Efficient calculation of 3N forces at N^3LO for ab initio studies

Kai Hebeler

Vancouver, February 17, 2015

TRIUMF workshop on
“Progress in ab initio Techniques in Nuclear Physics”

TECHNISCHE UNIVERSITÄT DARMSTADT

European Research Council
Established by the European Commission

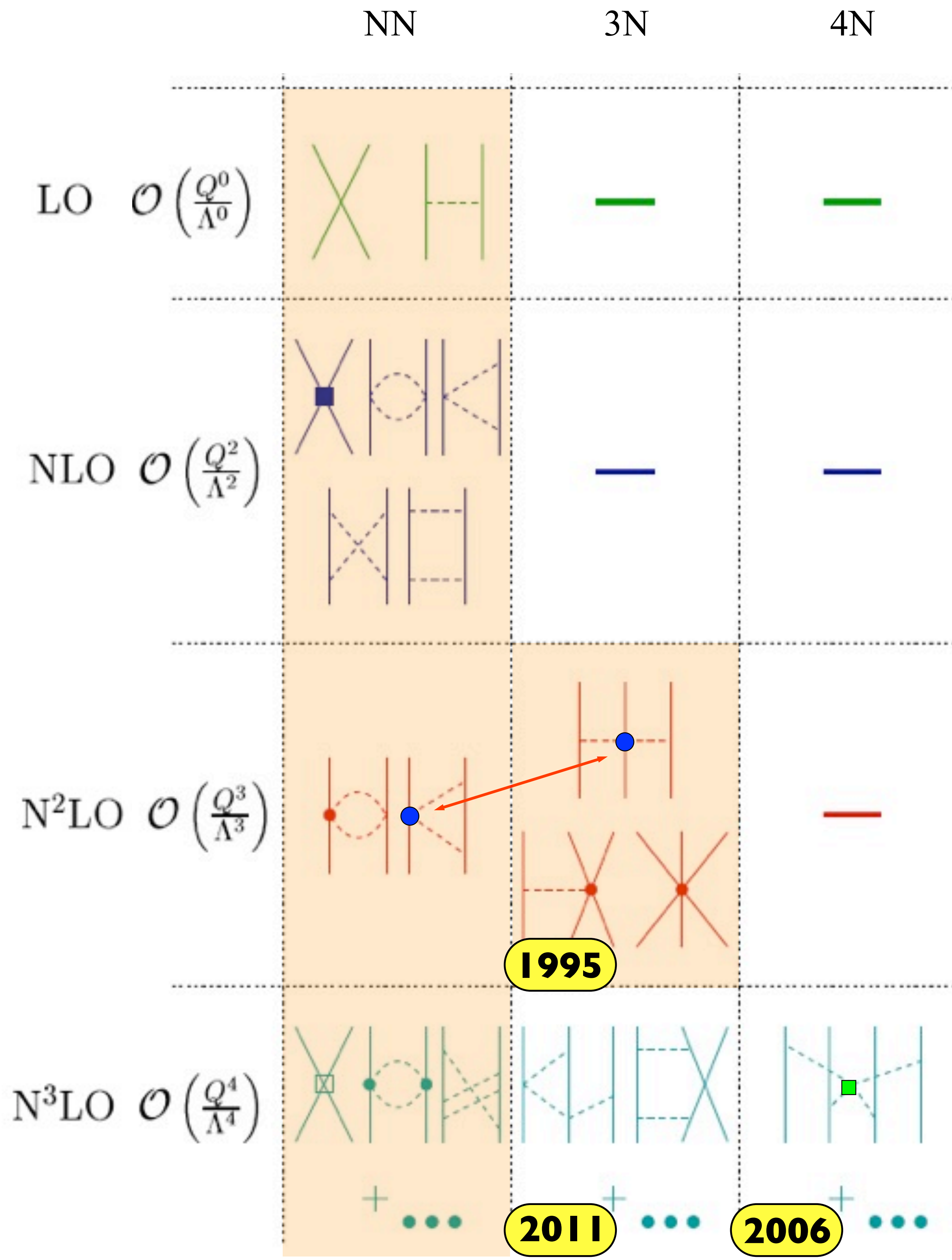
In collaboration with:
Hermann Krebs, Evgeny Epelbaum, Roman Skibinski, Jacek Golak

arXiv:1502.02977

Chiral effective field theory for nuclear forces

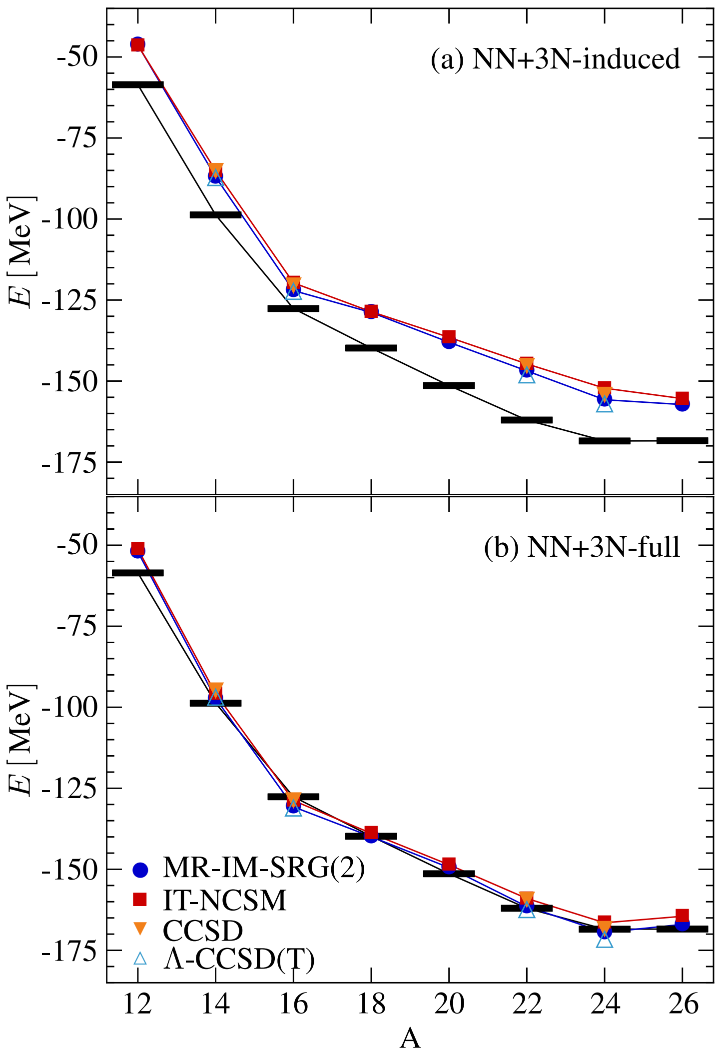
- choose relevant degrees of freedom: here nucleons and pions
- operators constrained by symmetries of QCD
- short-range physics captured in few short-range couplings
- separation of scales: Q << Λ_b, breakdown scale Λ_b~500 MeV
- power-counting: expand in powers Q/Λ_b
- systematic: work to desired accuracy,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

