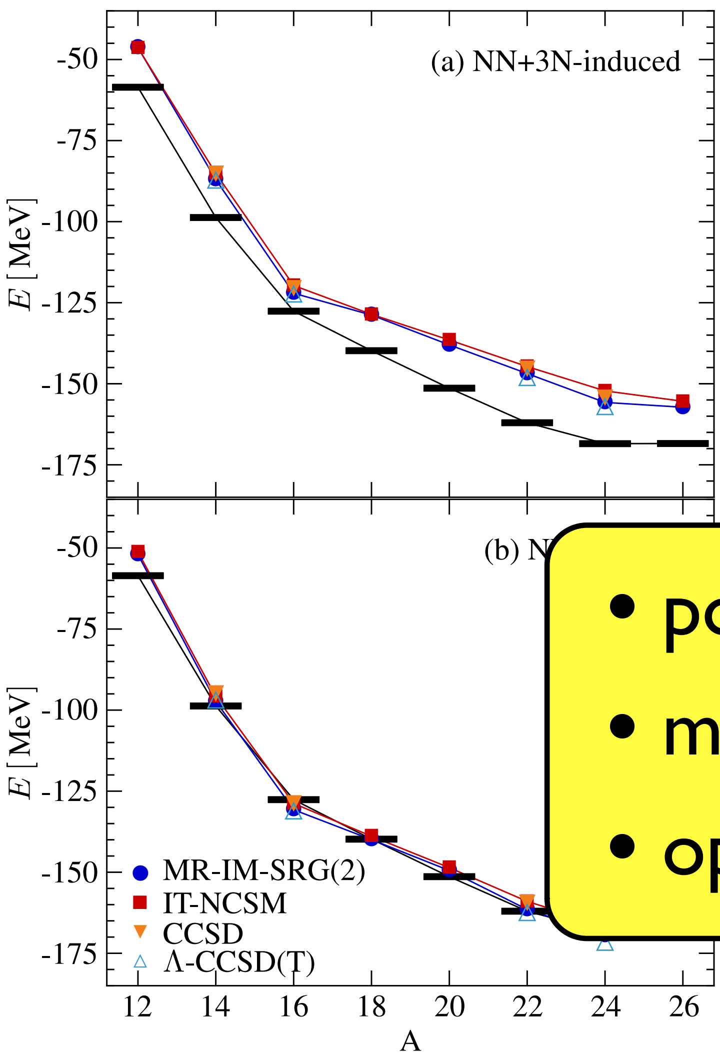


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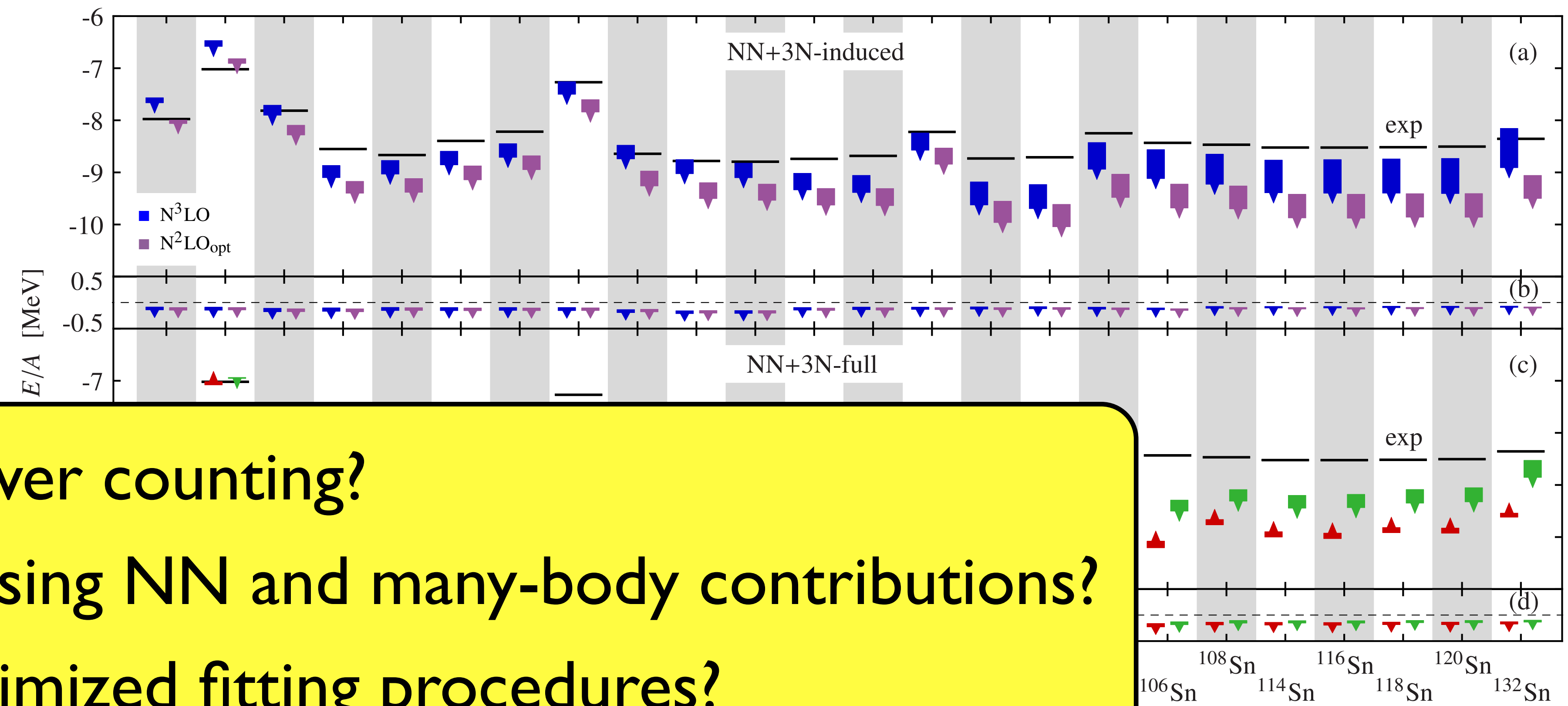


- power counting?
- missing NN and many-body contributions?
- optimized fitting procedures?

Hergert et al.,
PRL 110, 242501 (2013)

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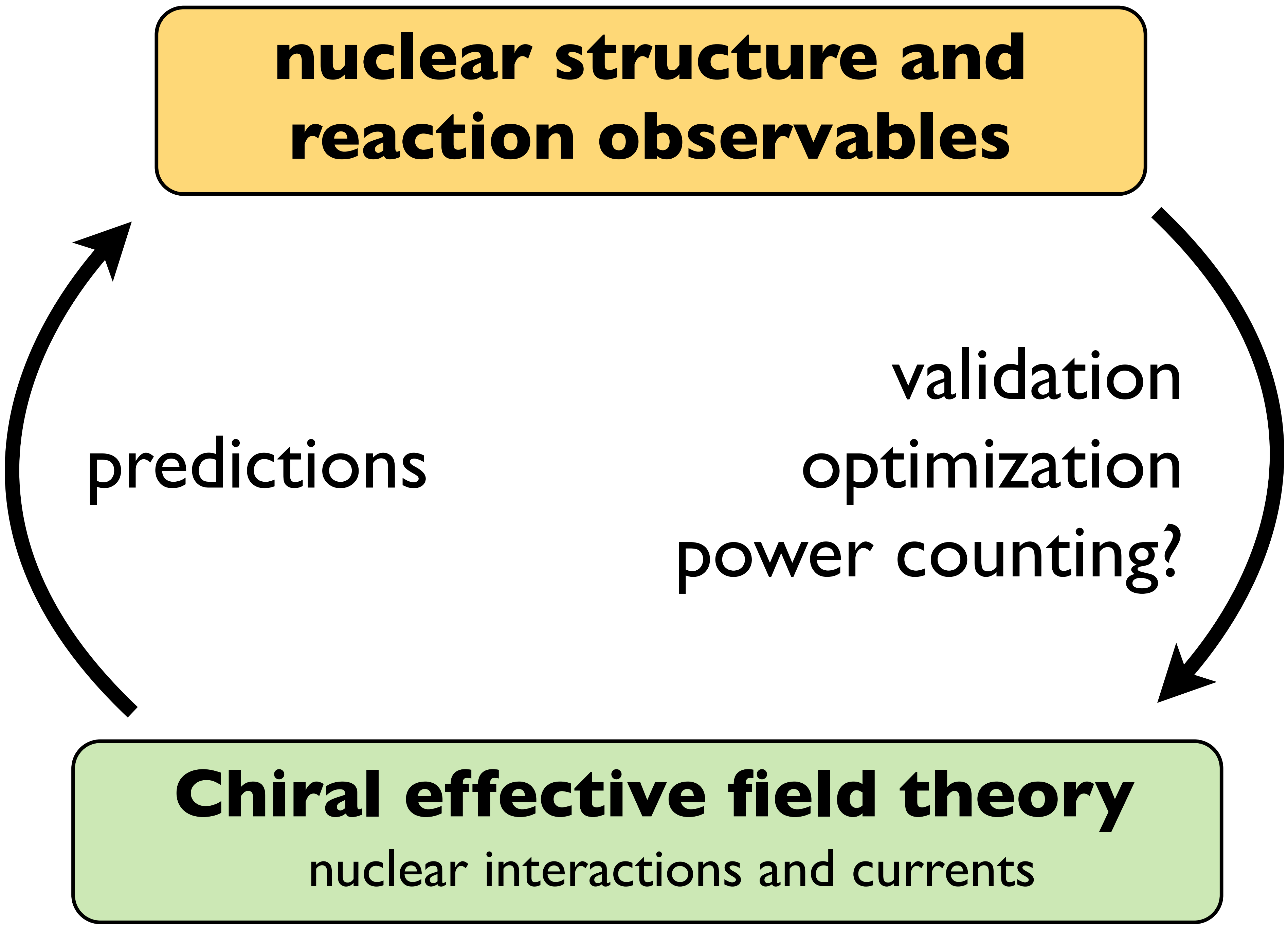
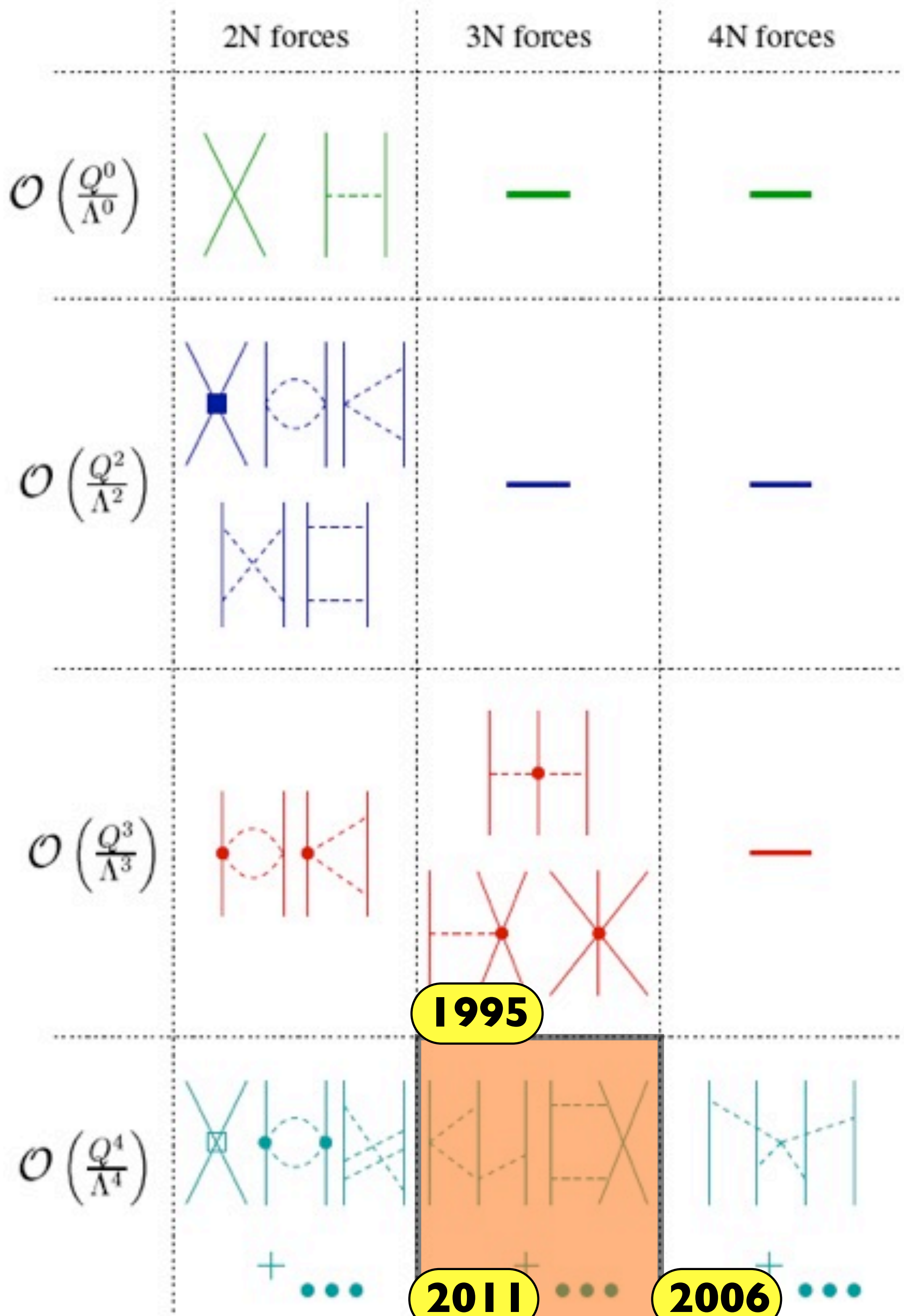
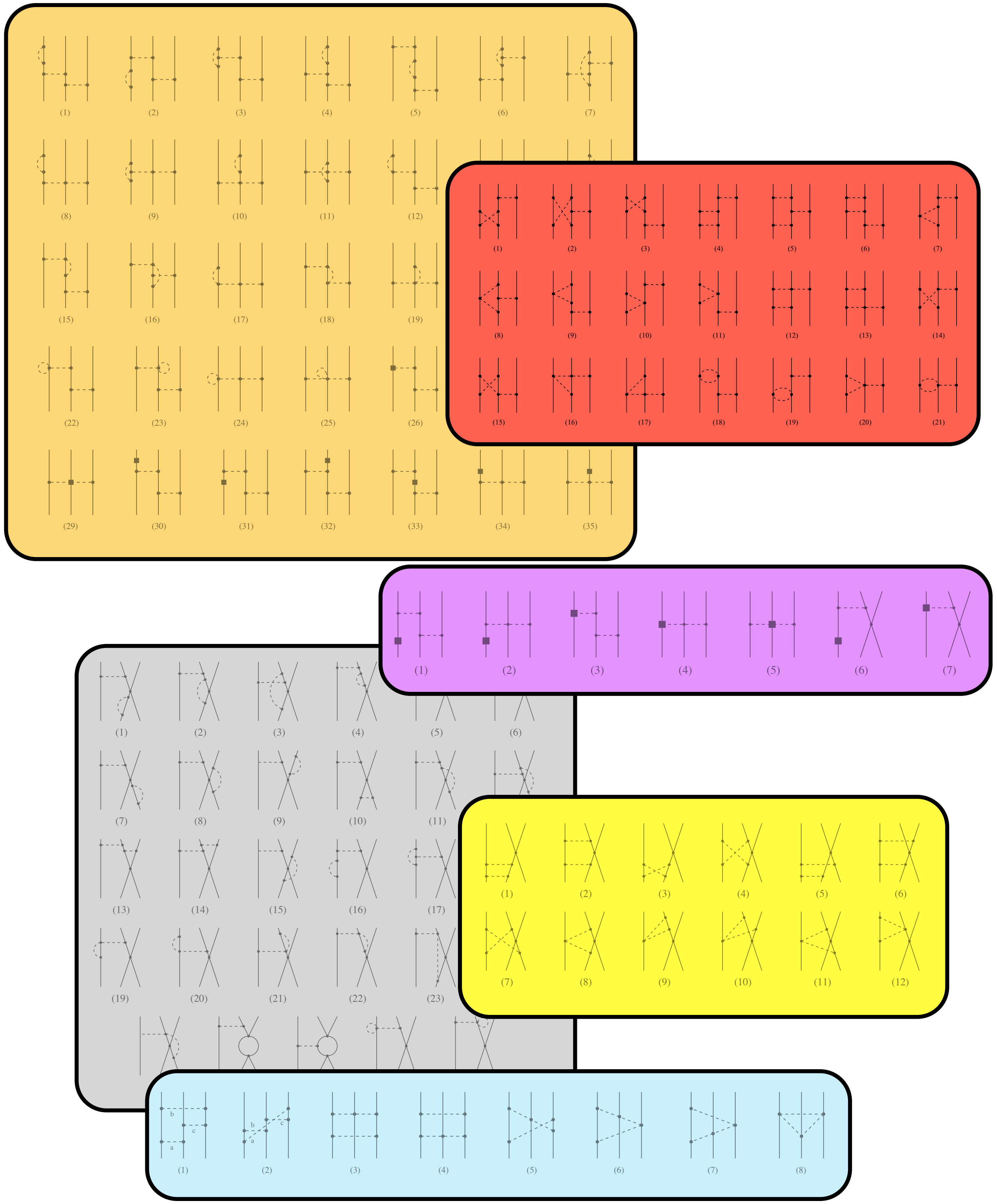
# Development of novel NN+3N chiral EFT potentials




study order-by-order convergence $\longrightarrow$ estimates of theoretical uncertainties