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



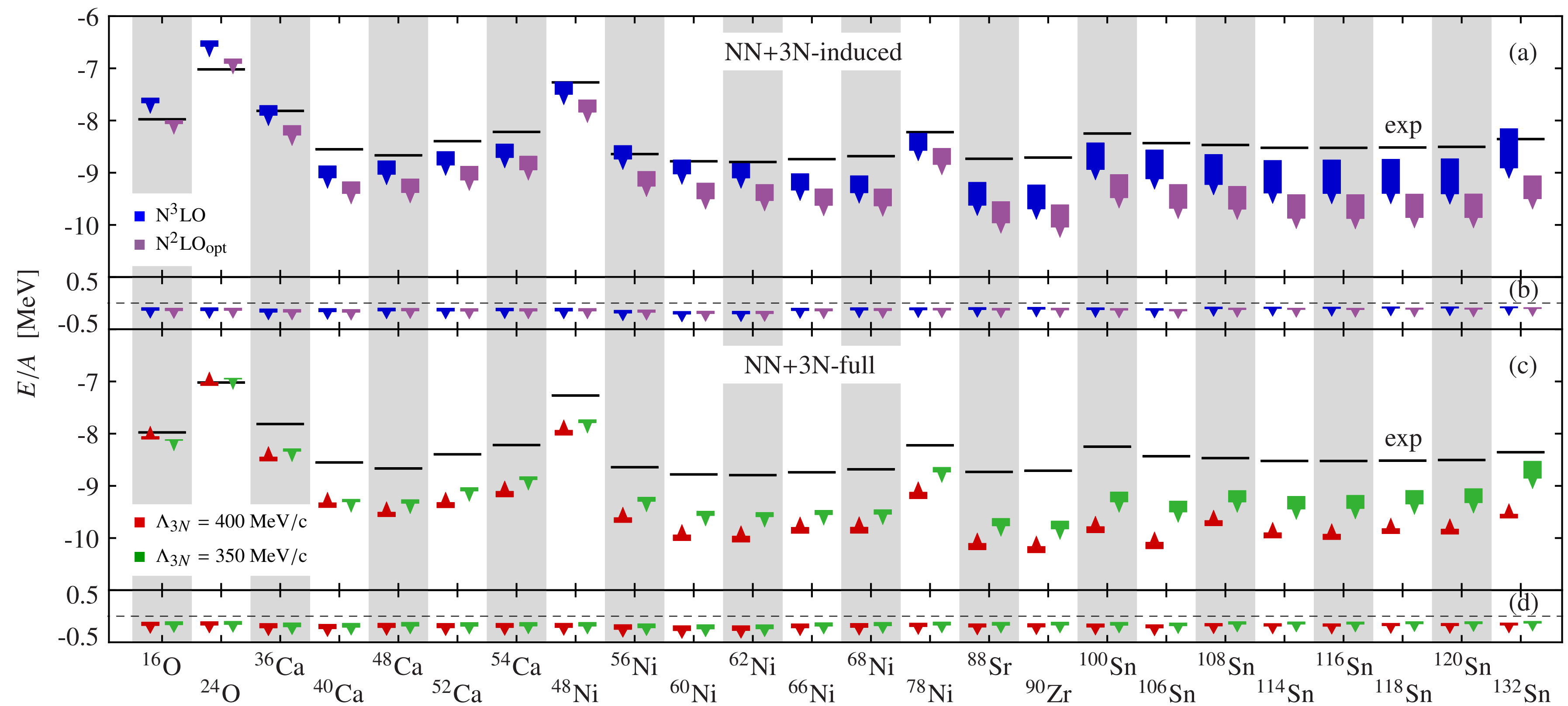
Open issues in nuclear interactions

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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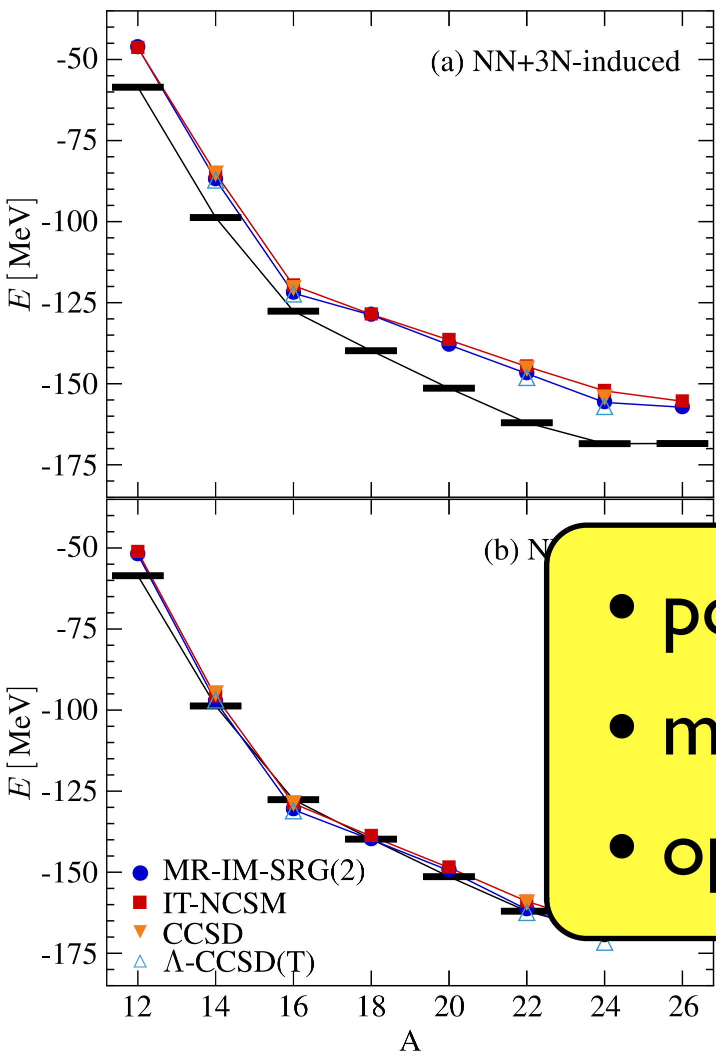

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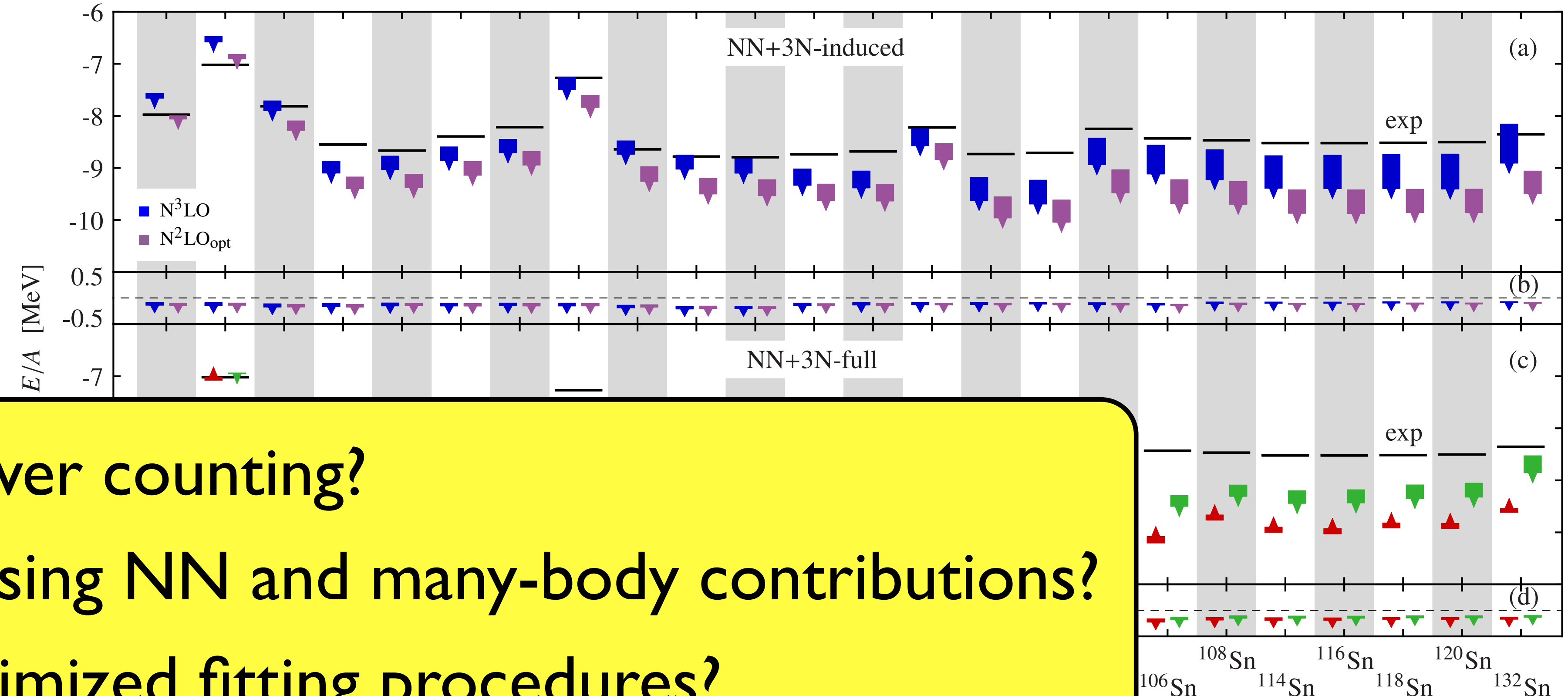
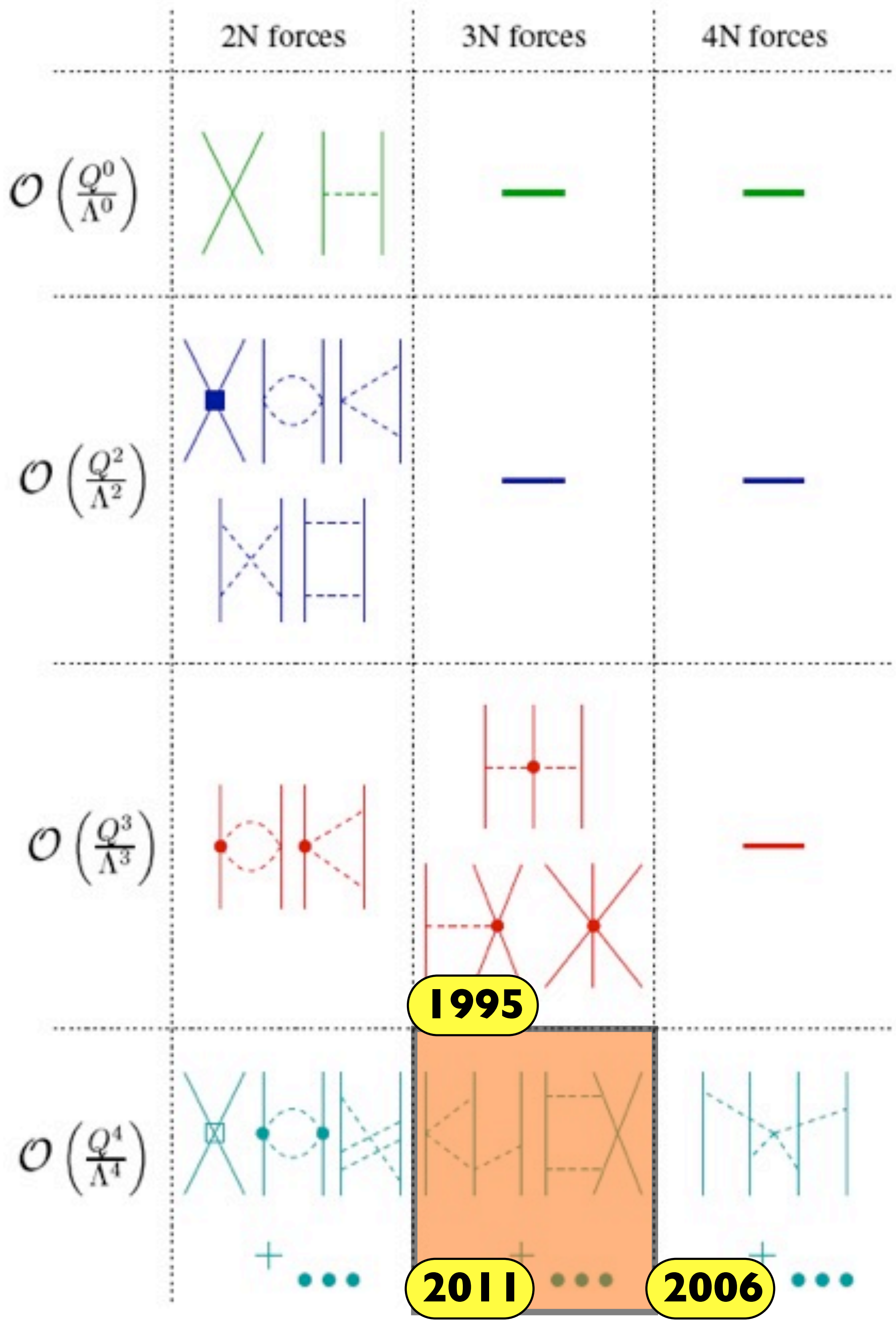
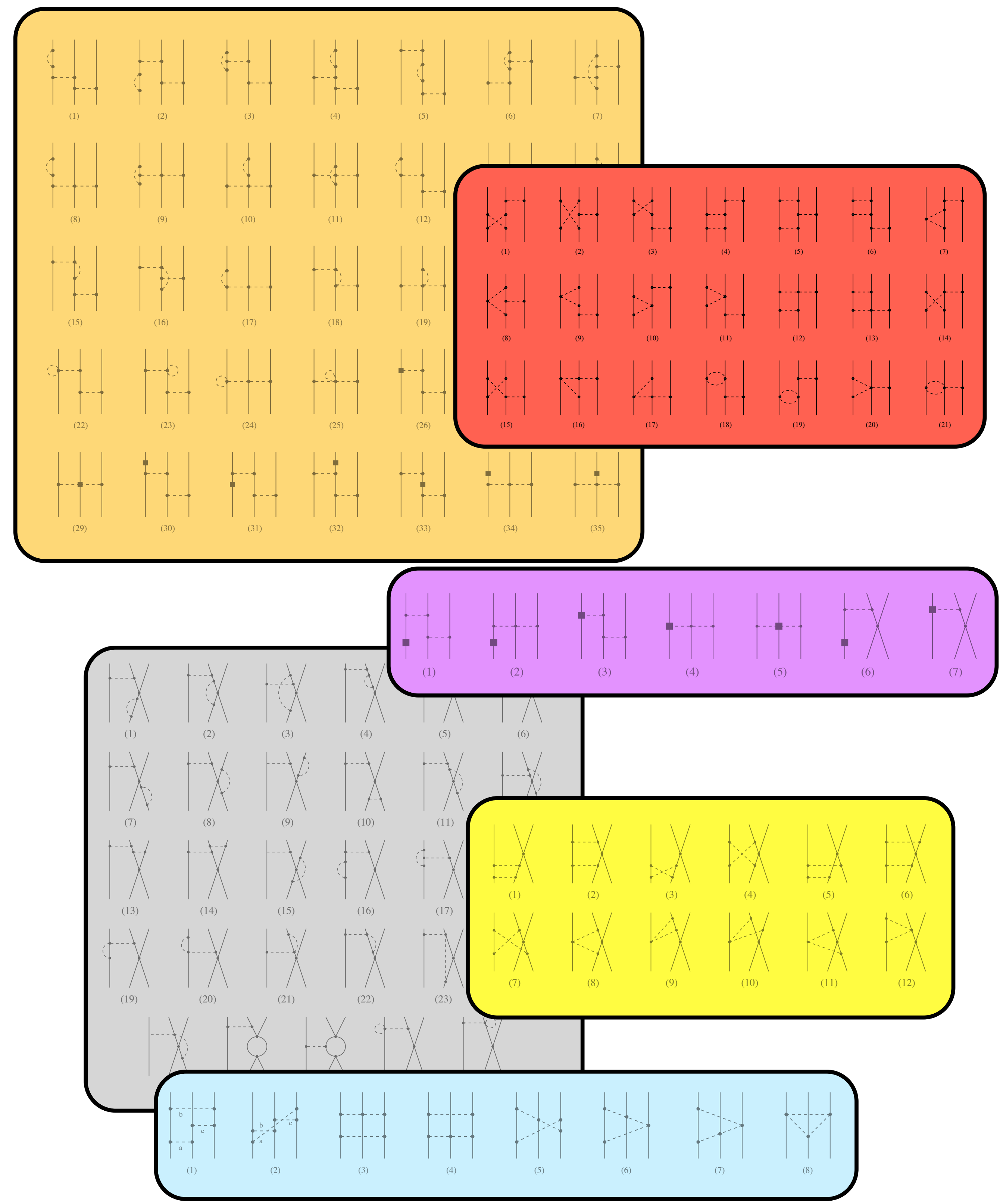