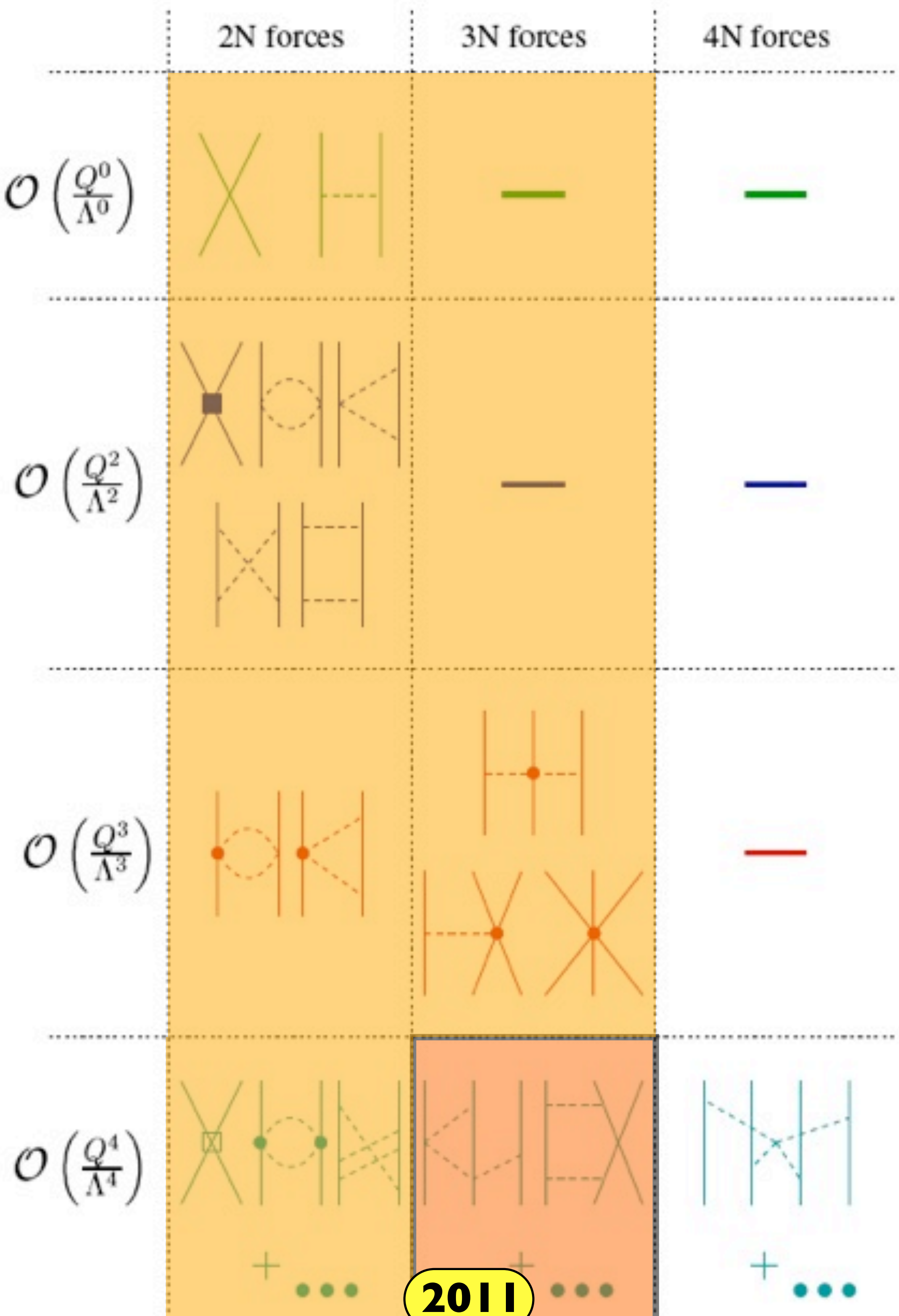
# Chiral 3N forces at subleading order ($N^3LO$)

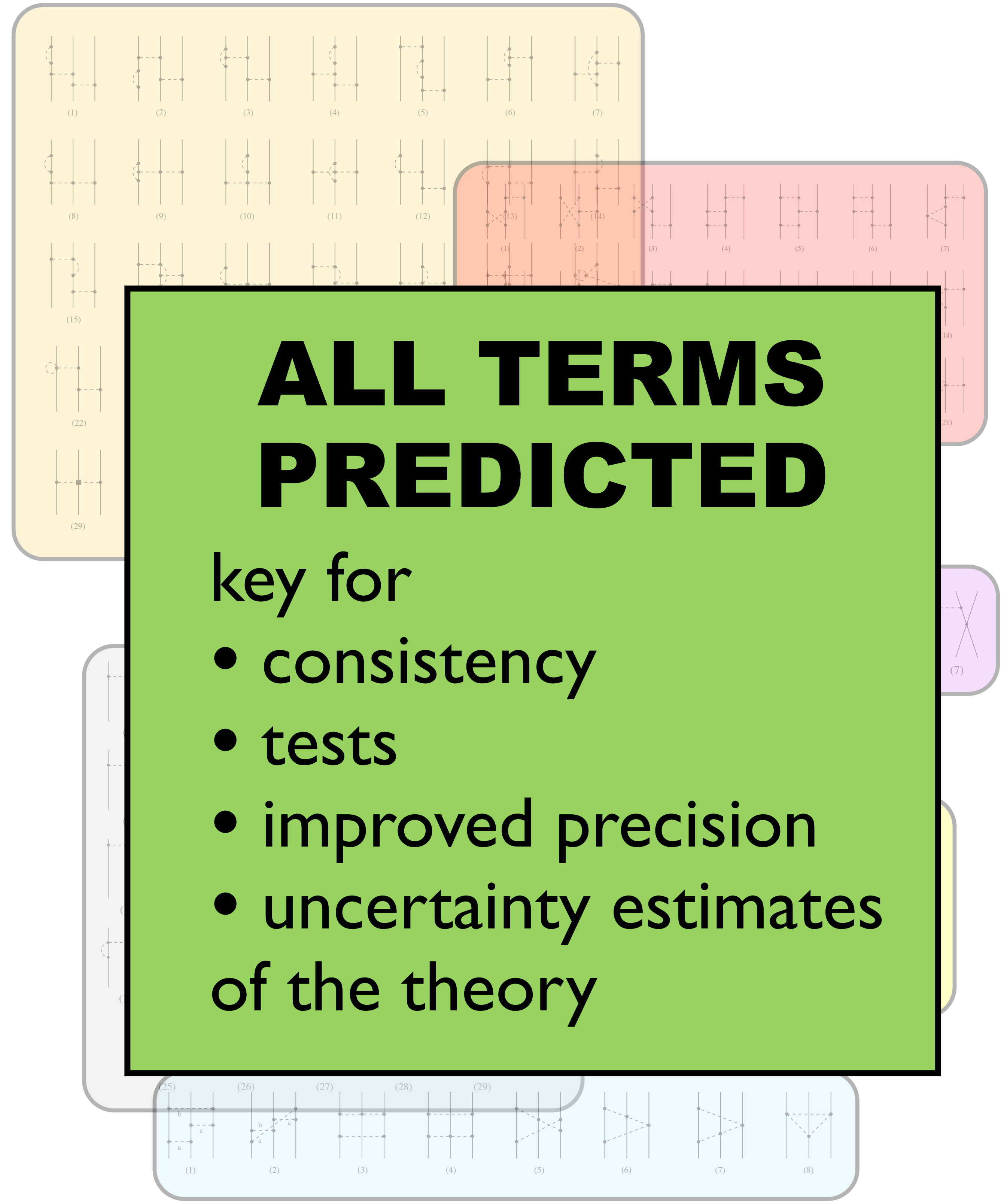



Bernard et al., PRC 77, 064004 (2008)
Bernard et al., PRC 84, 054001 (2011)
Krebs et al., PRC 85, 054006 (2012)
Krebs et al., PRC 87, 054007 (2013)

# Chiral 3N forces at subleading order (N$^3$LO)



**ALL TERMS PREDICTED**

key for
- consistency
- tests
- improved precision
- uncertainty estimates

of the theory


Bernard et al., PRC 77, 064004 (2008)
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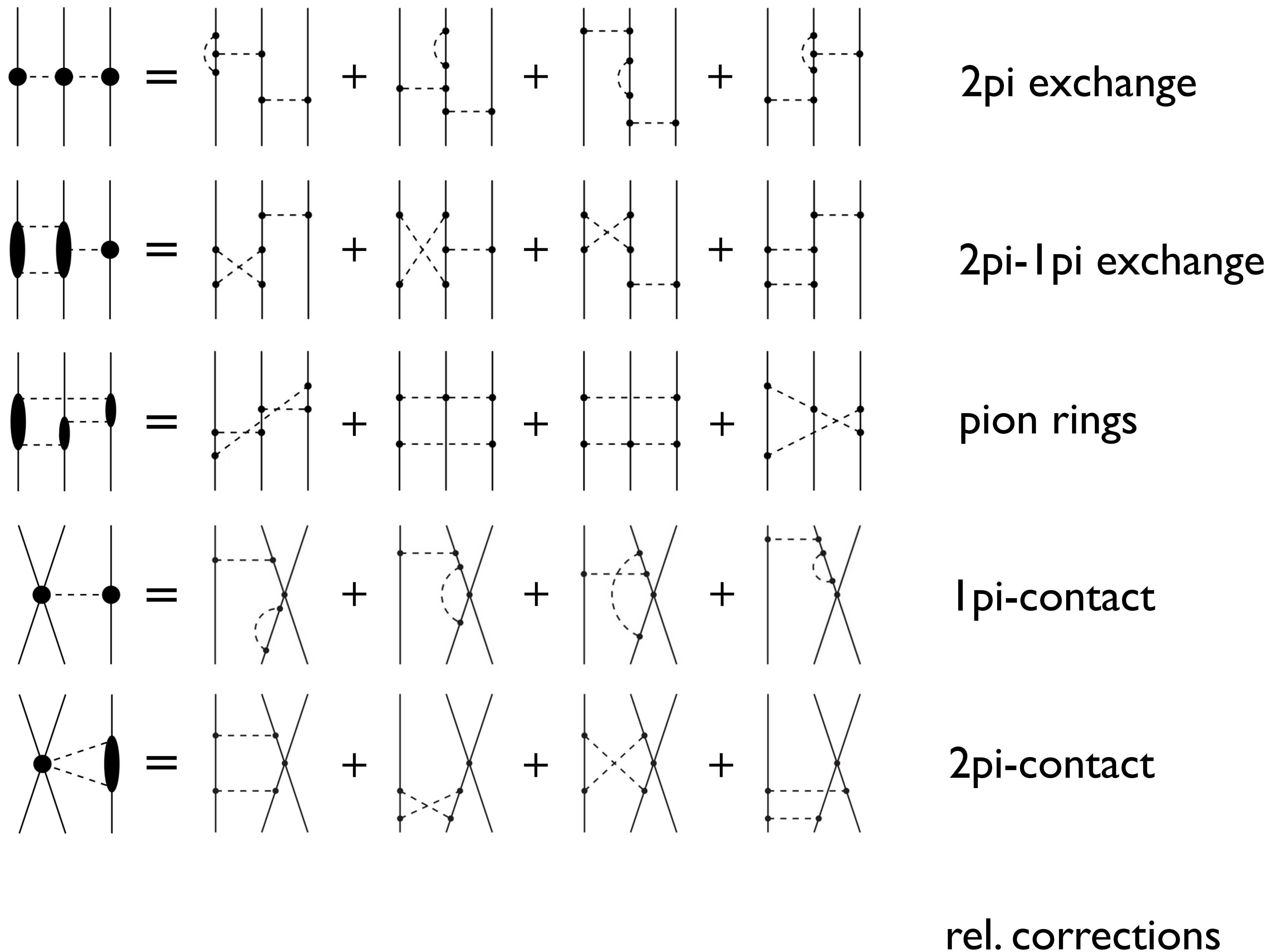
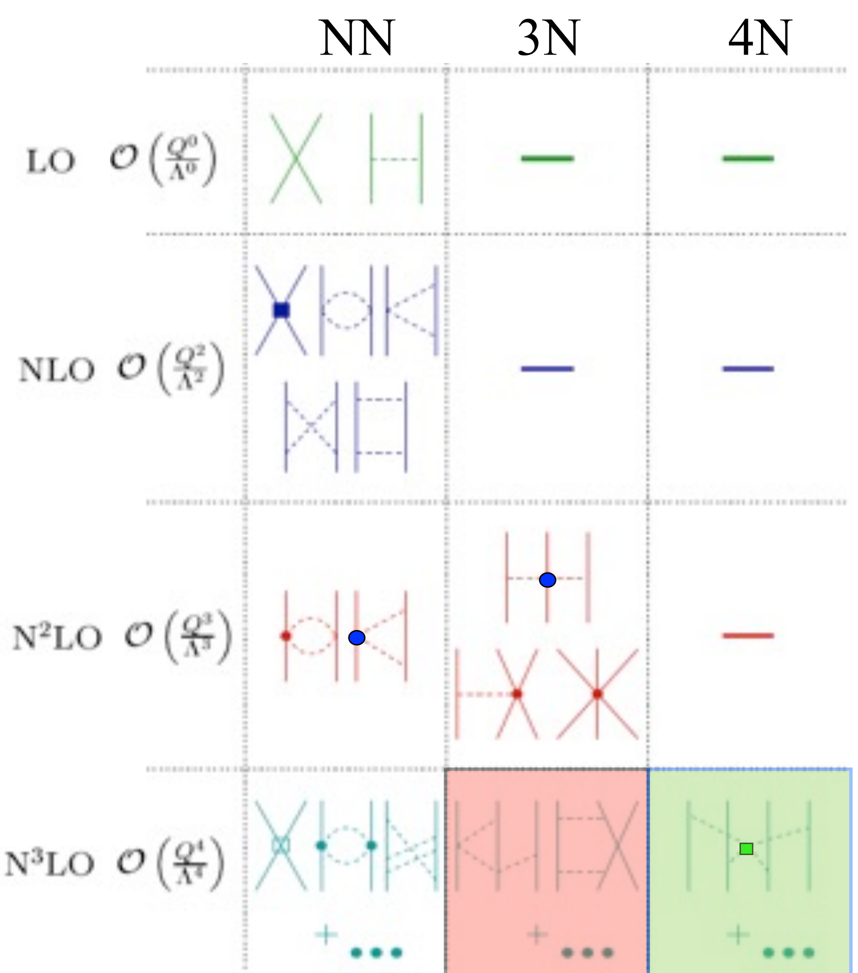
# Three-nucleon force contributions at $N^3LO$