- power counting?
- missing NN and many-body contributions?
- optimized fitting procedures?

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

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





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

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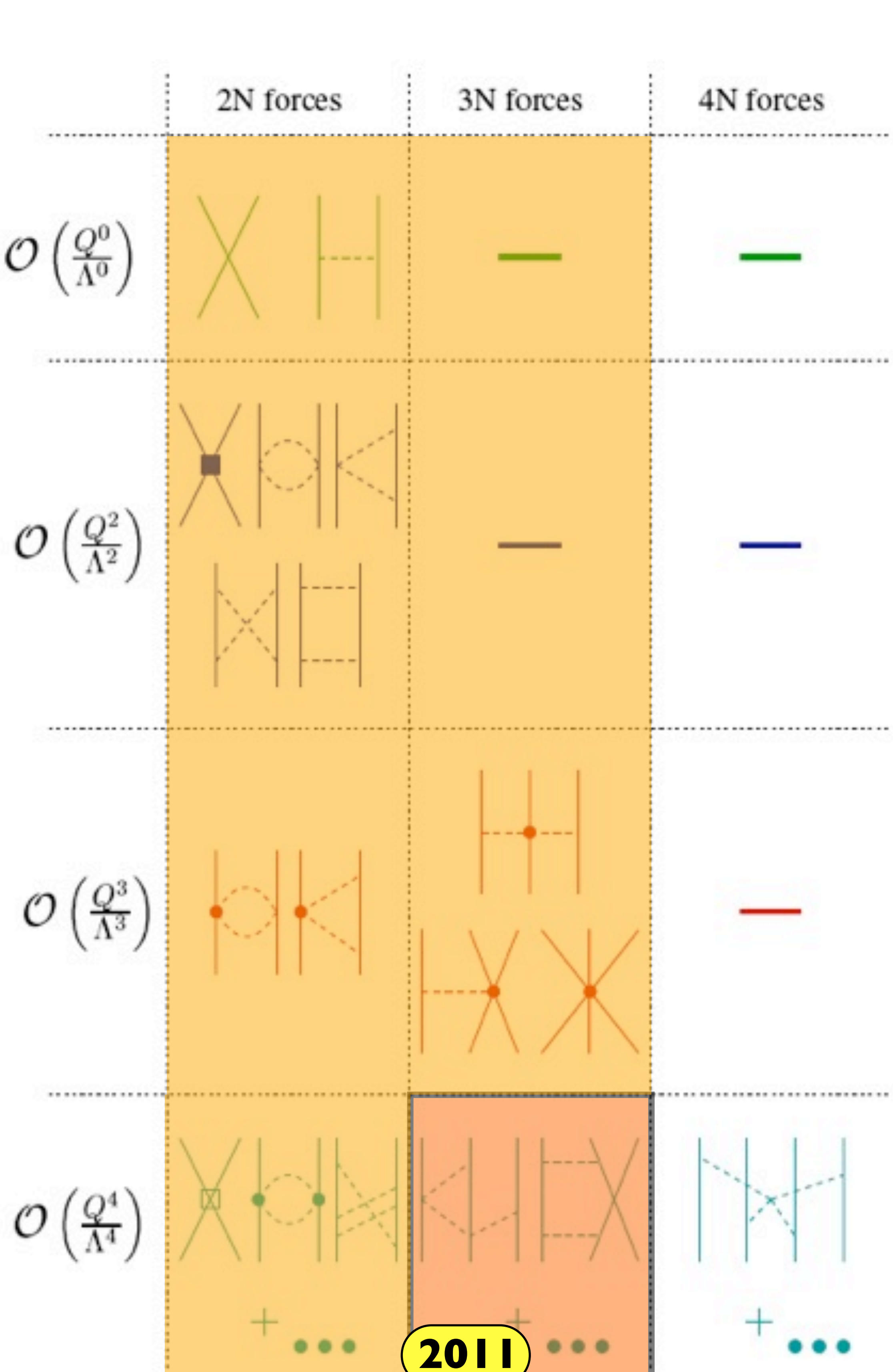
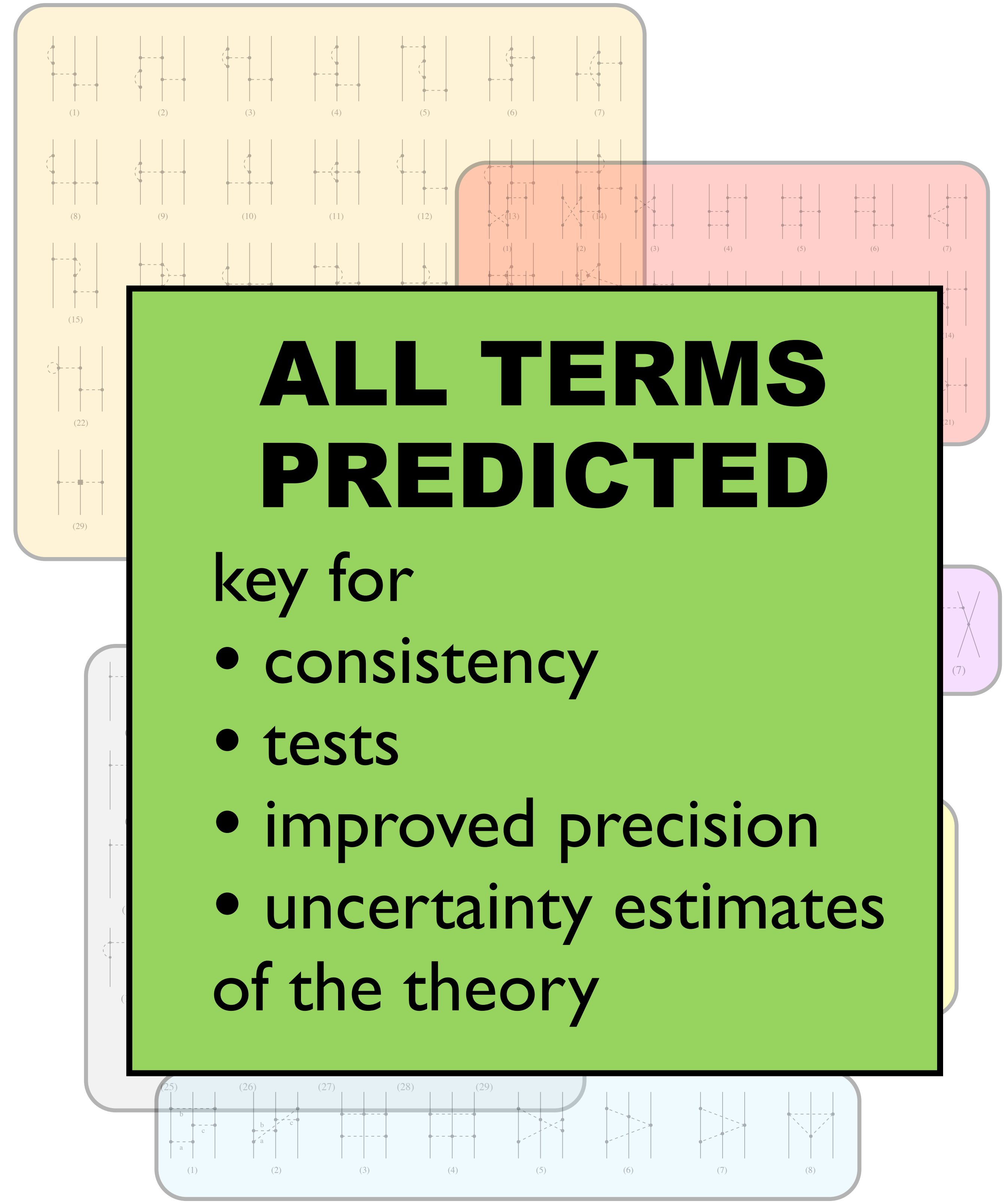




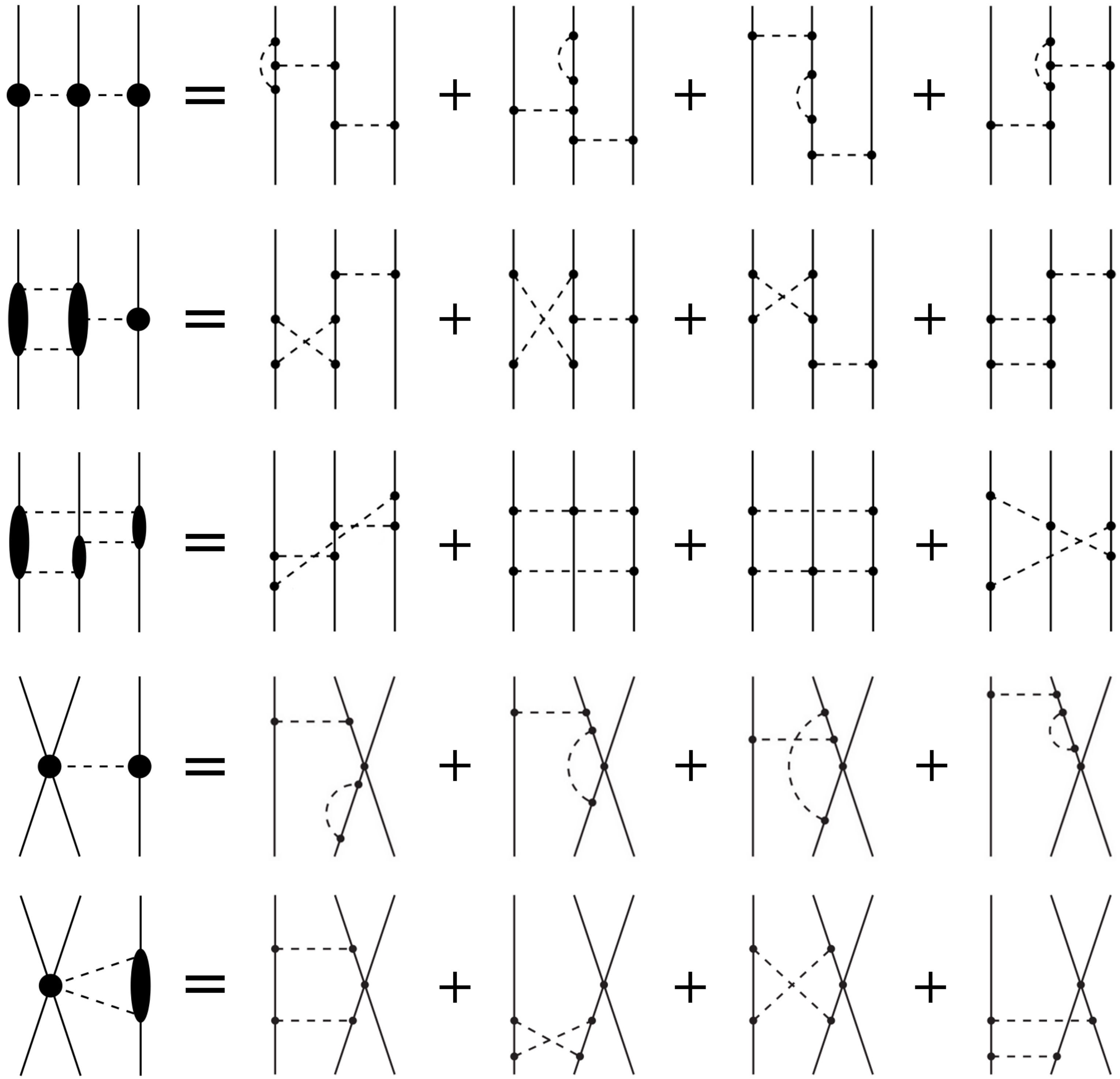
ALL TERMS PREDICTED

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

of the theory

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)