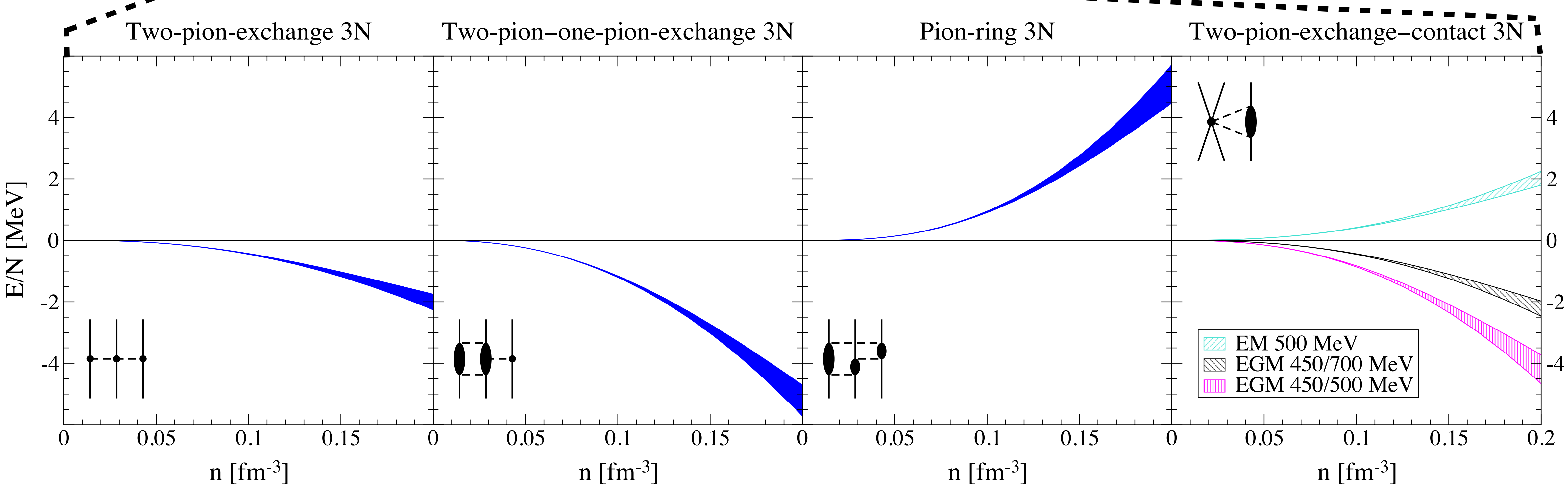


# Contributions of many-body forces at $N^3LO$ in neutron matter




- first calculations of $N^3LO$ 3NF and 4NF contributions to EOS of neutron matter
- found large contributions in Hartree Fock appr., comparable to size of $N^2LO$ contributions

Tews, Krüger, KH, Schwenk
PRL 110, 032504 (2013)



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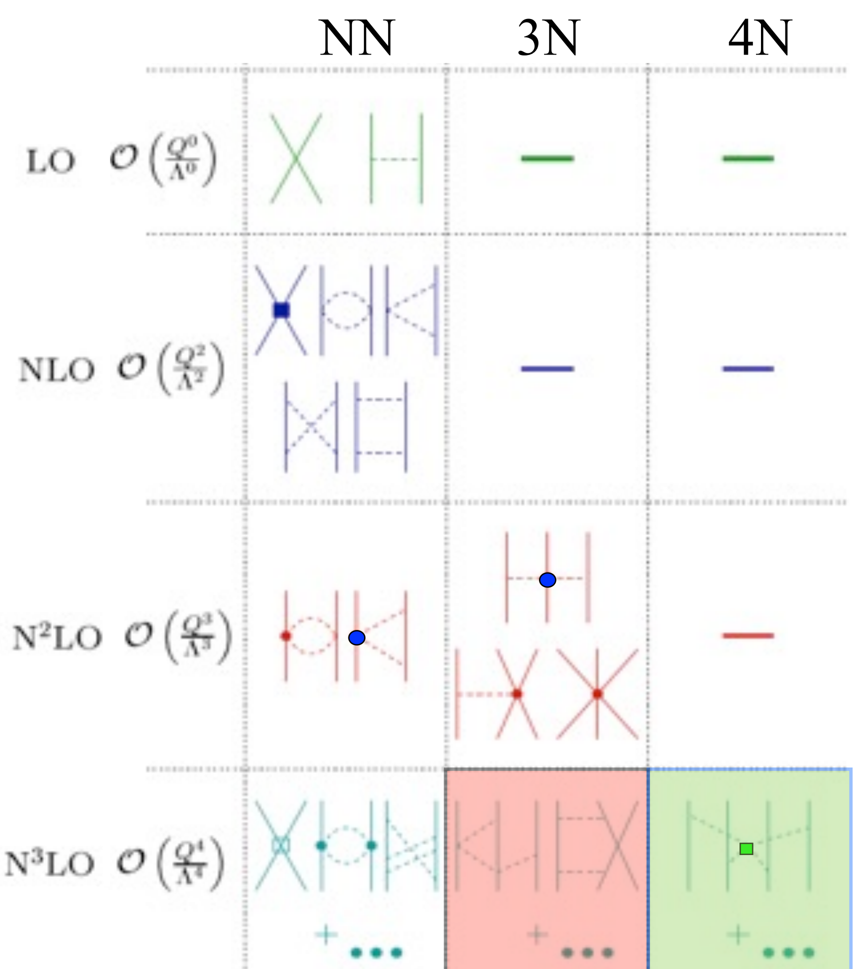


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- 4NF contributions small

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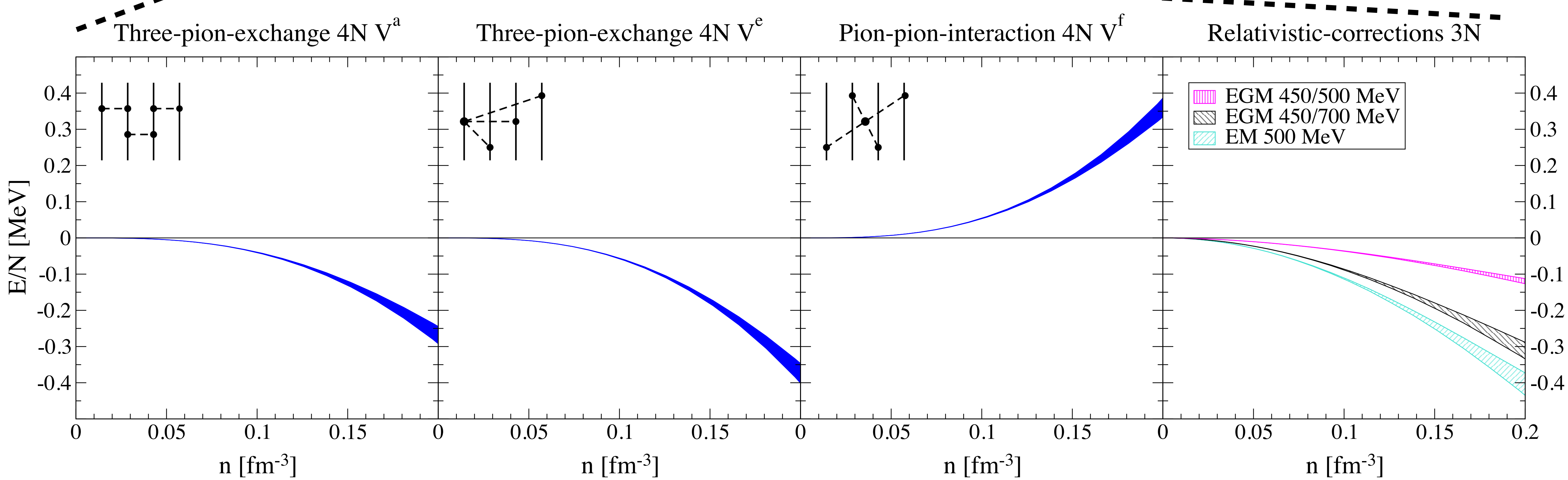
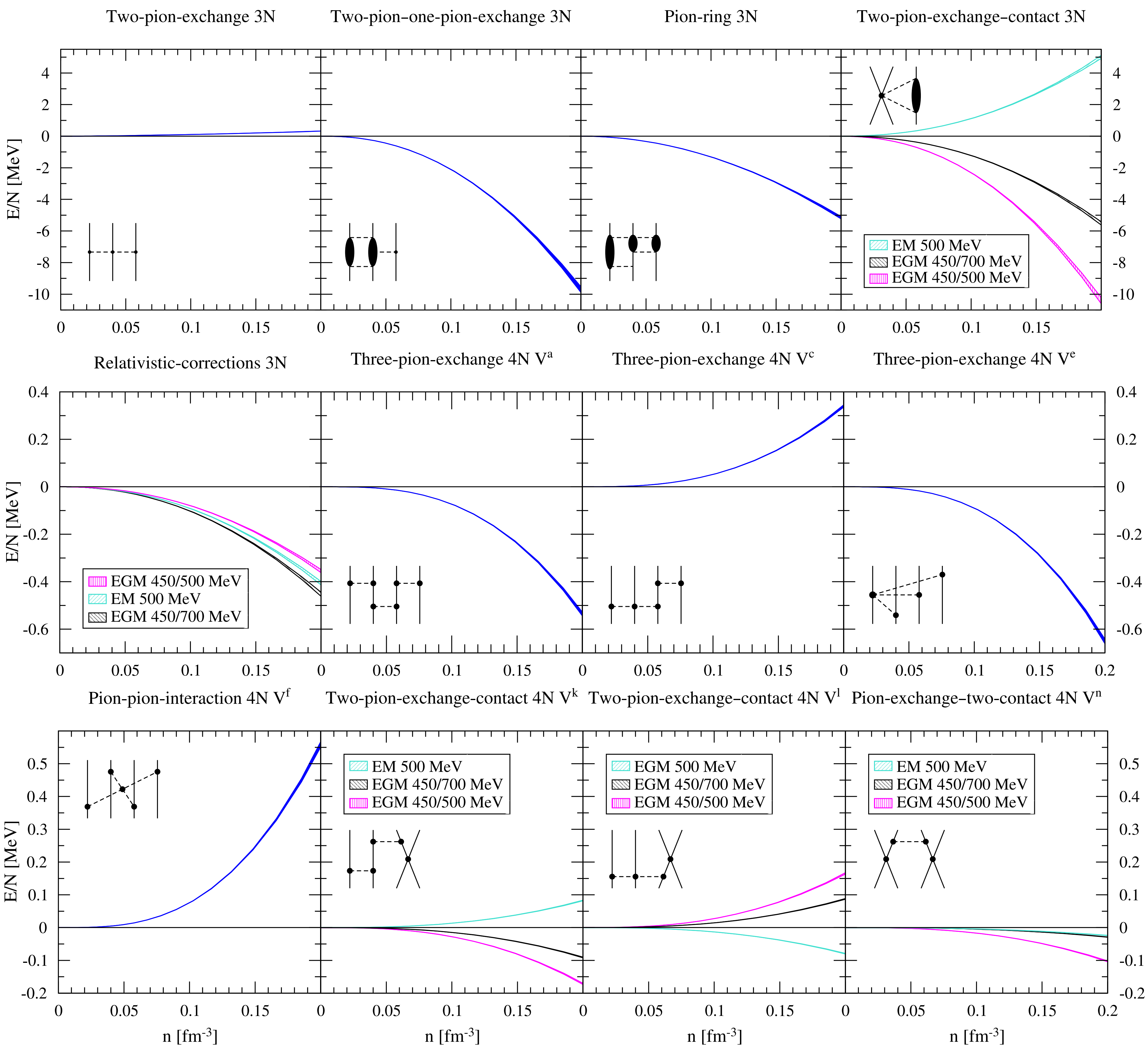


# $N^3LO$ contributions in nuclear matter (Hartree Fock)




Krüger, Tews, KH, Schwenk
PRC88, 025802 (2013)

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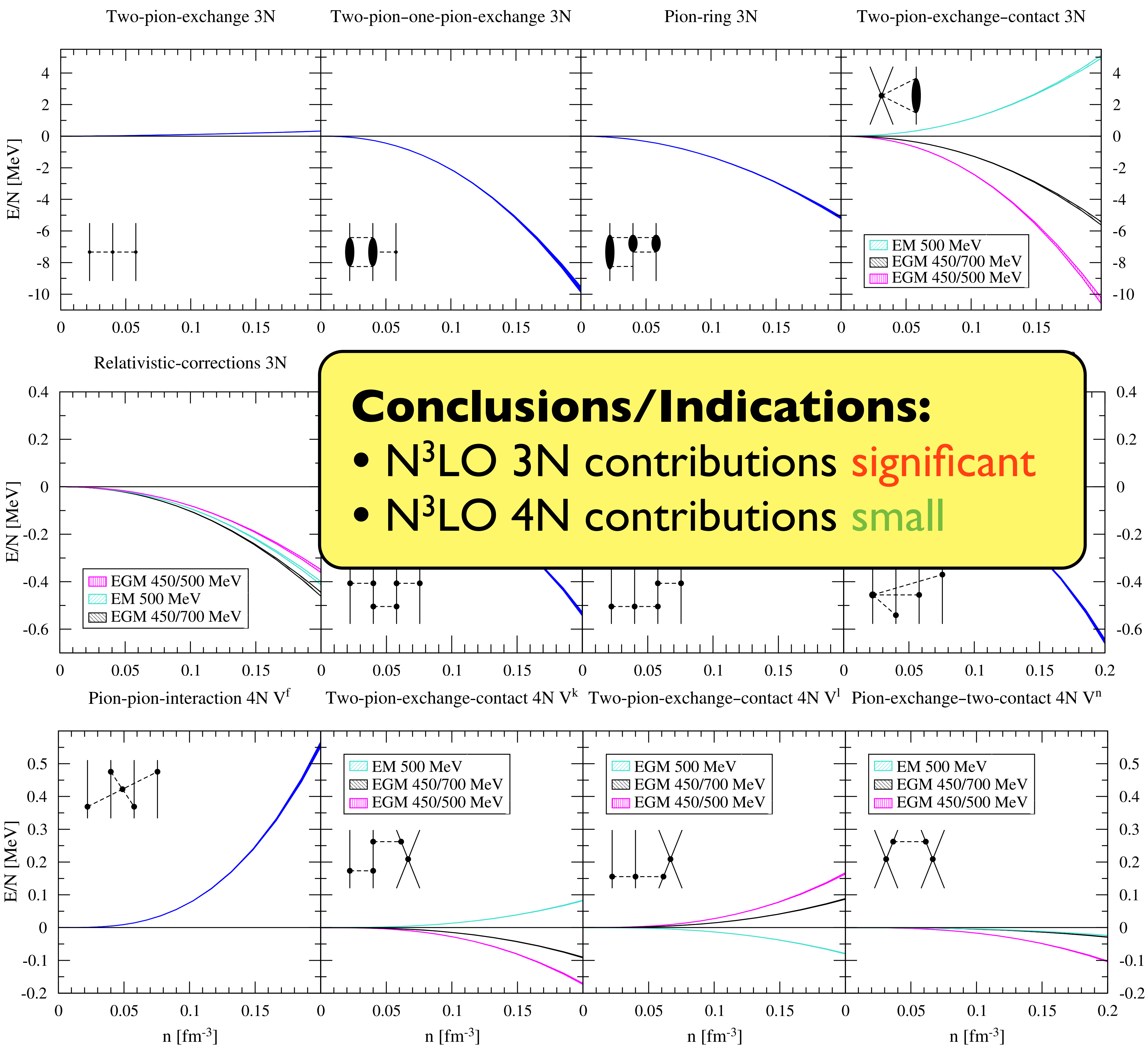


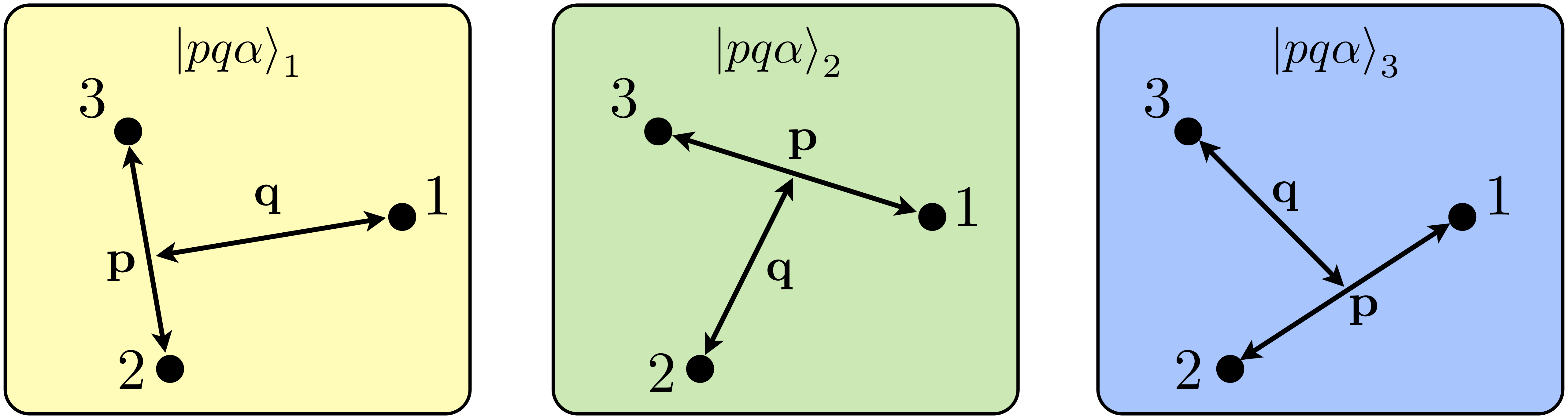

**Conclusions/Indications:**

- $N^3LO$ 3N contributions significant
- $N^3LO$ 4N contributions small

Krüger, Tews, KH, Schwenk
PRC88, 025802 (2013)

# Representation of 3N interactions in momentum space

$$|pq\alpha\rangle_i \equiv |p_i q_i; [(LS)J(ls_i)j]\,\mathcal{J}\mathcal{J}_z(Tt_i)\mathcal{T}\mathcal{T}_z\rangle$$




Due to the large number of matrix elements, the traditional way of computing matrix elements requires extreme amounts of computer resources.

$$N_p \simeq N_q \simeq 15$$
$$N_\alpha \simeq 30 - 180 \quad \longrightarrow \quad \dim[\langle pq\alpha|V_{123}|p'q'\alpha'\rangle] \simeq 10^7 - 10^{10}$$

Number of matrix elements was so far not sufficient for studies of $A \geq 4$ systems.

# Calculation of 3N forces in momentum partial-wave representation

$$\langle pq\alpha|V_{123}|p'q'\alpha'\rangle \sim \sum_{m_i} \int d\hat{\mathbf{p}}\, d\hat{\mathbf{q}}\, d\hat{\mathbf{p}}'\, d\hat{\mathbf{q}}' Y_l^m(\hat{\mathbf{p}}) Y_{\bar{l}}^{\bar{m}}(\hat{\mathbf{q}}) \, \langle \mathbf{p}\mathbf{q}ST|V_{123}|\mathbf{p}'\mathbf{q}'S'T'\rangle \, Y_{l'}^{m'}(\hat{\mathbf{p}}') Y_{\bar{l}'}^{\bar{m}'}(\hat{\mathbf{q}}')$$

**traditional method:**

- reduce dimension of angular integrals from 8 to 5 by using symmetry
- discretize angular integrals and perform all sums numerically

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**traditional method:**

- reduce dimension of angular integrals from 8 to 5 by using symmetry
- discretize angular integrals and perform all sums numerically

**new method:**

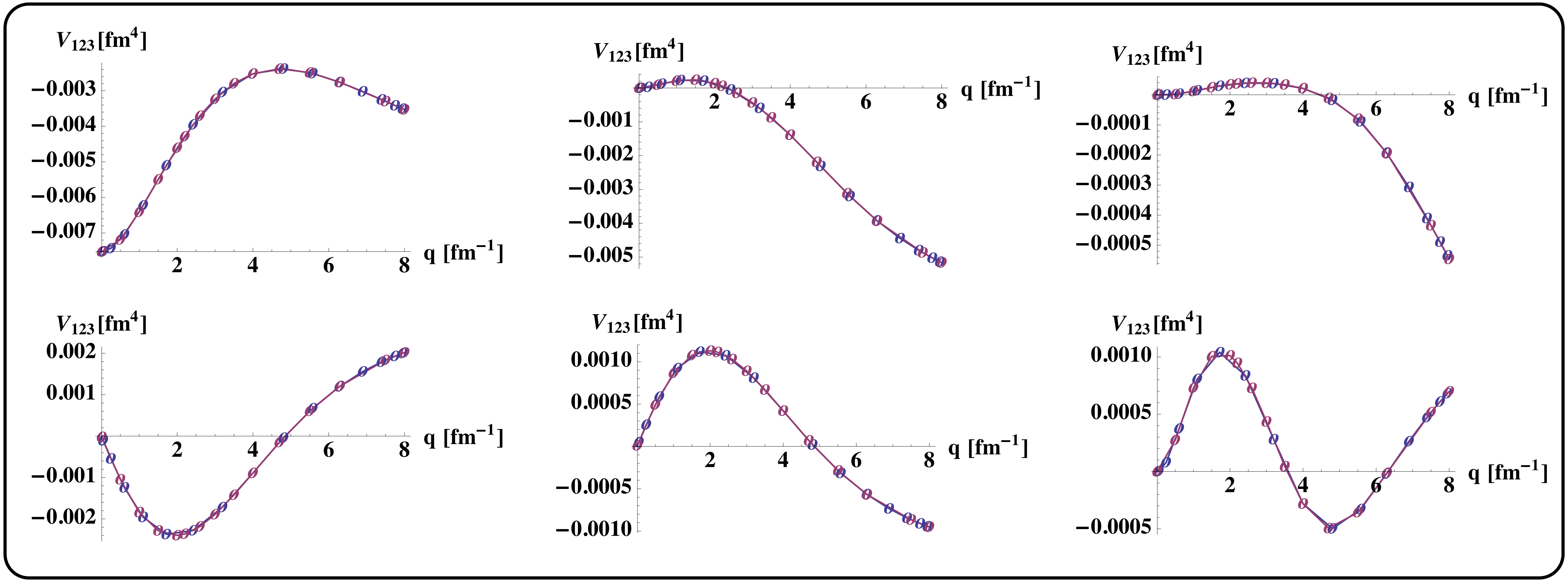
- use that all interaction contributions (except rel. corr.) are local:

$$\begin{aligned}\langle \mathbf{p}\mathbf{q}|V_{123}|\mathbf{p}'\mathbf{q}'\rangle &= V_{123}(\mathbf{p}-\mathbf{p}', \mathbf{q}-\mathbf{q}') \\ &= V_{123}(p-p', q-q', \cos\theta)\end{aligned}$$

$\longrightarrow$ allows to perform all except 3 integrals analytically

- only a few small discrete internal sums need to be performed for each external momentum and angular momentum

# Tests of the new framework




- **perfect agreement** with results based on traditional approach
- **speedup** factors of >1000
- **very general**, can also be applied to
  - pion-full EFT
  - $N^4LO$ terms
  - currents?
- **efficient:** allows to study systematically alternative regulators

# Current status of calculations

- all 3N topologies are calculated and stored separately, allows to easily adjust values of LECs and the cutoff value and form of non-local regulators

- calculated matrix elements of Faddeev components

$$\langle pq\alpha | V_{123}^{i} | p'q'\alpha' \rangle$$

  as well as antisymmetrized matrix elements

$$\langle pq\alpha | (1 + P_{123} + P_{132}) V_{123}^{i} (1 + P_{123} + P_{132}) | p'q'\alpha' \rangle$$

- HDF5 file format for efficient I/O

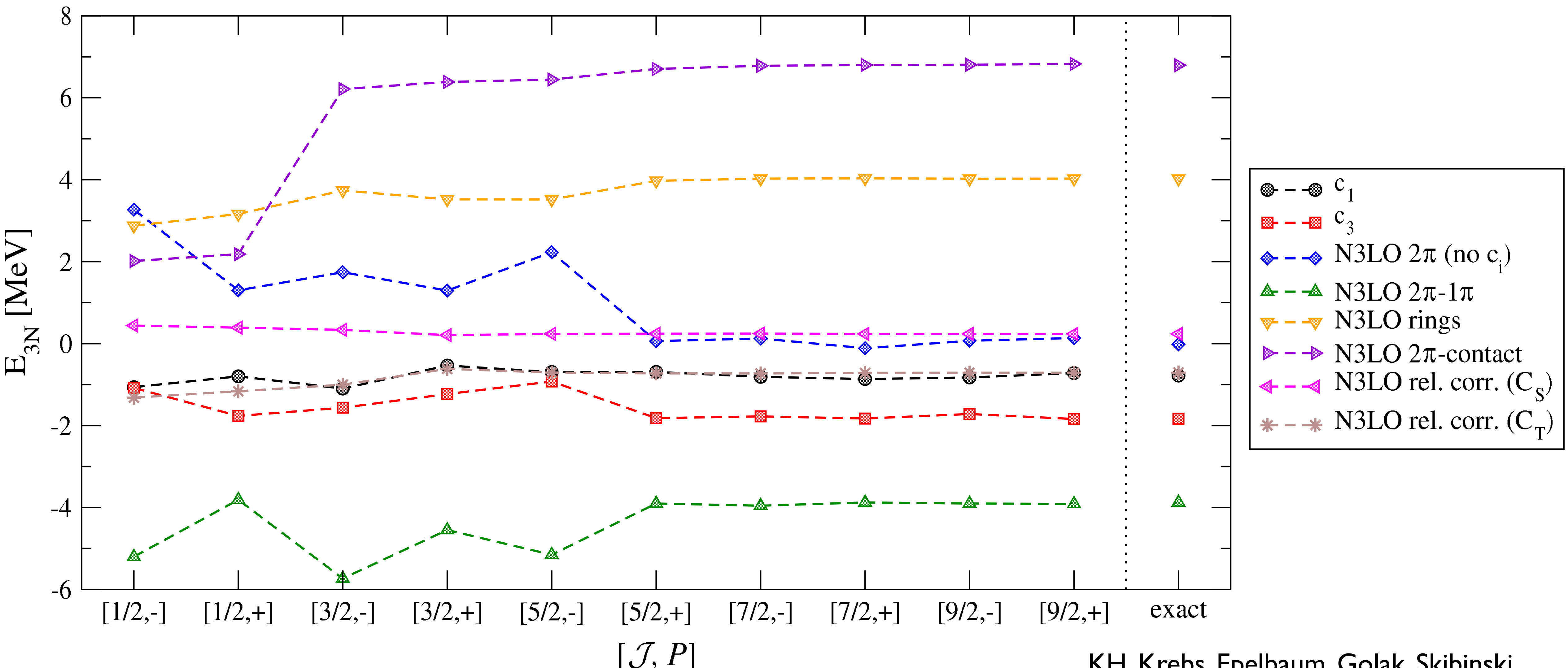
  *http://www.hdfgroup.org*

- current model space limits:

| $\mathcal{J}$ | $\mathcal{T}$ | $J_{\max}^{12}$ | size [GB] |
|---|---|---|---|
| 1/2 | 1/2 | 8 | 1.0 |
| 3/2 | 1/2 | 8 | 3.2 |
| 5/2 | 1/2 | 8 | 6.2 |
| 7/2 | 1/2 | 7 | 6.9 |
| 9/2 | 1/2 | 6 | 6.2 |
| 1/2 | 3/2 | 8 | 0.3 |
| 3/2 | 3/2 | 8 | 0.8 |
| 5/2 | 3/2 | 8 | 1.8 |
| 7/2 | 3/2 | 7 | 1.8 |
| 9/2 | 3/2 | 6 | 1.8 |
| | | | $\sim 0.5$ TB |

# Partial wave convergence: energy of infinite matter in Hartree-Fock approximation

## neutron matter:

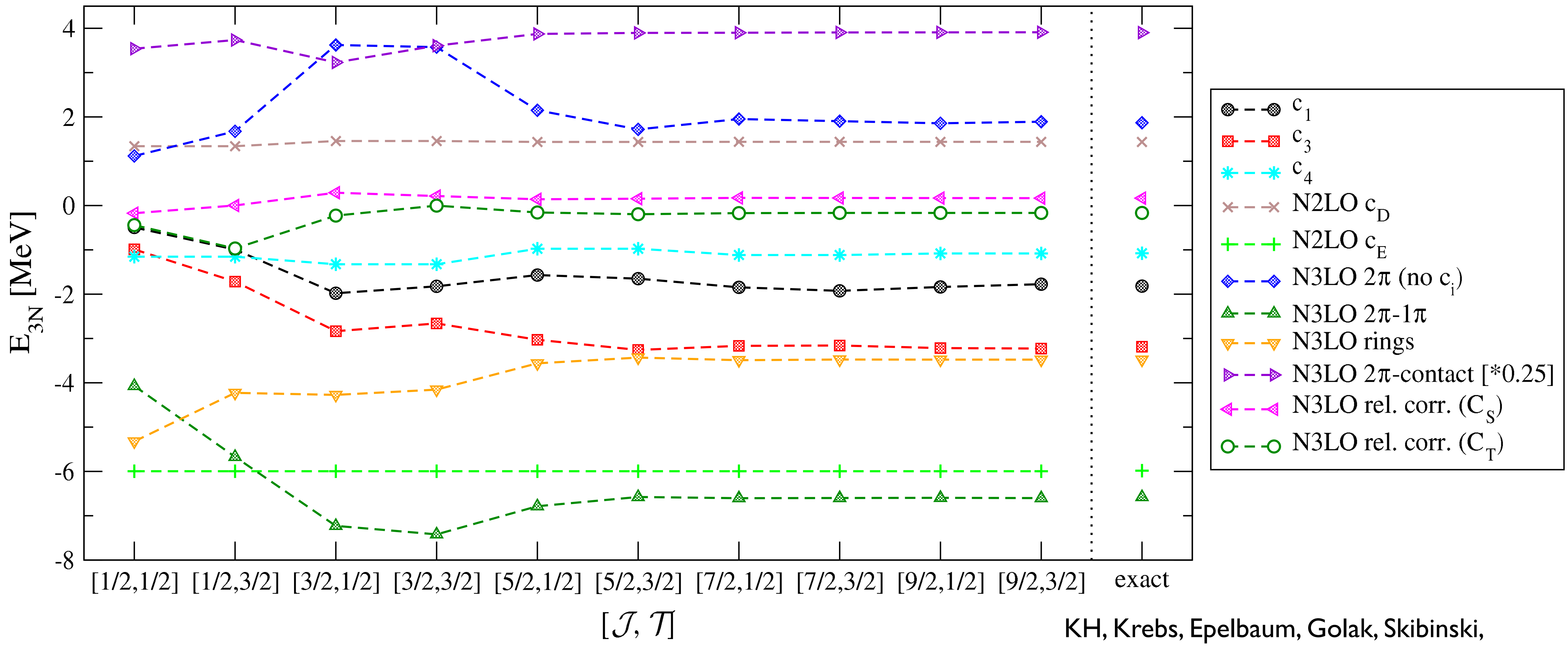



KH, Krebs, Epelbaum, Golak, Skibinski, PRC 91, 044001 (2015)

- in PNM only matrix elements with $\mathcal{T} = 3/2$ contribute
- resummation up to $\mathcal{J} = 9/2$ leads to well converged results
- essentially perfect agreement with 'exact' results (cf. PRC88, 025802)

# Partial wave convergence: energy of infinite matter in Hartree-Fock approximation

symmetric nuclear matter:




KH, Krebs, Epelbaum, Golak, Skibinski, PRC 91, 044001 (2015)

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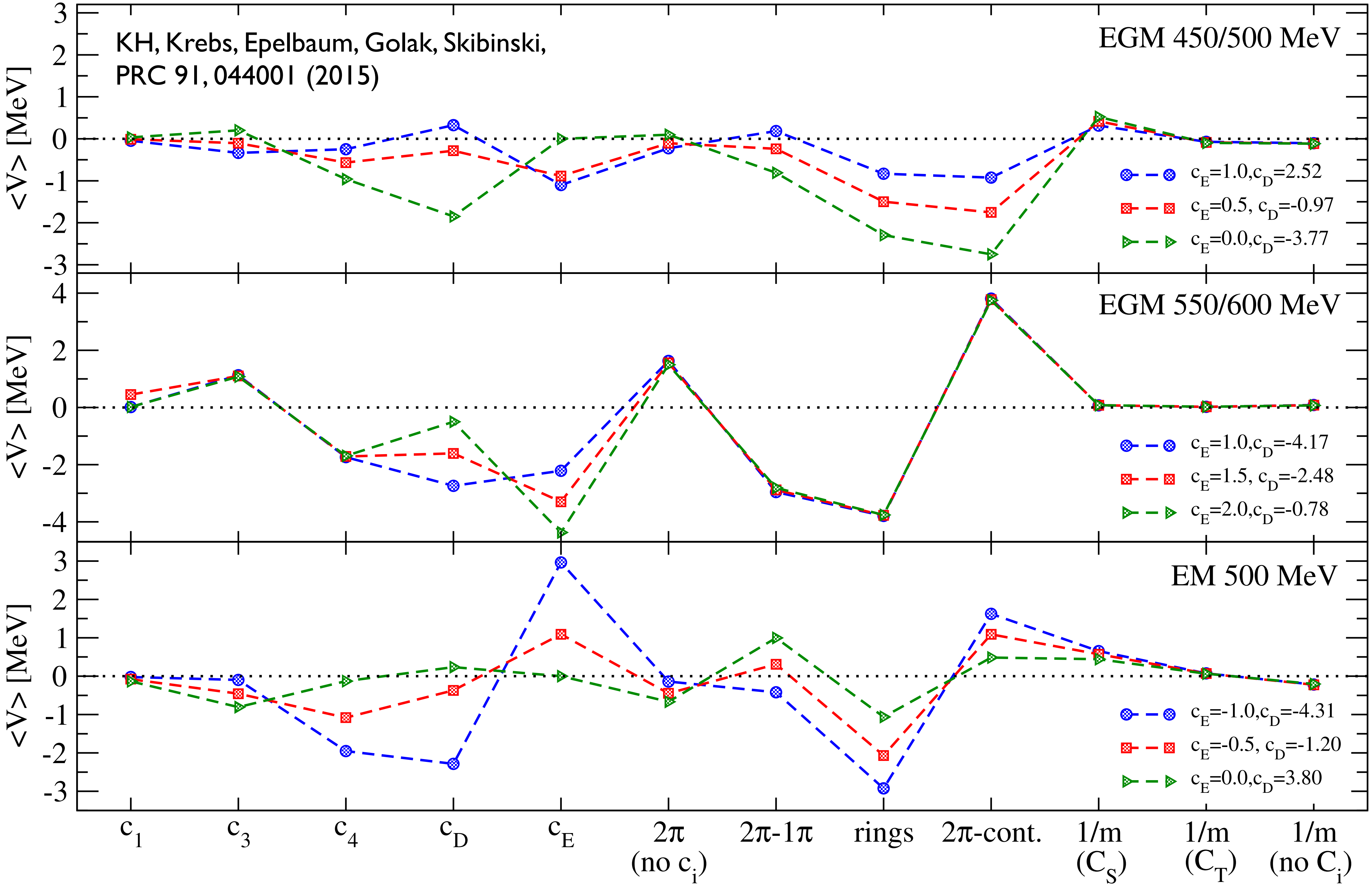
# Contributions of individual topologies in $^3H$