Three-nucleon force contributions at N^3LO



2pi exchange

2pi-1pi exchange

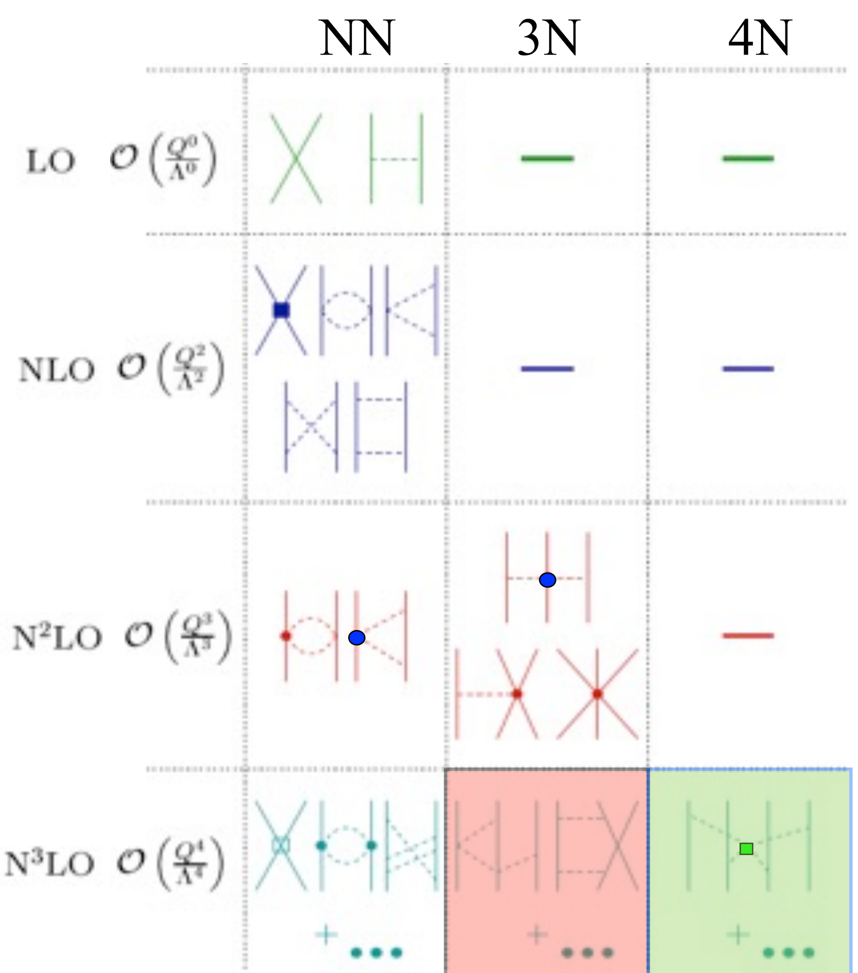
pion rings

1pi-contact

2pi-contact

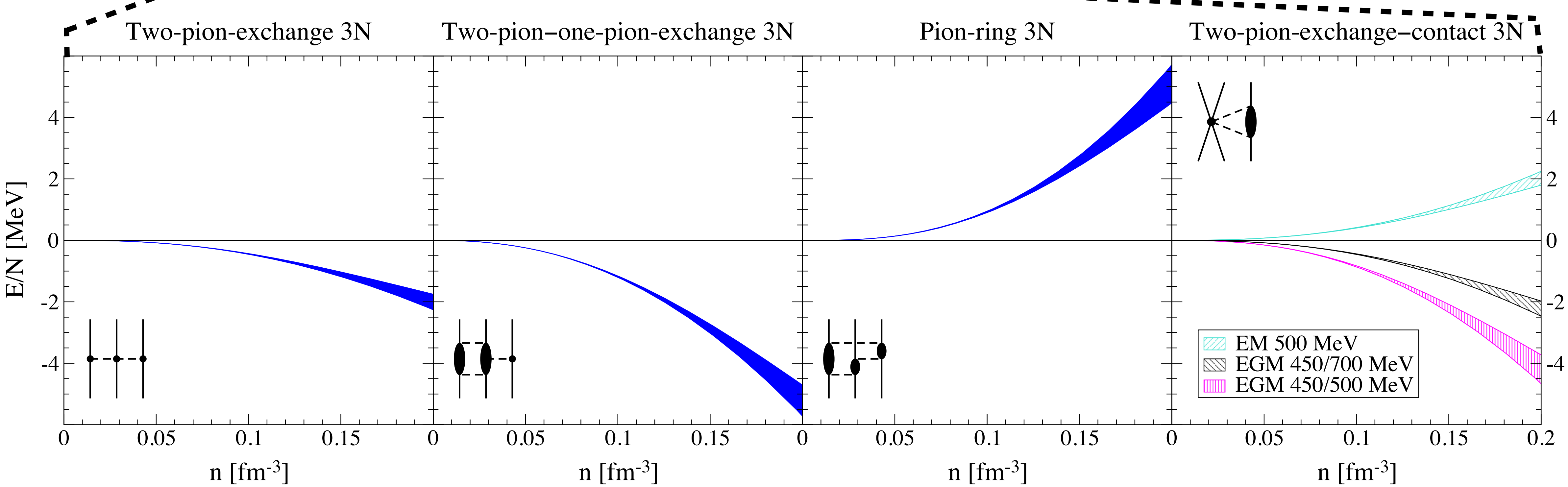
rel. corrections

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

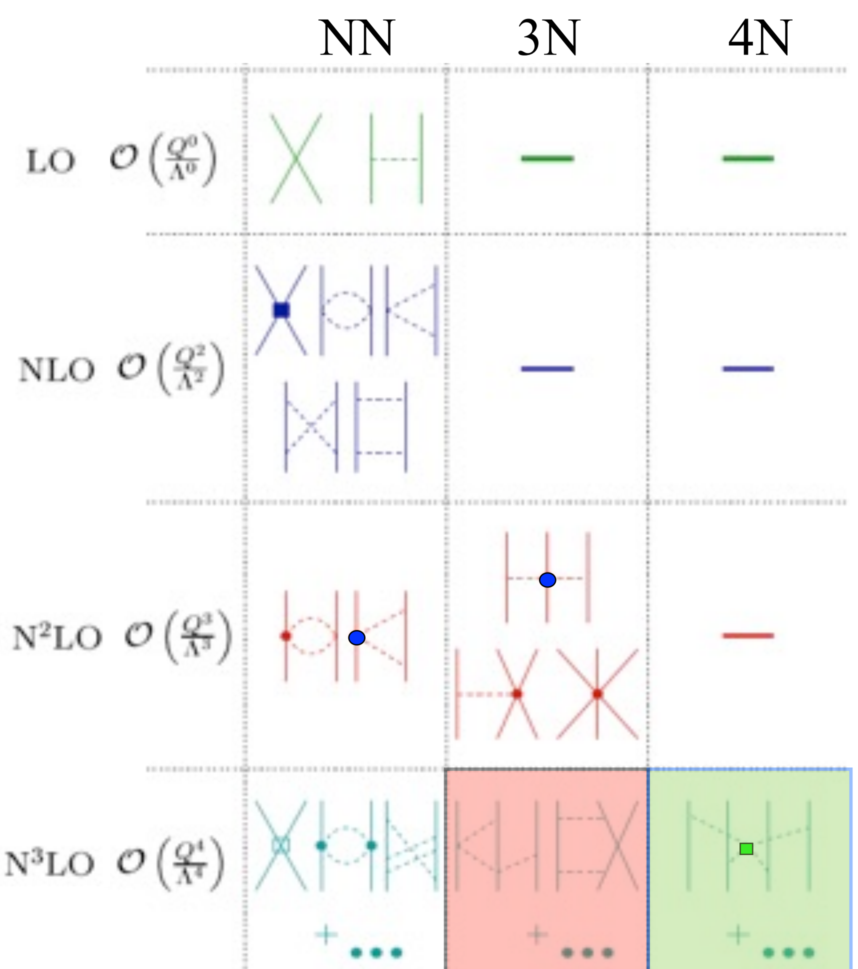


- first calculations of N^3LO 3NF and 4NF contributions to EOS of neutron matter
- found large contributions in Hartree Fock appr., comparable to size of N^2LO contributions

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



Contributions of many-body forces at N^{3}LO in neutron matter



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- 4NF contributions small

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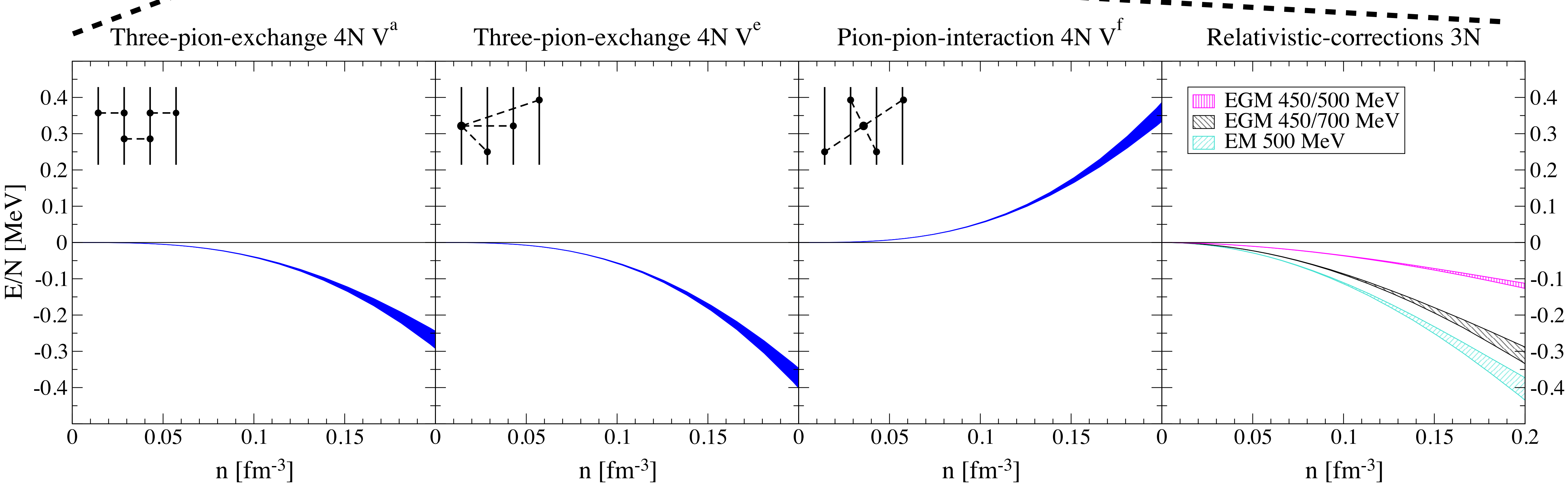
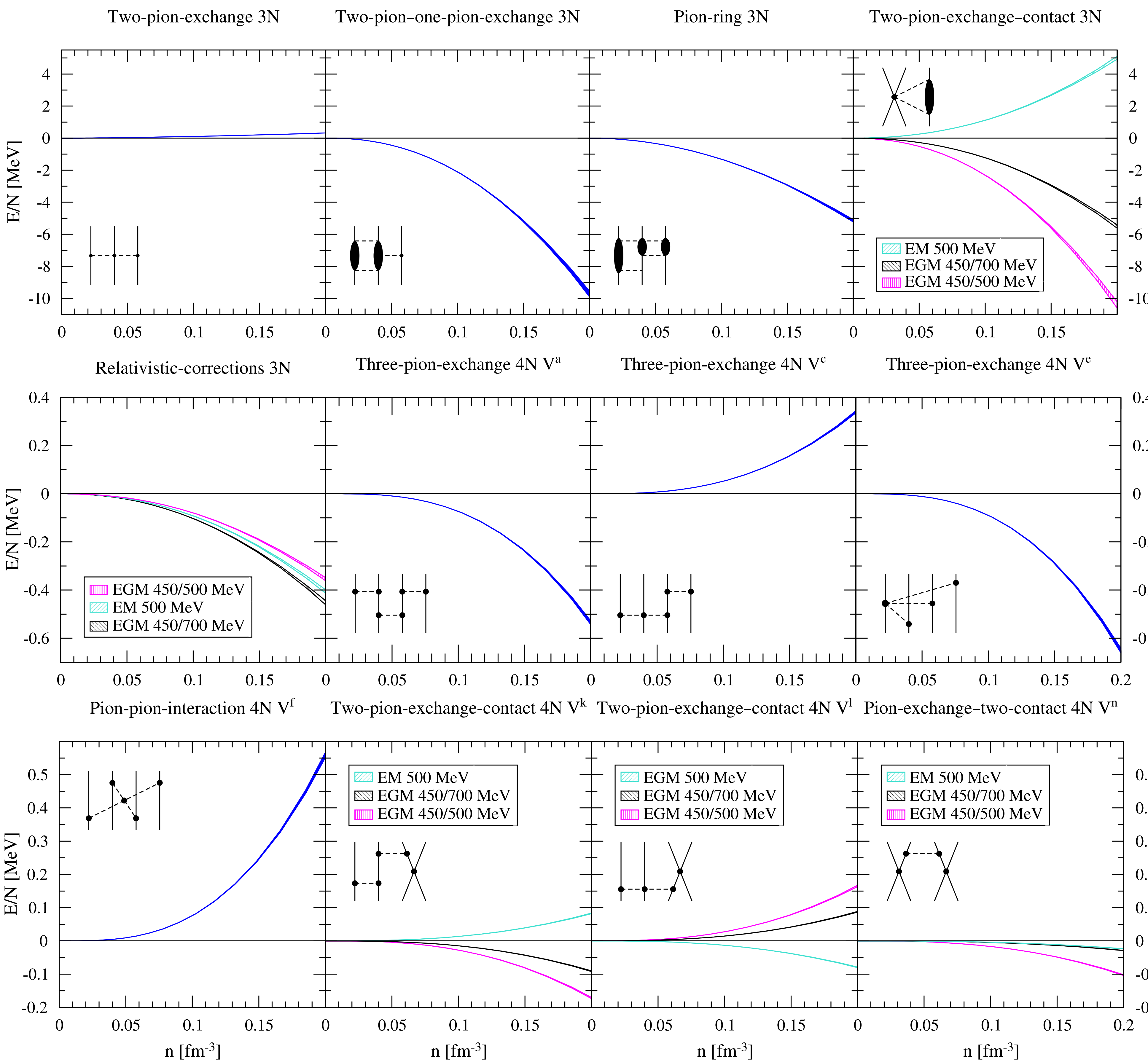