## for specific choices of NN interactions and regulator functions!




- contributions of individual contributions depend sensitively on details
- N3LO contributions not suppressed compared to N2LO
- perturbativeness of 3NF strongly depends on NN interaction

# Future directions:
# Incorporation in different many-body frameworks

Hyperspherical harmonics


Faddeev,
Faddeev-Yakubovski

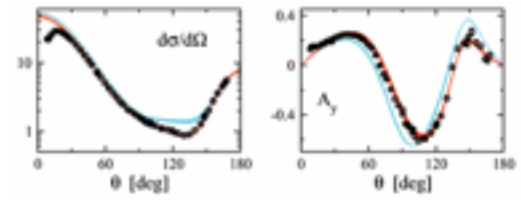


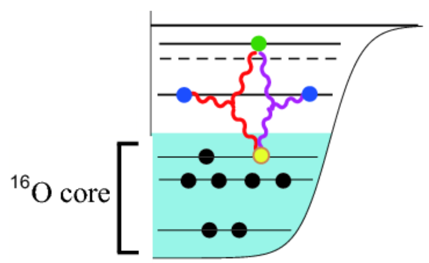

FIG. 4: Nd elastic observables at 65 MeV.

no-core shell model

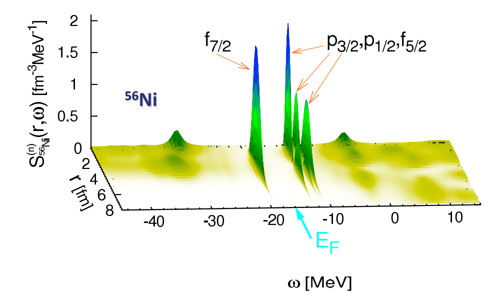
coupled cluster method

$$|\Psi\rangle = e^{\hat{T}}|\Phi_0\rangle = \left(1 + \hat{T} + \frac{1}{2}\hat{T}^2 + \frac{1}{3!}\hat{T}^3 + \cdots\right)|\Phi_0\rangle,$$

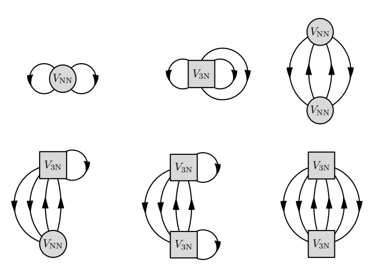
valence shell model



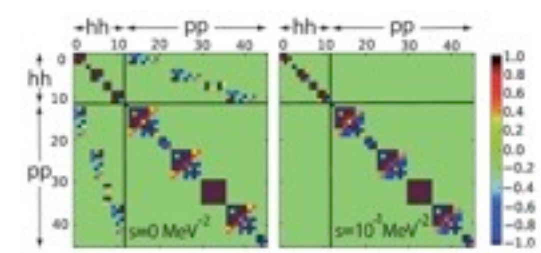

Self-consistent
Greens function




Many-body
perturbation theory



In-medium SRG




Required inputs:

1. consistent NN and 3N forces at N$^3$LO in partial-wave-decomposed form
2. softened forces for judging approximations and pushing to heavier nuclei

# Different regularization schemes

Goal of regularization:
**Separate long- from short-range physics**

1. non-local regularization: $V_{\rm NN}(p,p') \sim \exp\left[-\frac{p^{2n}+p'^{2n}}{\Lambda^{2n}}\right]$

2. local regularization: $V_{\rm NN}(r) \sim \left(1-\exp\left[-\frac{r^n}{R_0^n}\right]\right)$

3. hybrid strategy: regularize long-range parts locally and short-range distance non-locally

---

- different choices regulate short range physics in different ways
- important to explore various alternatives
- **need to implement according regularizations in 3NF**

# Regularization schemes for 3NF

## 1. non-local regularization:

$$V_{3\mathrm{N}}(p,q,p',q') \sim \exp\left[-\frac{p^2+3/4q^2}{\Lambda^2}\right]\exp\left[-\frac{p'^2+3/4q'^2}{\Lambda^2}\right]$$

- multiplicative (no partial-wave mixing), trivial to apply
- calculated matrix elements up to $N^3LO$ can be used immediately

## 2. local regularization:

$$V_{3\mathrm{N}}(\mathbf{r}_{12},\mathbf{r}_{23},\mathbf{r}_{13}) \sim \left(1-\exp\left[\frac{r_{12}^2}{R_0^2}\right]\right)^n\left(1-\exp\left[\frac{r_{23}^2}{R_0^2}\right]\right)^n\left(1-\exp\left[\frac{r_{13}^2}{R_0^2}\right]\right)^n$$

- partial wave mixing, application of regulator non-trivial in partial-wave basis
- different possibilities to calculate 3NF partial wave matrix elements:
  - ⋆ decompose 3N in coordinate space and then fourier transform
  - ⋆ perform convolution integrals in momentum space partial wave basis

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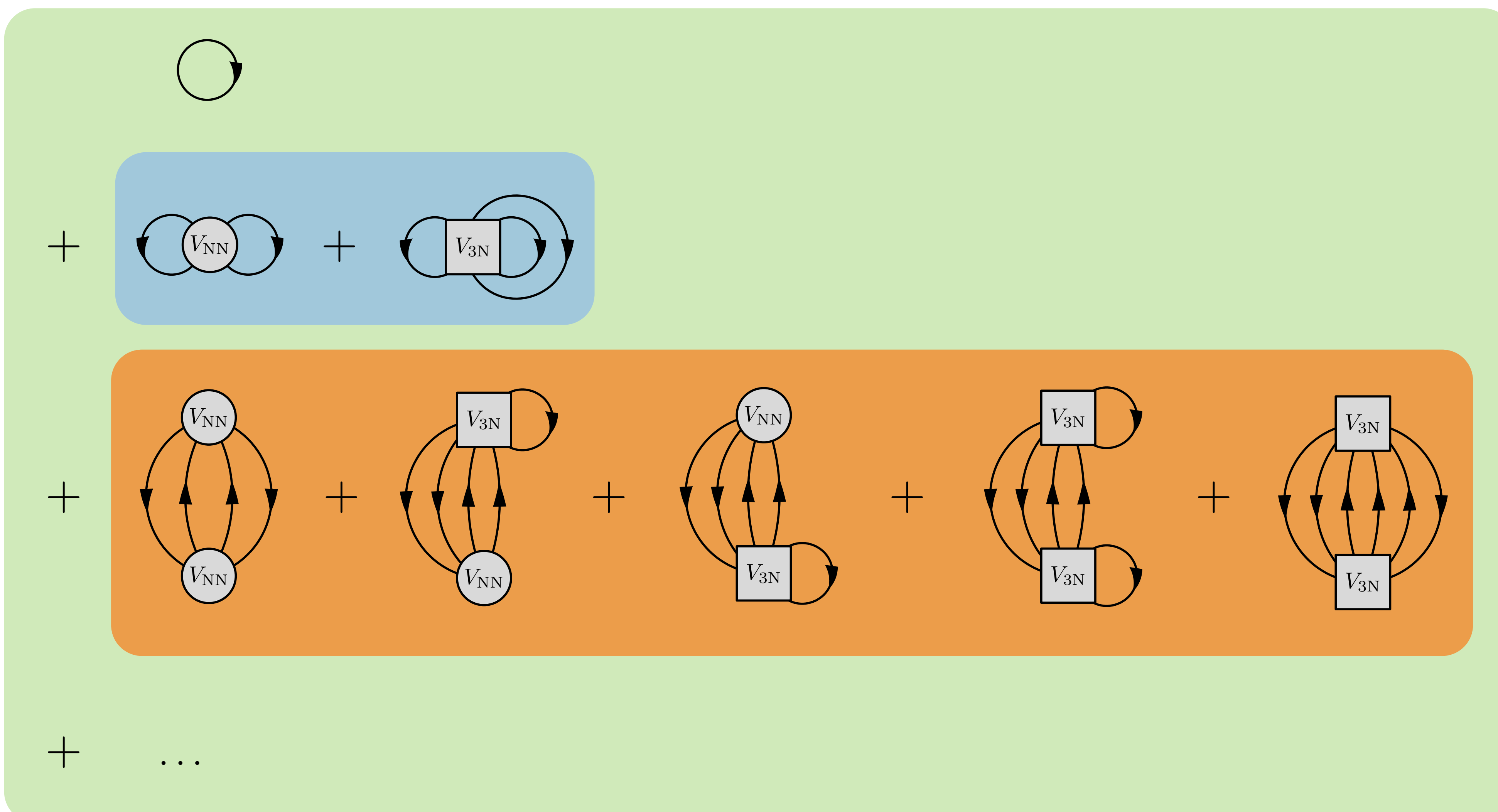
**Work in progress. Stay tuned!**

# Equation of state: Many-body perturbation theory

central quantity of interest: energy per particle $E/N$

$$H(\lambda) = T + V_{\text{NN}}(\lambda) + V_{3\text{N}}(\lambda) + \ldots$$

$E =$




kinetic energy

Hartree-Fock

2nd-order

3rd-order
and beyond

- "hard" interactions require non-perturbative summation of diagrams
- with low-momentum interactions much more perturbative
- inclusion of 3N interaction contributions crucial!

# Improved normal ordering of 3NF in infinite matter

- involves summation of one particle over occupied states in the Fermi sphere

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

- so far, an approximate normal ordering (P=0) has been developed specifically for individual 3NF topologies (so far up to $\mathrm{N}^2\mathrm{LO}$)

Holt, Kaiser, Weise
PRC 81, 024002 (2010)

KH and Schwenk
PRC 82, 014314 (2010)

Carbone, Polls, Rios
PRC 90, 054322 (2014)

- following this approach, the treatment of more general 3NF becomes very tedious

**Strategy:**

Develop general normal ordering based on partial-wave-decomposed 3NF

Drischler, KH, Schwenk, in preparation

# Improved normal ordering of 3NF in infinite matter

$$\overline{V}_{3\mathrm{N}} = \left(\frac{3}{2}\right)^3 \mathrm{Tr}_{\sigma_3} \mathrm{Tr}_{\tau_3} \int \frac{d\mathbf{q}}{(2\pi)^3} n^{\tau_3}_{(3\vec{q}+\vec{P})/2} \mathcal{A}_{123} V_{3\mathrm{N}}$$

- generalize normal ordering to finite P:

$$n^{\tau}_{(3\vec{q}+\vec{P})/2} \longrightarrow \Gamma^{\tau}(q,P) = \frac{1}{4\pi} \int d\Omega_{\vec{P}}\, n^{\tau}_{(3\vec{q}+\vec{P})/2}$$

$$\begin{aligned}
&\left\langle p(LS)JTm_T | \overline{V}^{\mathrm{as}}_{3\mathrm{N}}(P) | p'(L'S')JT'm_T \right\rangle \\
&= \frac{(-i)^{L'-L}}{(4\pi)^2} \left(\frac{3}{4\pi}\right)^3 3 \int dq\, q^2\; f_{\mathrm{R}}(p,q) f_{\mathrm{R}}(p',q) \\
&\quad \times \sum_{\tau} \mathcal{C}^{m_T+\tau}_{Tm_T 1/2\tau \mathcal{T}} \mathcal{C}^{\mathcal{T} m_T+\tau}_{T'm_T 1/2\tau}\; \Gamma^{\tau}(q,P) \\
&\quad \times \sum_{\substack{l,j \\ \mathcal{J},\mathcal{T}}} \frac{2\mathcal{J}+1}{2J+1} \delta_{ll'} \delta_{jj'} \delta_{JJ'}\; \langle pq\alpha | V^{\mathrm{as}}_{3\mathrm{N}} | p'q\alpha' \rangle
\end{aligned}$$

Drischler, KH, Schwenk, in preparation

# Improved normal ordering of 3NF in infinite matter

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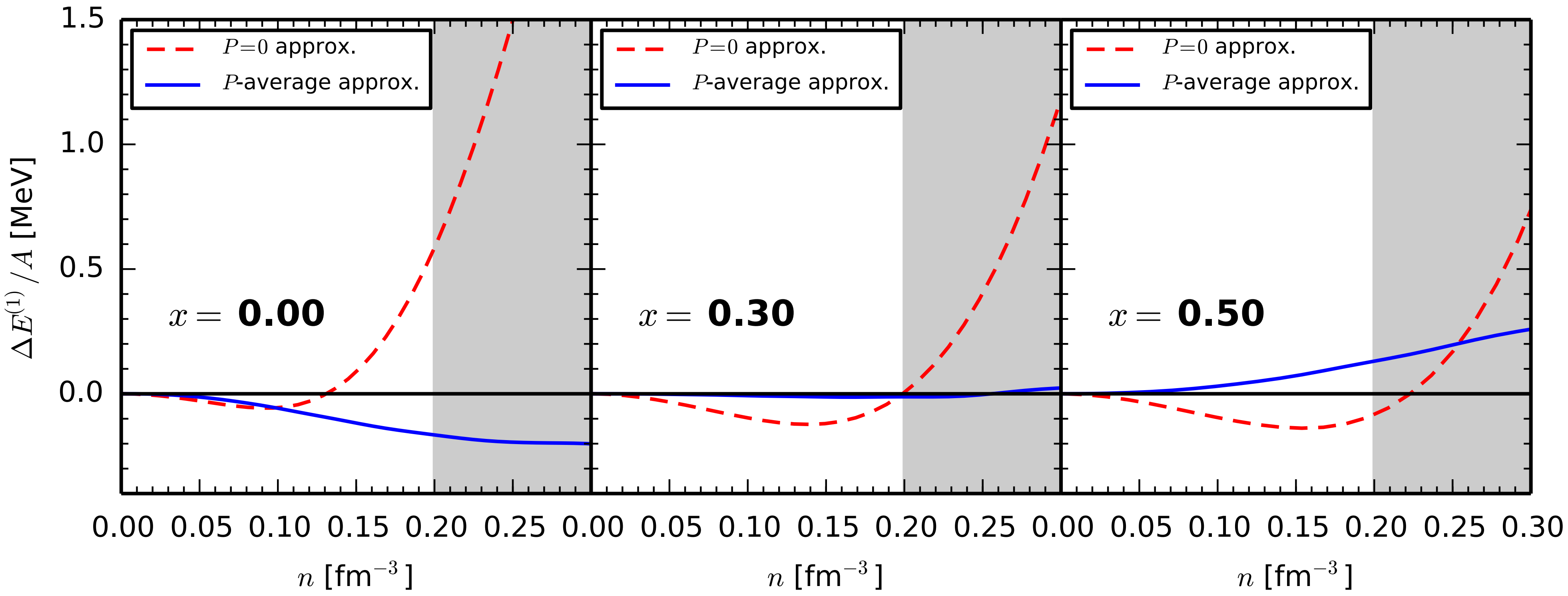


Drischler, KH, Schwenk
in preparation

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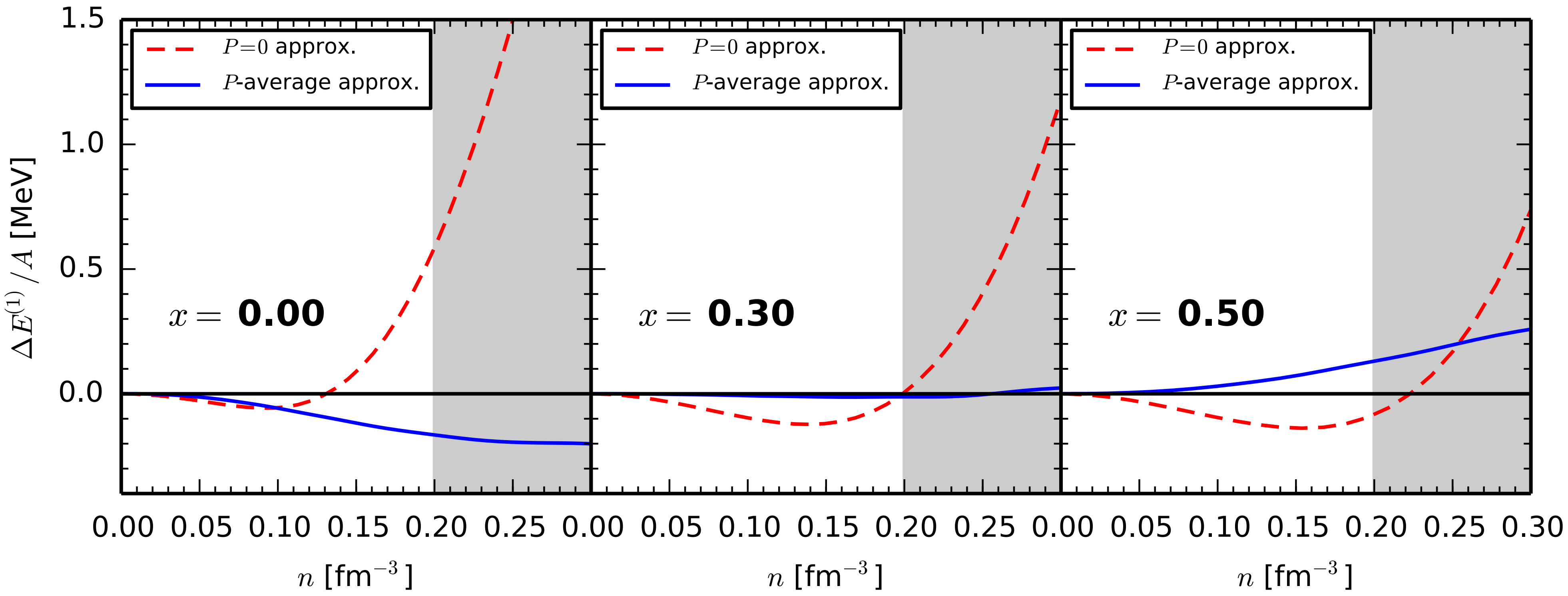
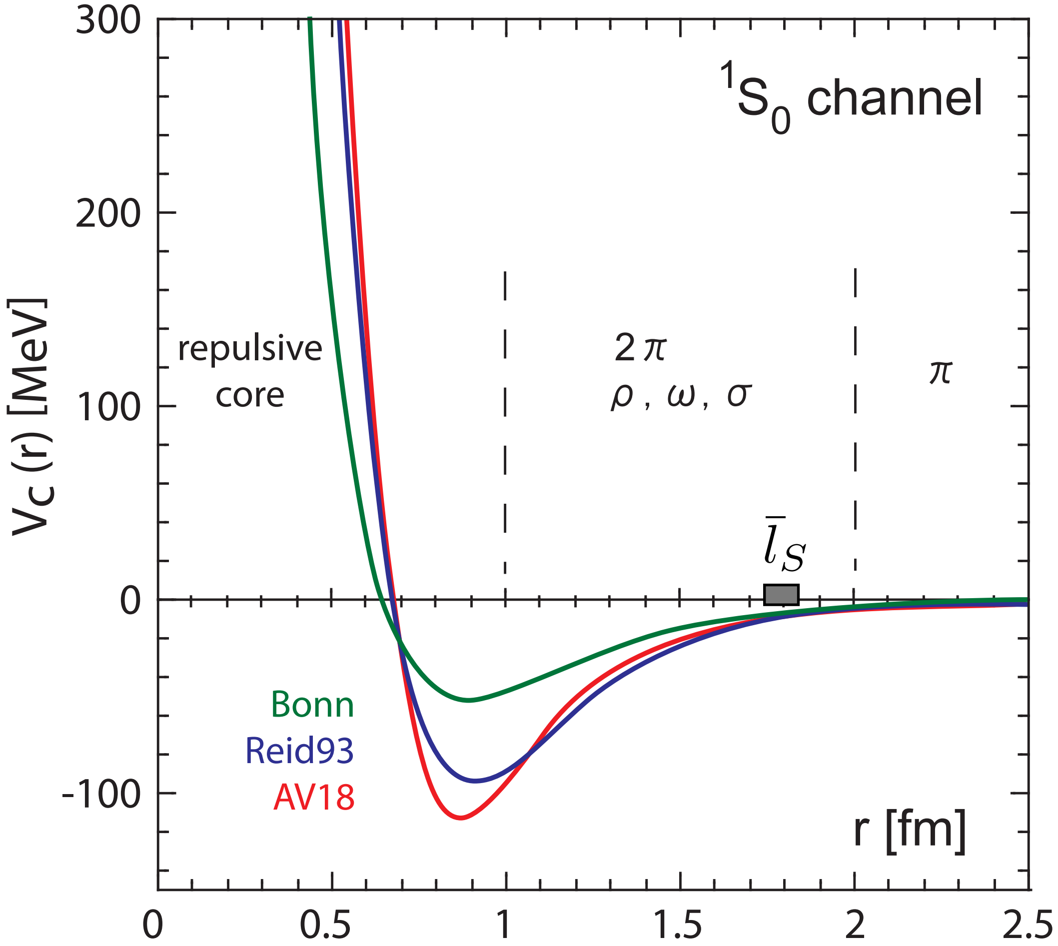


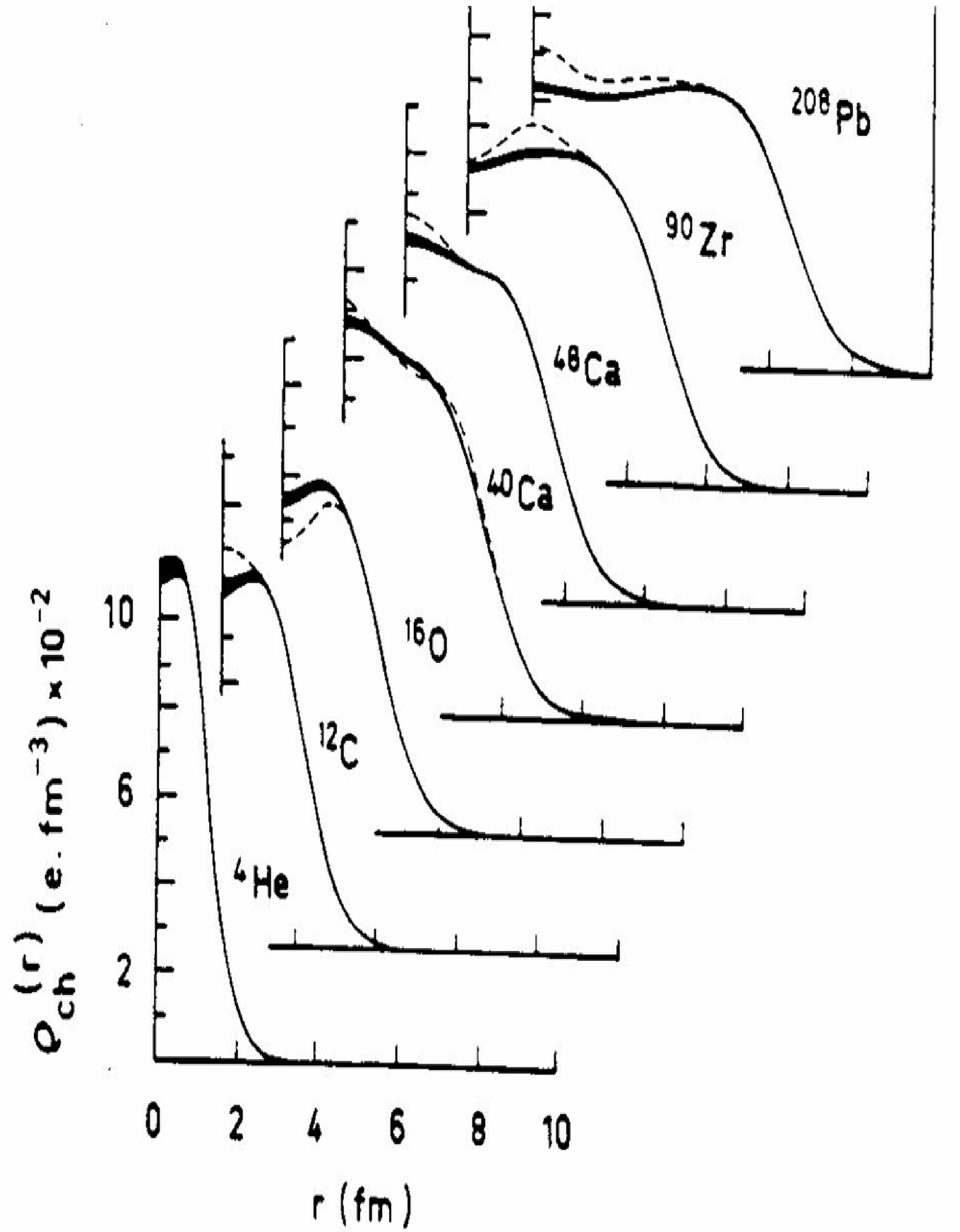

Drischler, KH, Schwenk
in preparation

- makes it possible to treat also SRG-evolved 3NF in momentum space

KH, PRC 85, 021002 (2012)

# Equation of state of symmetric nuclear matter, nuclear saturation

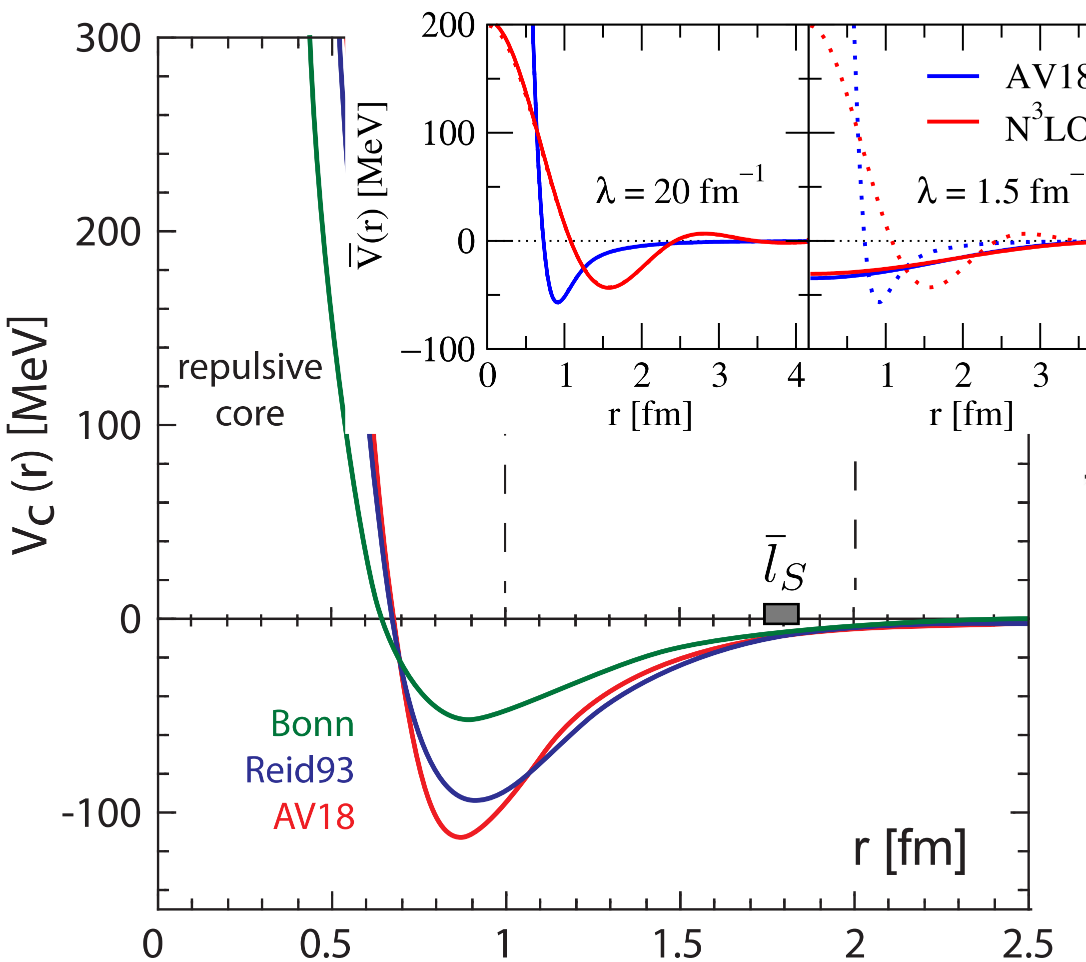


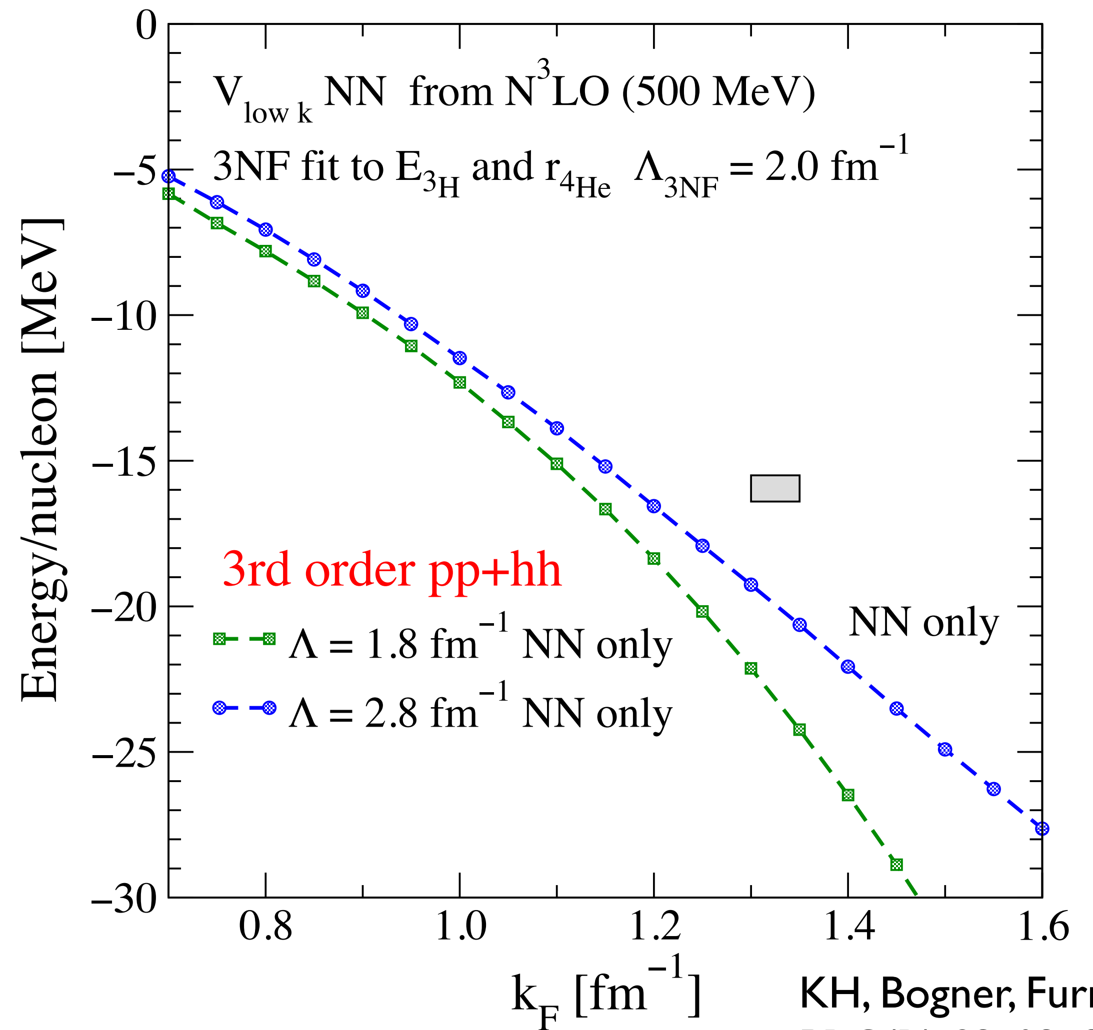




*"Very soft potentials must be excluded because they do not give saturation; they give too much binding and too high density. In particular, a substantial tensor force is required."*