N^3LO contributions in nuclear matter (Hartree Fock)



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

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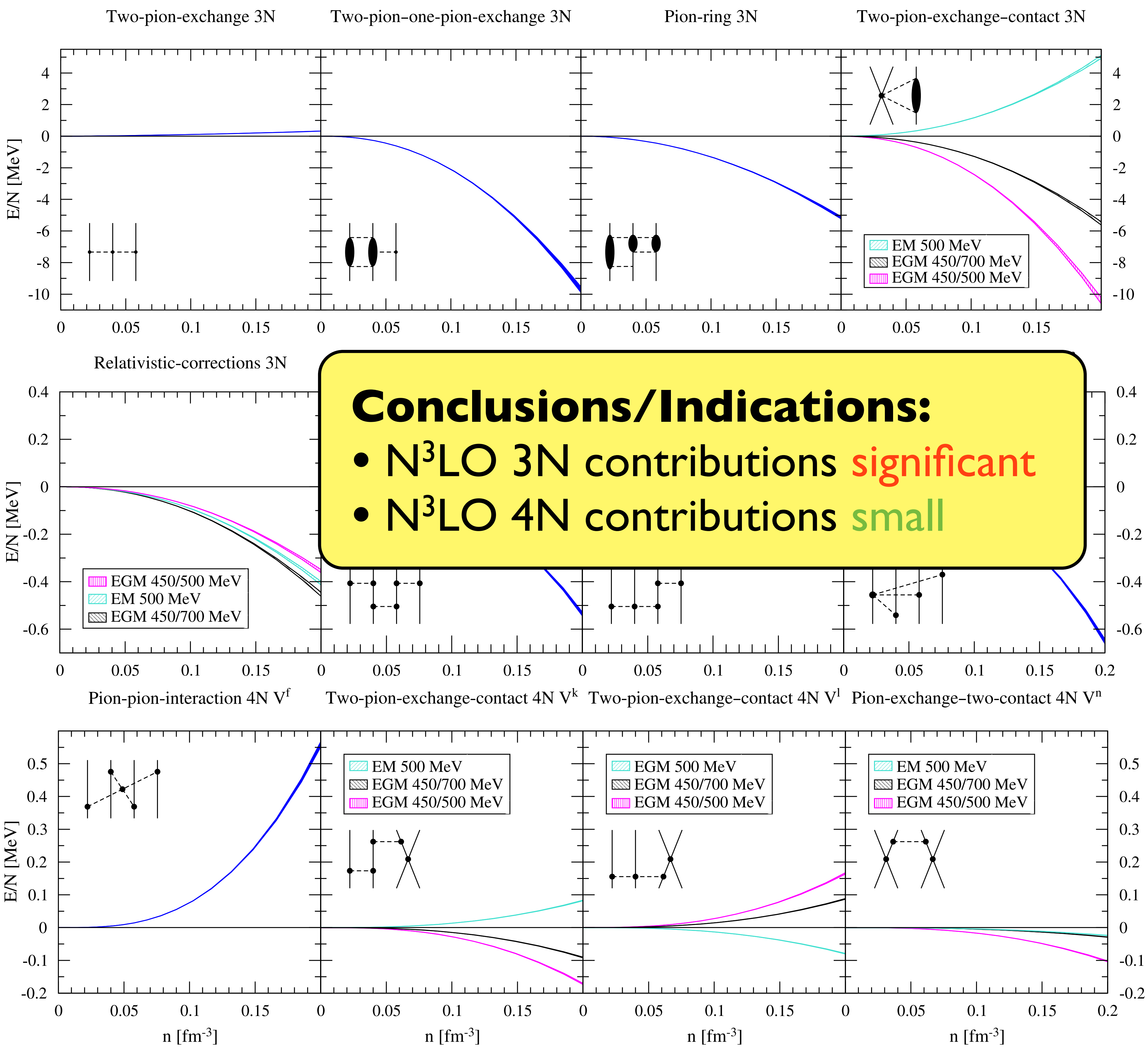


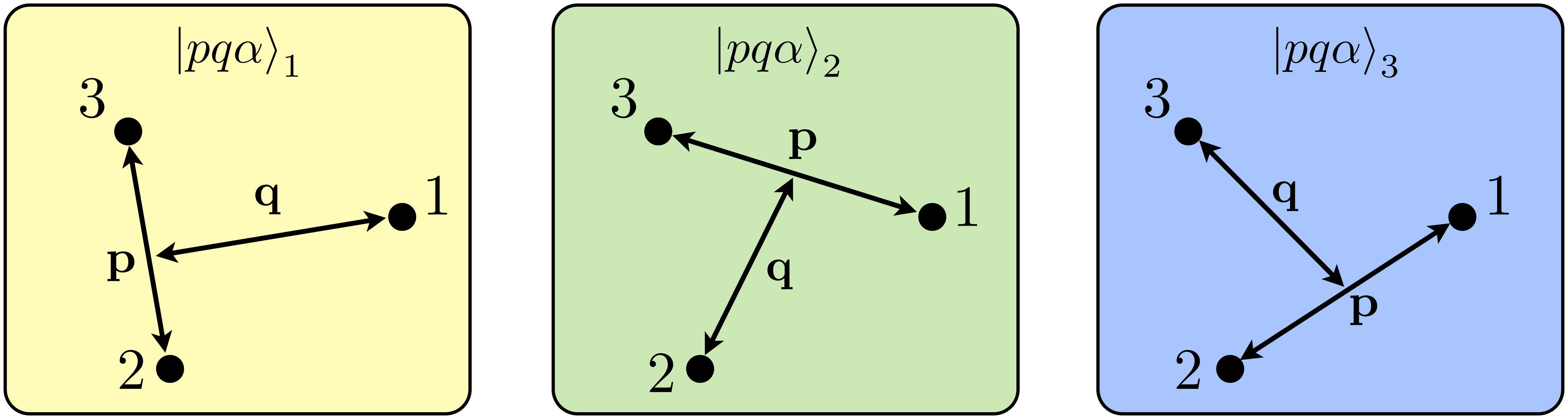
Conclusions/Indications:

- 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:

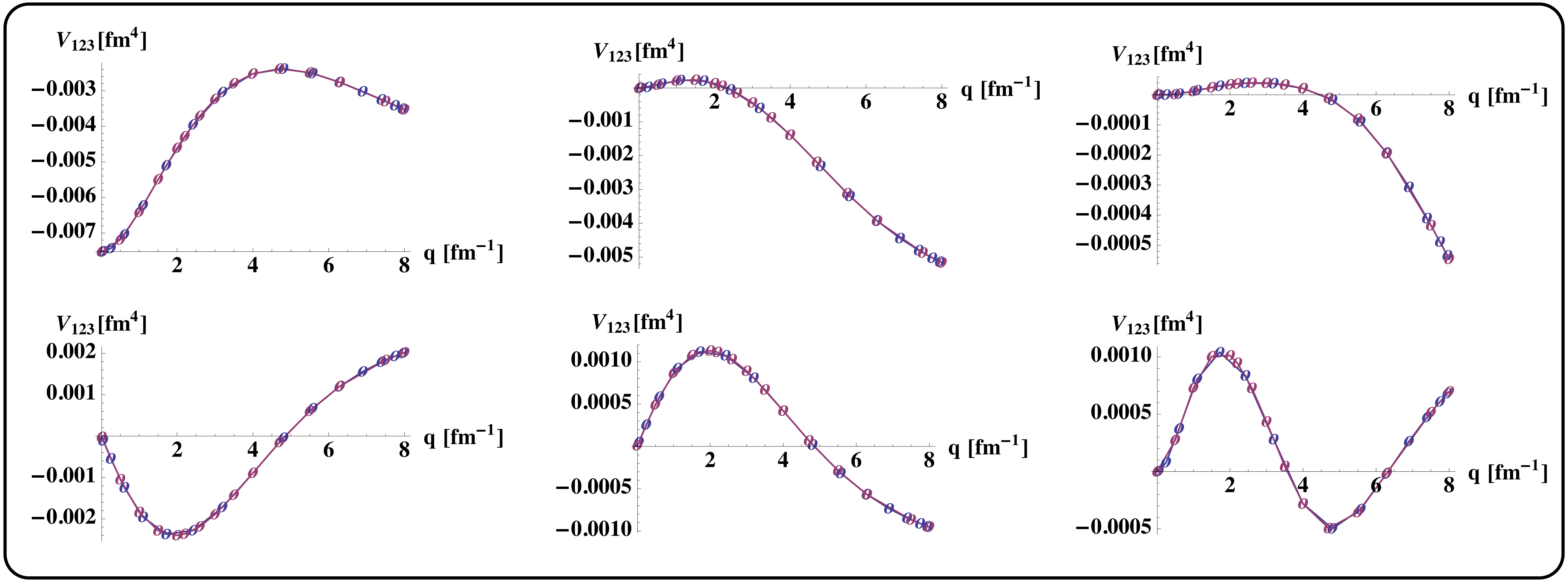
- use that all interaction contributions (except rel. corr.) are local:

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

$\longrightarrow$ 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

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

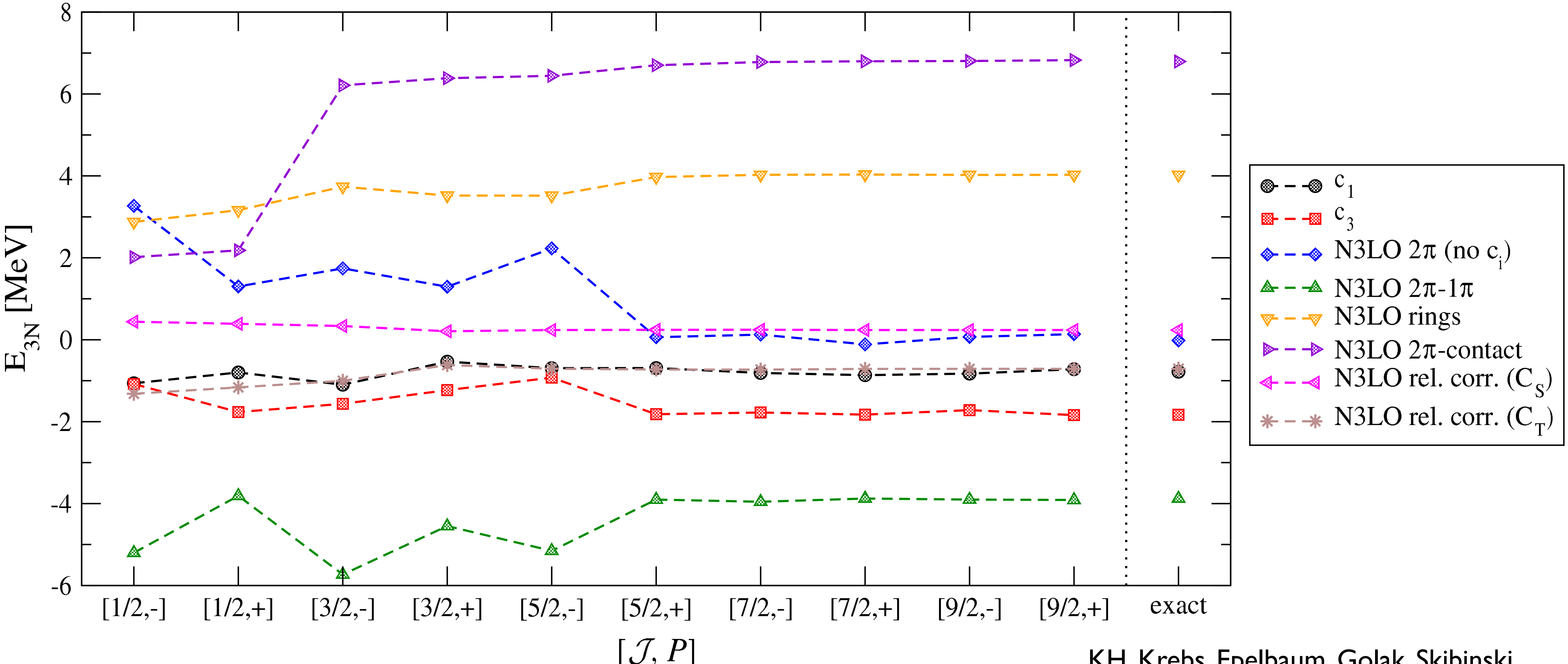
- HDF5 file format for efficient I/O   *http://www.hdfgroup.org*

- 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
			~ 0.5 TB

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

neutron matter:

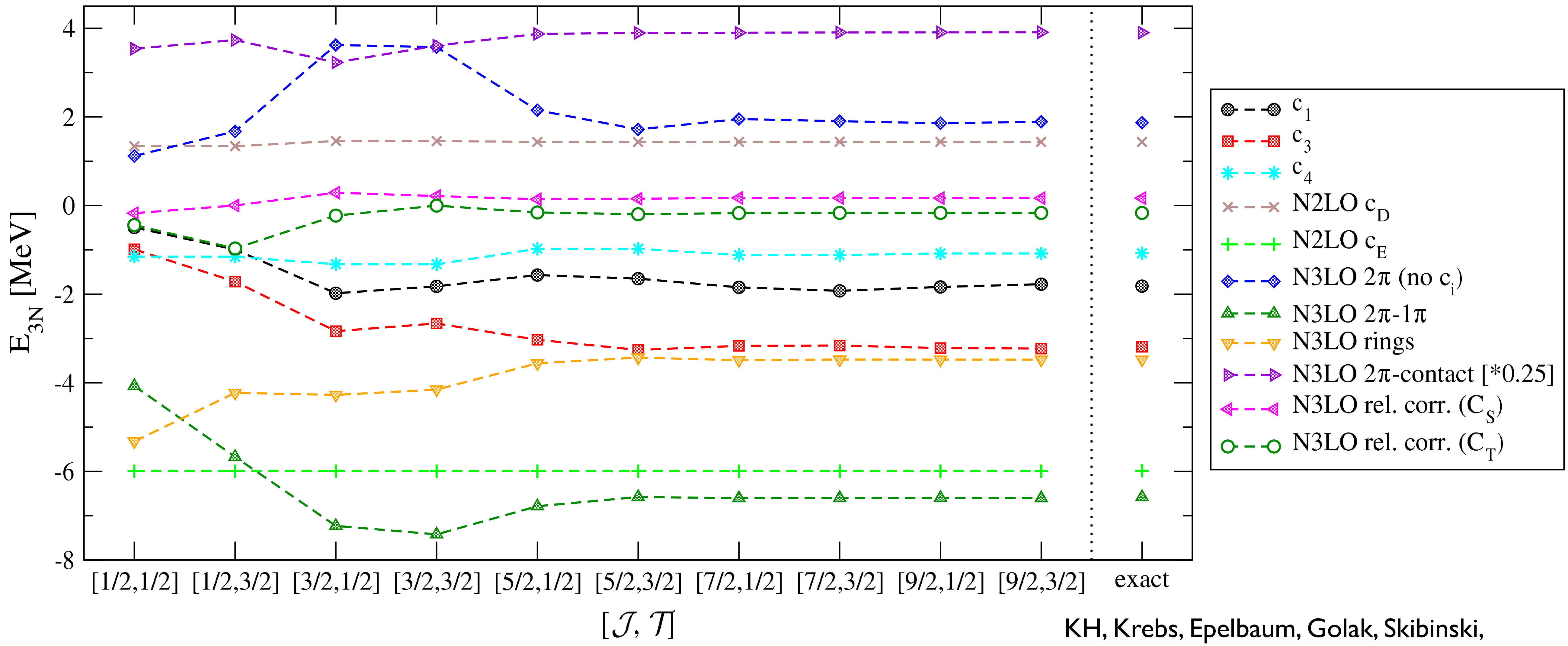


KH, Krebs, Epelbaum, Golak, Skibinski, arXiv:1502.02977

- 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:



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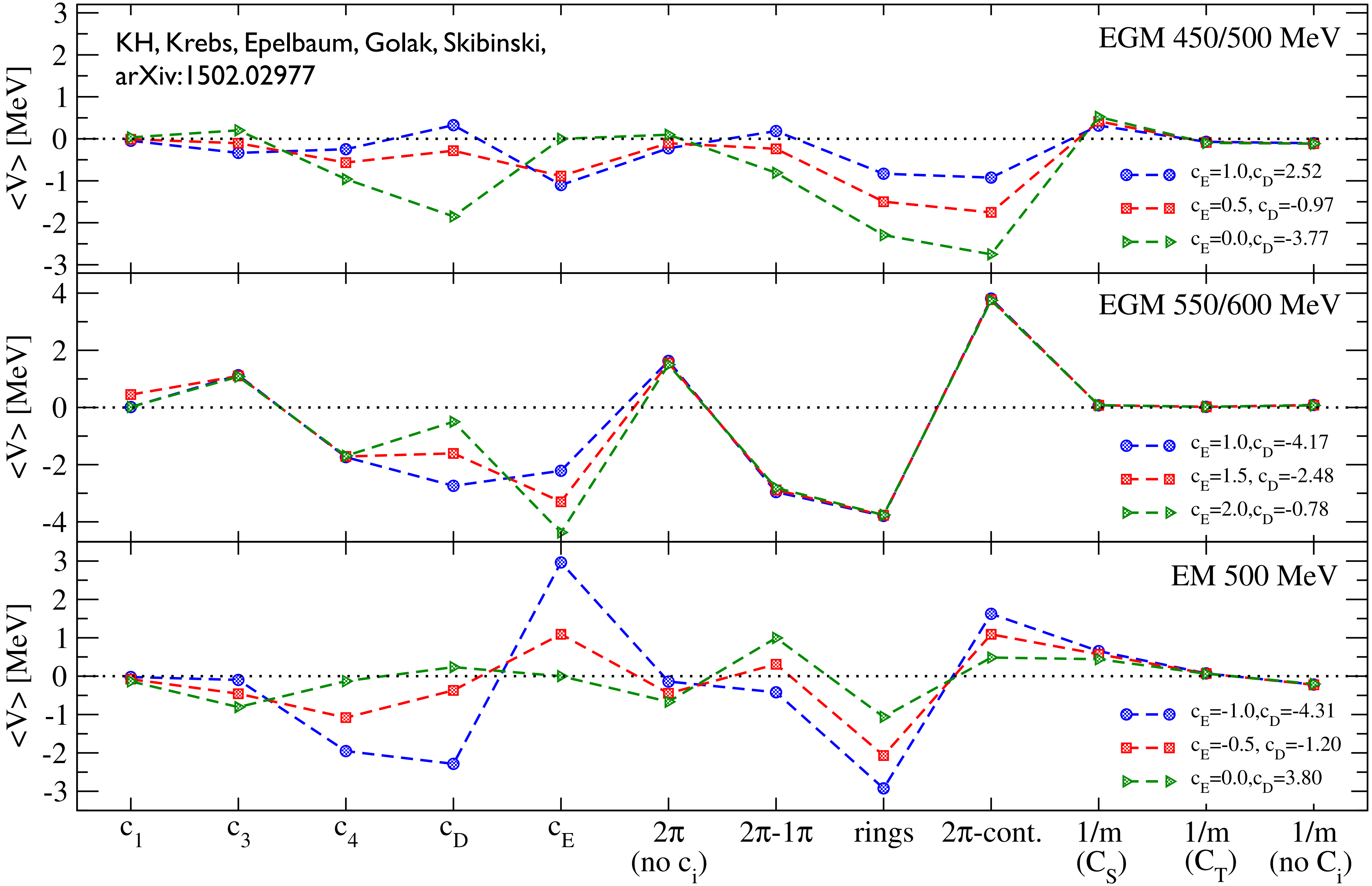
Contributions of individual topologies in ^3H