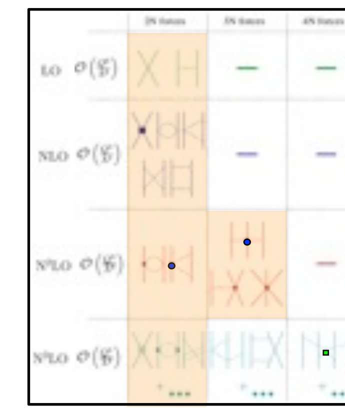
**Hans Bethe** (1971)

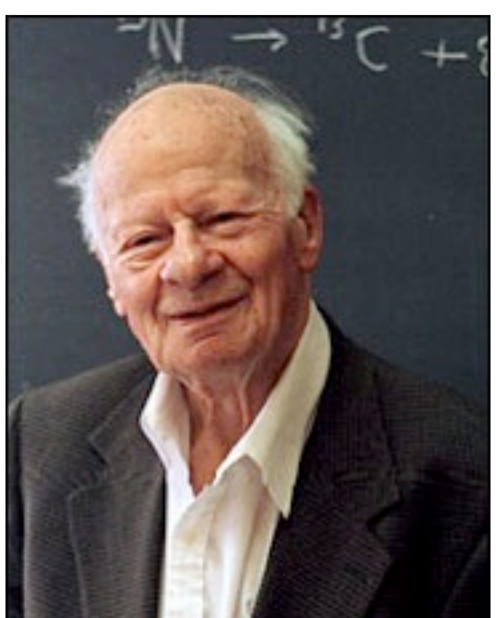
# Fitting the 3NF LECs at low resolution scales




KH, Bogner, Furnstahl, Nogga,
PRC(R) 83, 031301 (2011)



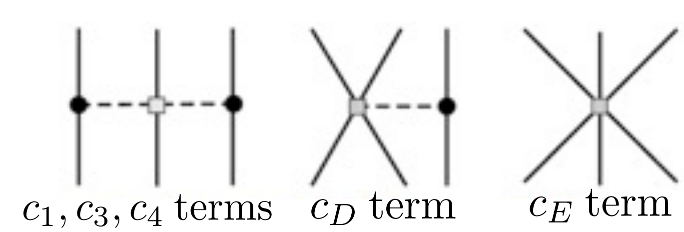


*"Very soft potentials must be excluded because they do not give saturation;*
*they give too much binding and too high density. In particular, a substantial tensor force is required."*

**Hans Bethe** (1971)

intermediate ($c_D$) and short-range ($c_E$) 3NF couplings fitted to few-body systems at different resolution scales:

$$E_{^3\mathrm{H}} = -8.482\,\mathrm{MeV} \qquad r_{^4\mathrm{He}} = 1.464\,\mathrm{fm}$$



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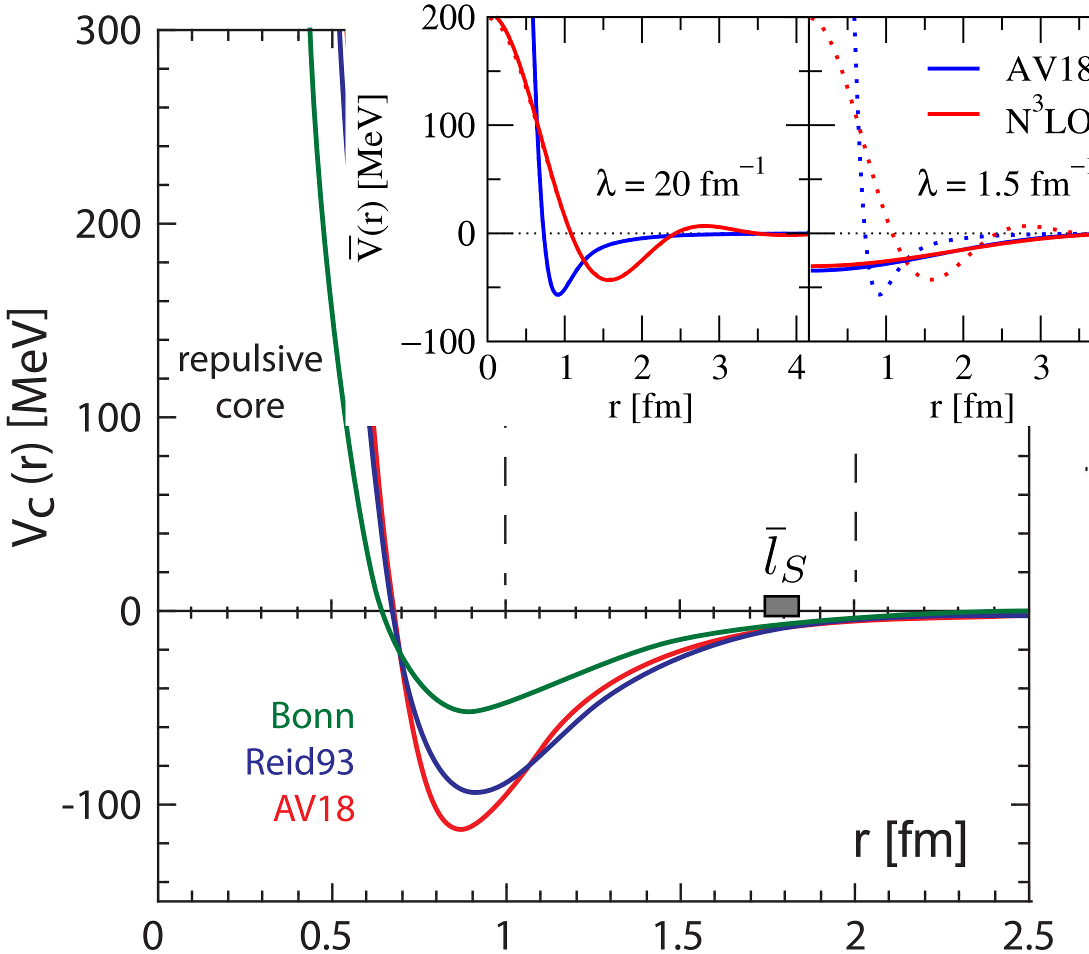
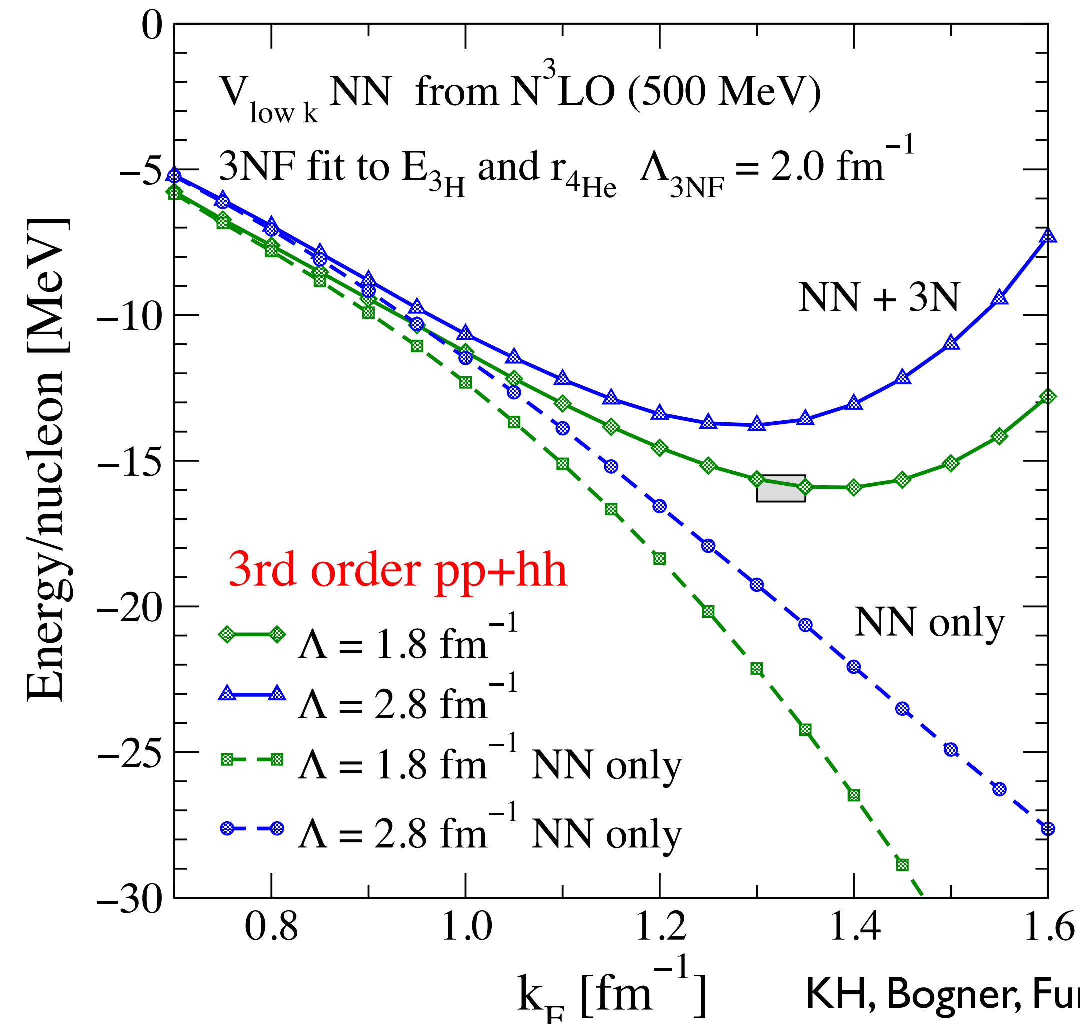
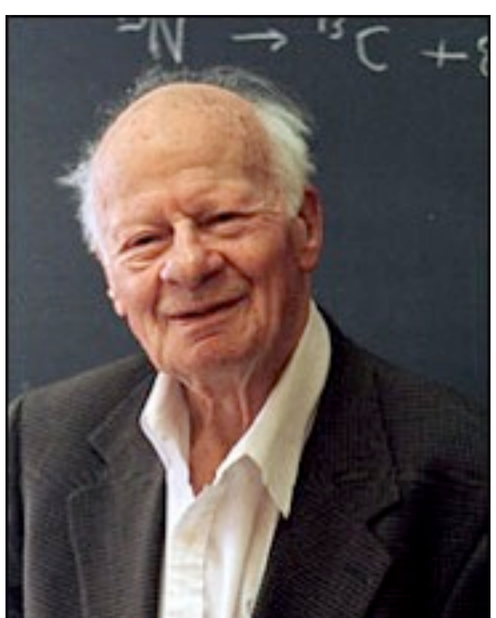



KH, Bogner, Furnstahl, Nogga, PRC(R) 83, 031301 (2011)

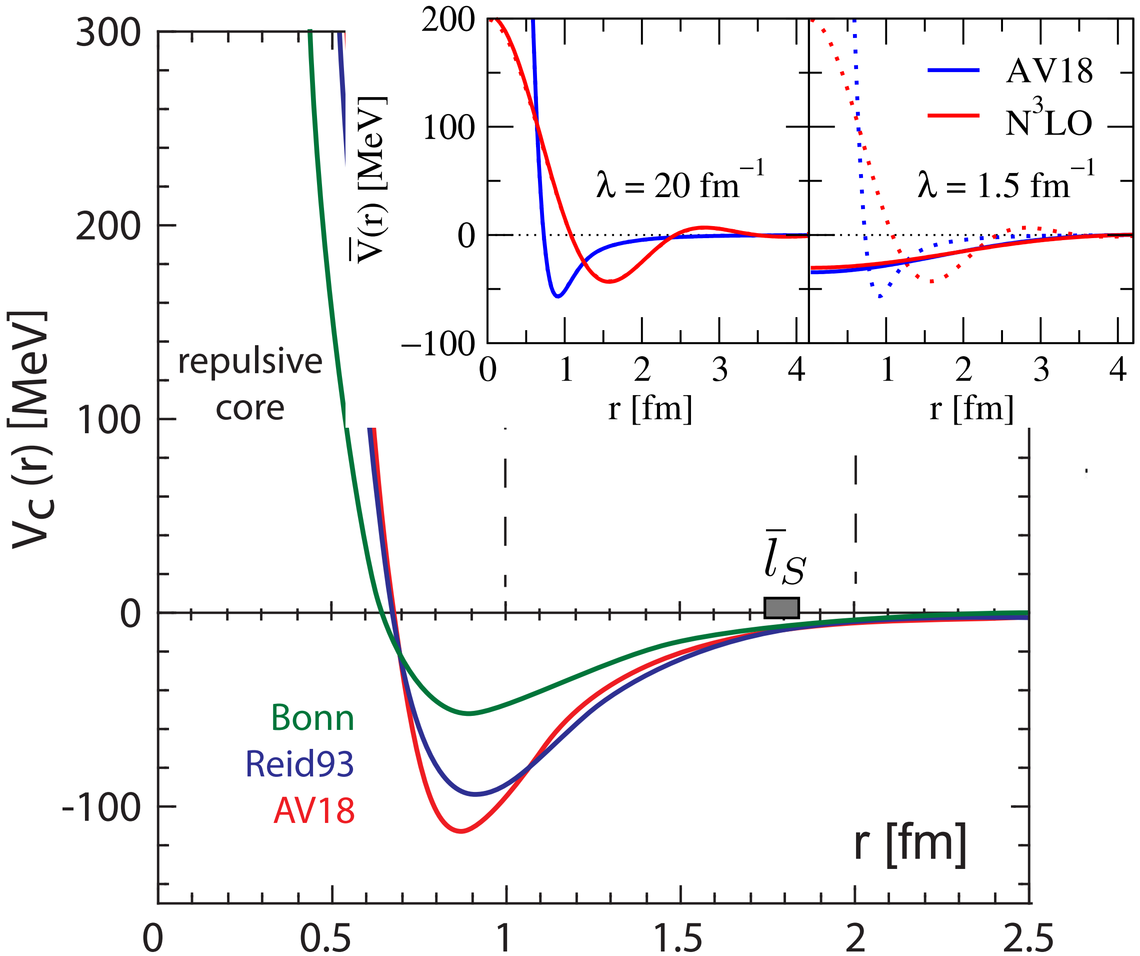


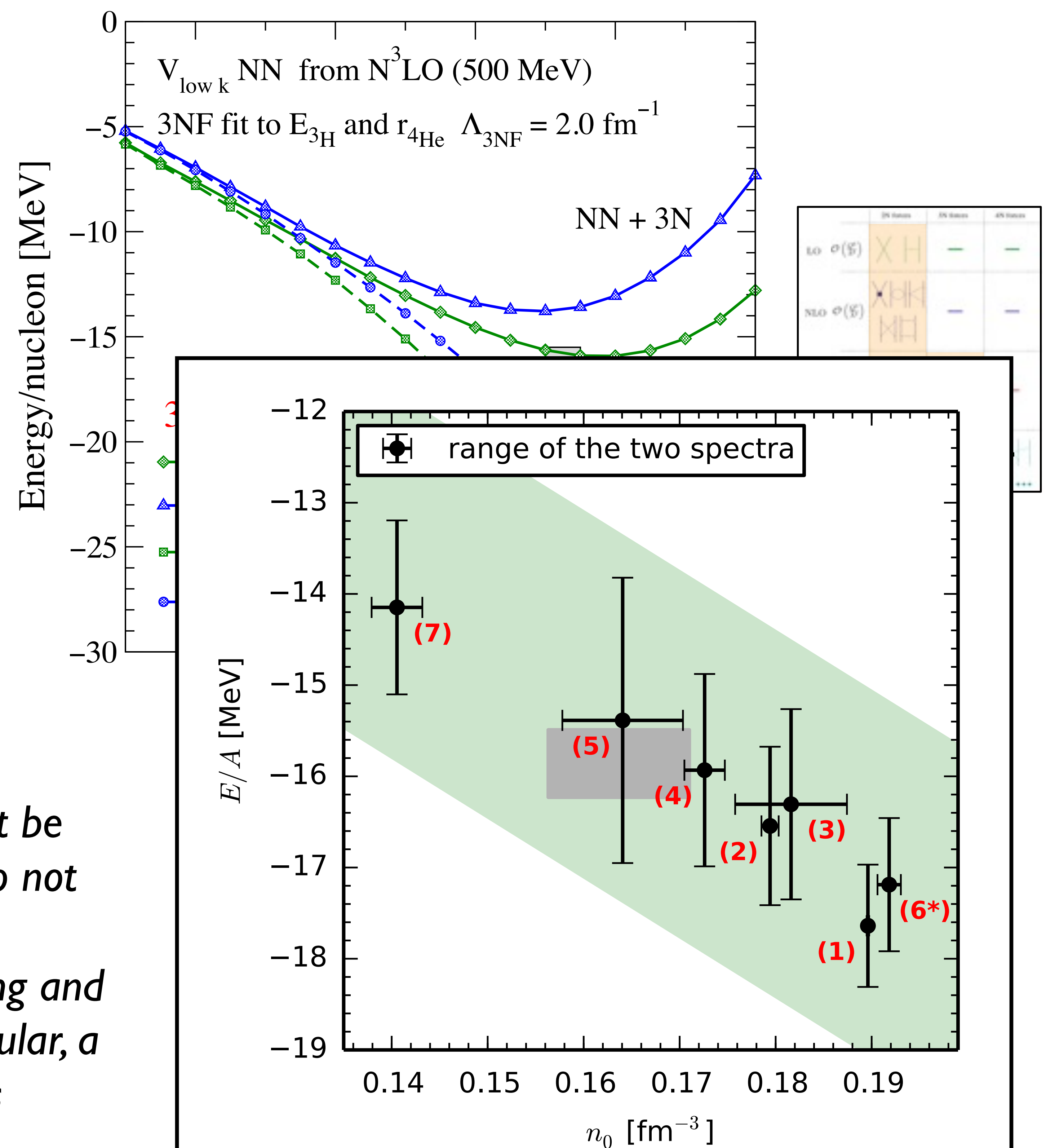
*"Very soft potentials must be excluded because they do not give saturation; they give too much binding and too high density. In particular, a substantial tensor force is required."*

**Hans Bethe** (1971)

Reproduction of saturation point without readjusting parameters!

# Fitting the 3NF LECs at low resolution scales




Drischler, KH, Schwenk,
in preparation

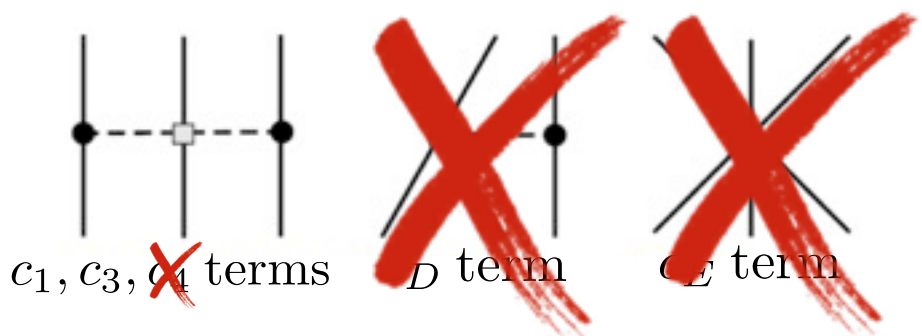
*"Very soft potentials must be excluded because they do not give saturation;*
*they give too much binding and too high density. In particular, a substantial tensor force is required."*

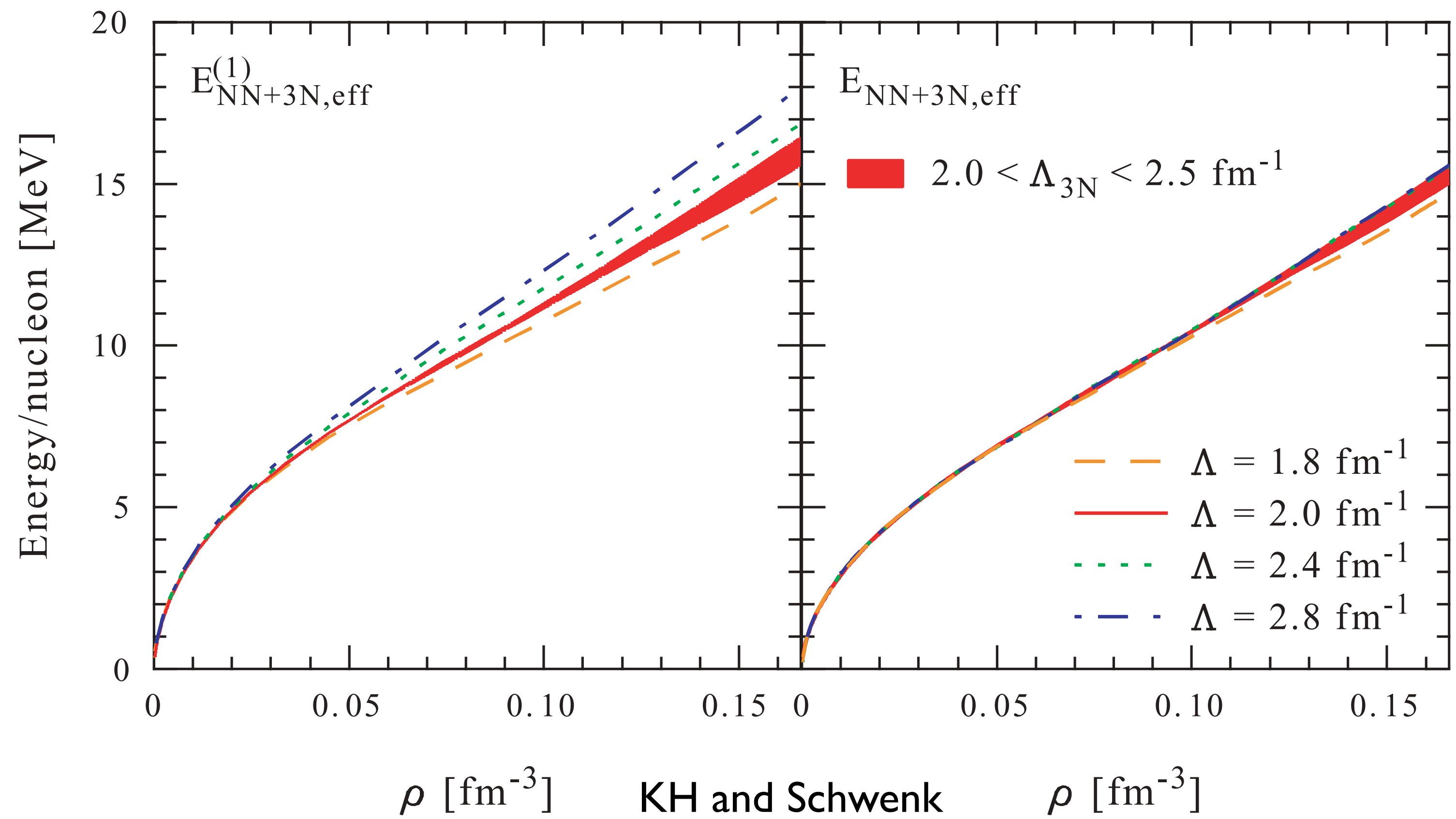
**Hans Bethe** (1971)

# Results for the neutron matter equation of state

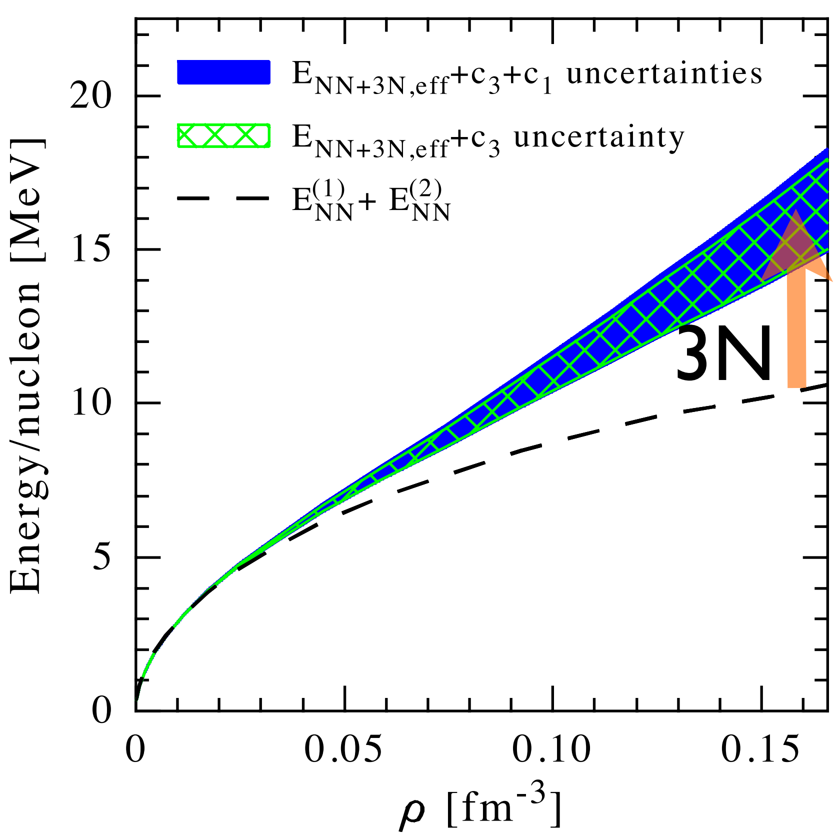
neutron matter is a **unique system** for chiral EFT:

only long-range 3NF contribute in leading order



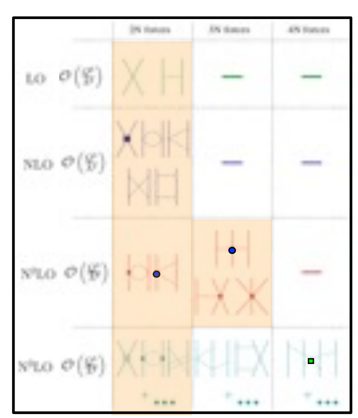




KH and Schwenk
PRC 82, 014314 (2010)



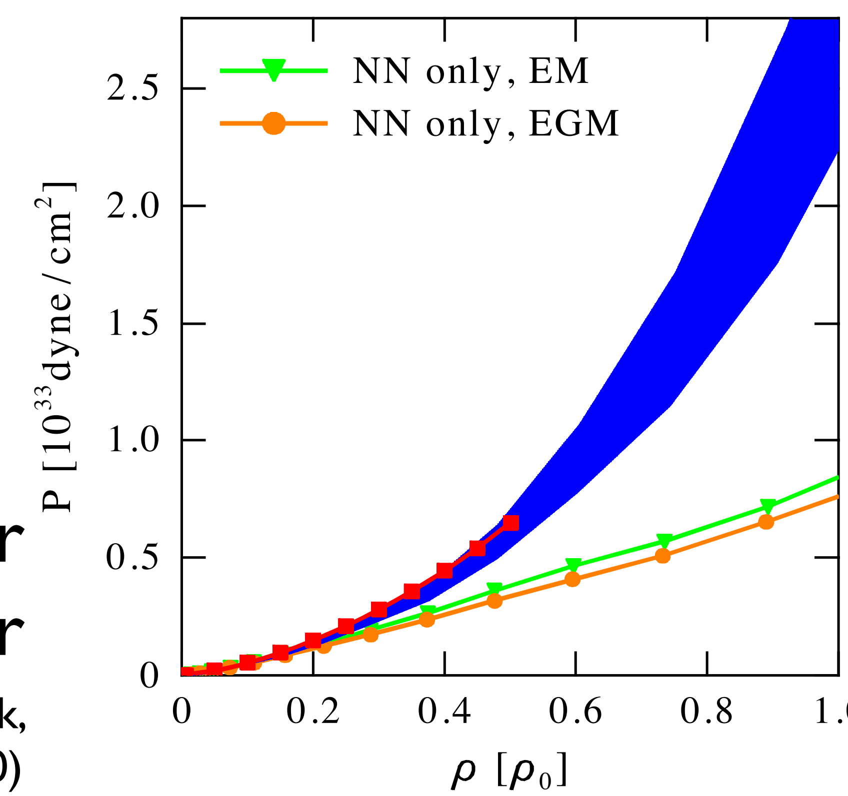

## pure neutron matter

KH and Schwenk PRC 82, 014314 (2010)

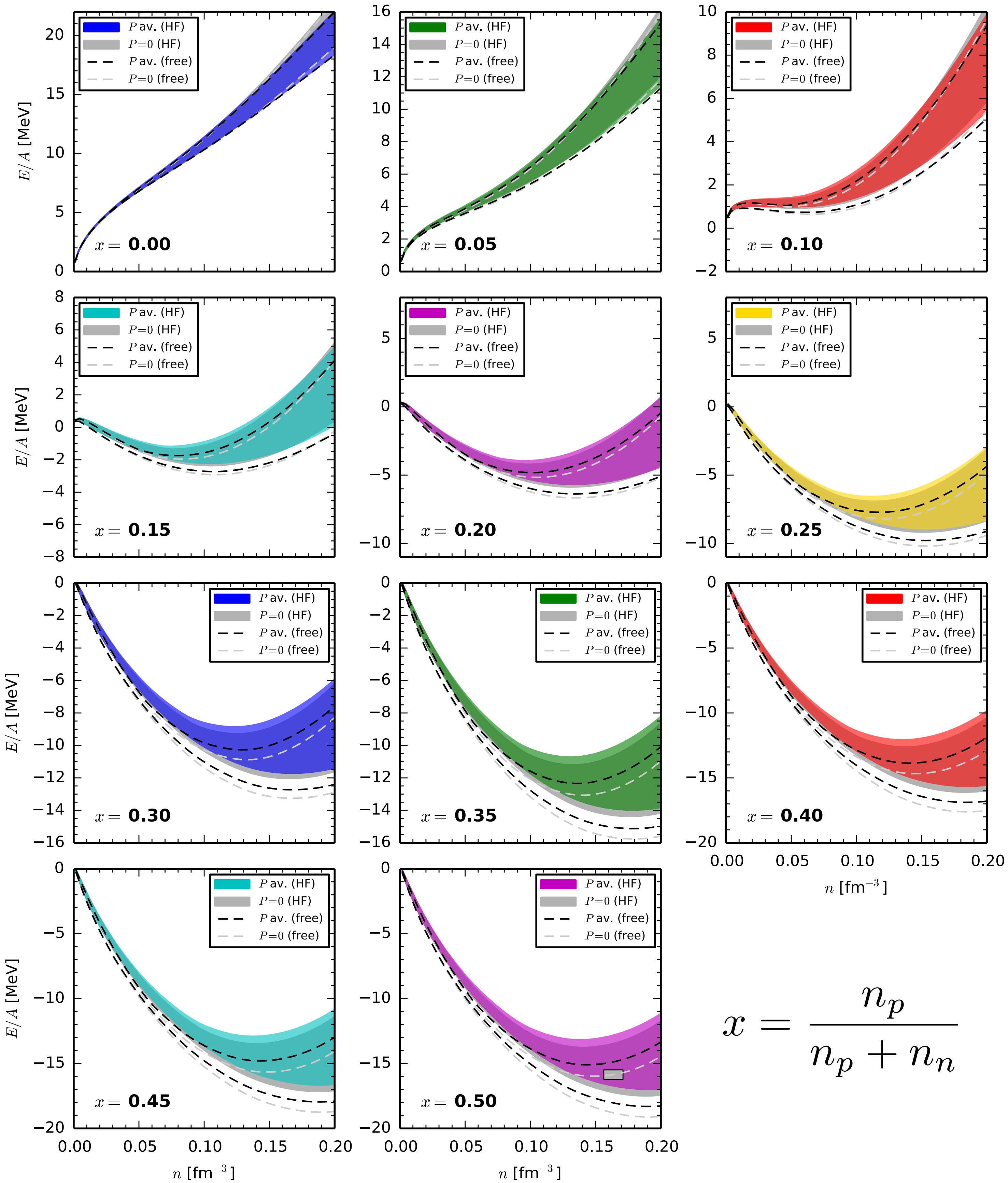


## neutron star matter

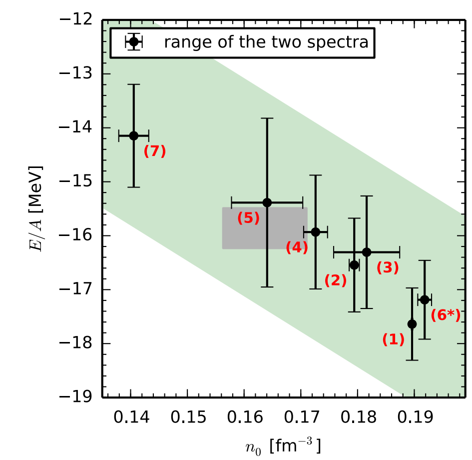
KH, Lattimer, Pethick, Schwenk,
PRL 105, 161102 (2010)



# First application to isospin asymmetric nuclear matter




- uncertainty bands determined by set of 7 Hamitonians




$$x = \frac{n_p}{n_p + n_n}$$

Drischler, KH, Schwenk,
in preparation

# Current and future directions

LENPIC

- derivation of systematic uncertainty estimates for many-body observables, order-by-order convergence studies

- benchmarks of different many-body frameworks based on a set of common Hamiltonians, from light nuclei to nuclear matter

- exploration of different fitting strategies, include bayesian analysis for statistical interpretation of uncertainties?

- role of regulators, clean separation of short- and long-range physics, naturalness of coupling constants, power counting schemes, inclusion of delta excitations