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

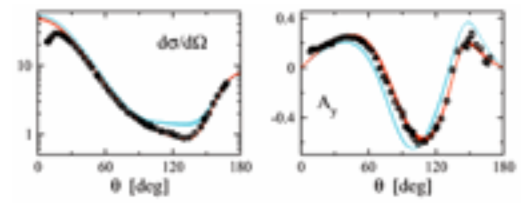


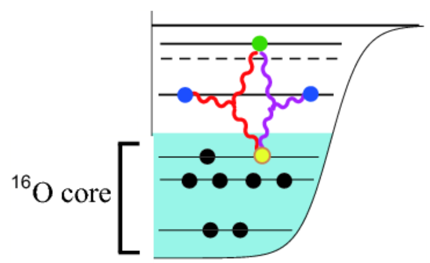
FIG. 4: Nd elastic observables at 65 MeV.

no-core shell model

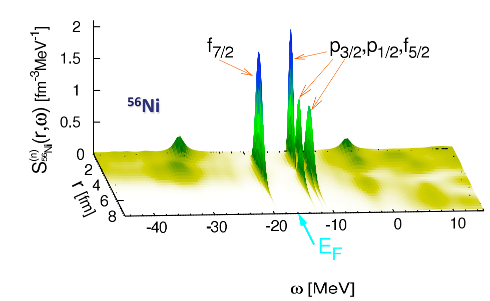
coupled cluster method

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

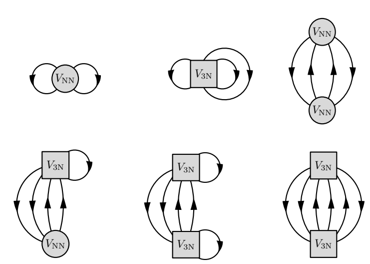
valence shell model



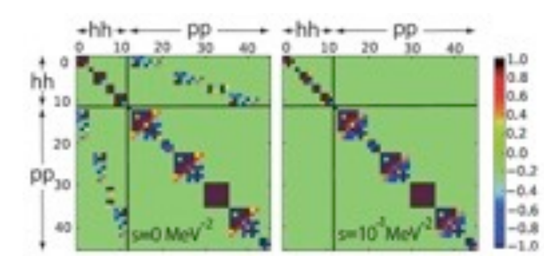
Self-consistent
Greens function



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

Future directions: 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 (see talk by H. Krebs)

- 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 N3LO 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 folding integrals in momentum space partial wave basis

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Work in progress. Stay tuned!

Summary

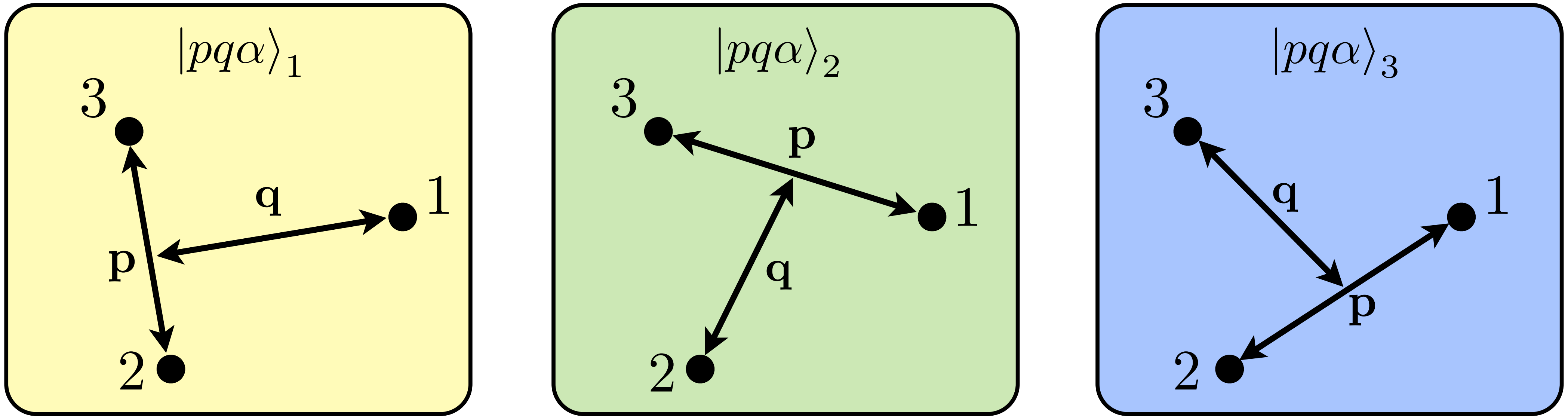
- calculated unregularized partial-wave matrix elements of chiral 3NF up to N3LO
- tested partial wave convergence in nuclear matter (Hartree-Fock appr.)
- contributions to ^{3}H of individual 3NF topologies scheme dependent
- transformation of matrix elements to HO basis straightforward
  $\longrightarrow$ calculations of finite nuclei (shell model, coupled cluster, IM-SRG, SCGF...)

Outlook

- inclusion of non-local regulators trivial, impl. of local regulators in progress
- efficient calculation of nuclear currents?
- chiral forces based on other power counting?
- chiral forces at N4LO?
- delta-full EFT?

Thank you!

RG evolution of 3N interactions in momentum space



- represent interaction in basis $|pq\alpha\rangle_i \equiv |p_i q_i; [(LS)J(ls_i)j]\, \mathcal{J}\mathcal{J}_z (Tt_i)\mathcal{T}\mathcal{T}_z\rangle$
- explicit equations for NN and 3N flow equations

$$
\begin{aligned}
\frac{dV_{ij}}{ds} &= [[T_{ij}, V_{ij}], T_{ij} + V_{ij}], \\
\frac{dV_{123}}{ds} &= [[T_{12}, V_{12}], V_{13} + V_{23} + V_{123}] \\
&+ [[T_{13}, V_{13}], V_{12} + V_{23} + V_{123}] \\
&+ [[T_{23}, V_{23}], V_{12} + V_{13} + V_{123}] \\
&+ [[T_{\rm rel}, V_{123}], H_s]
\end{aligned}
$$

Bogner, Furnstahl, Perry PRC 75, 061001(R) (2007)

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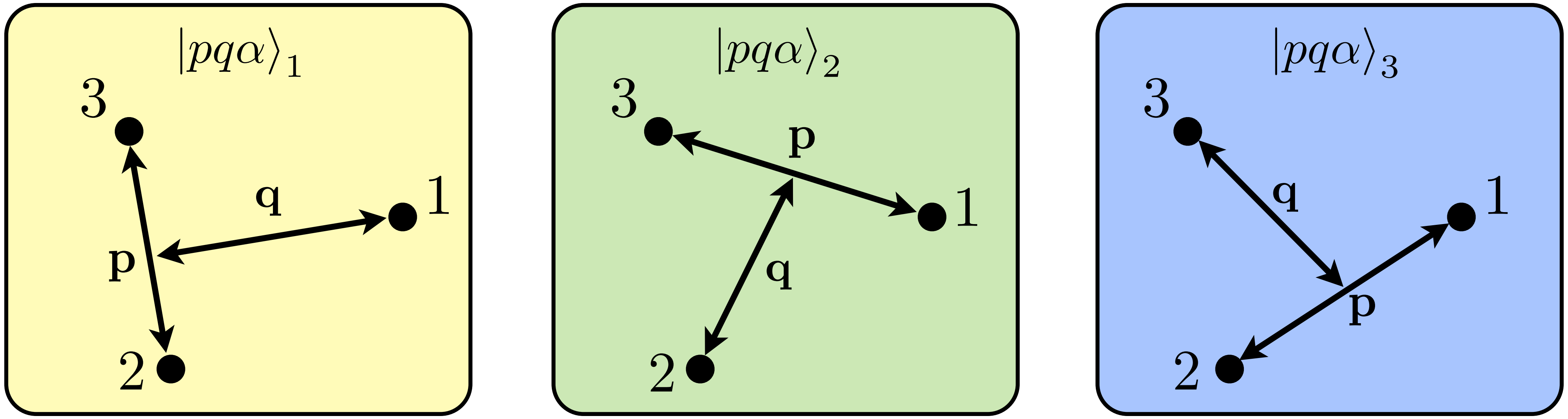

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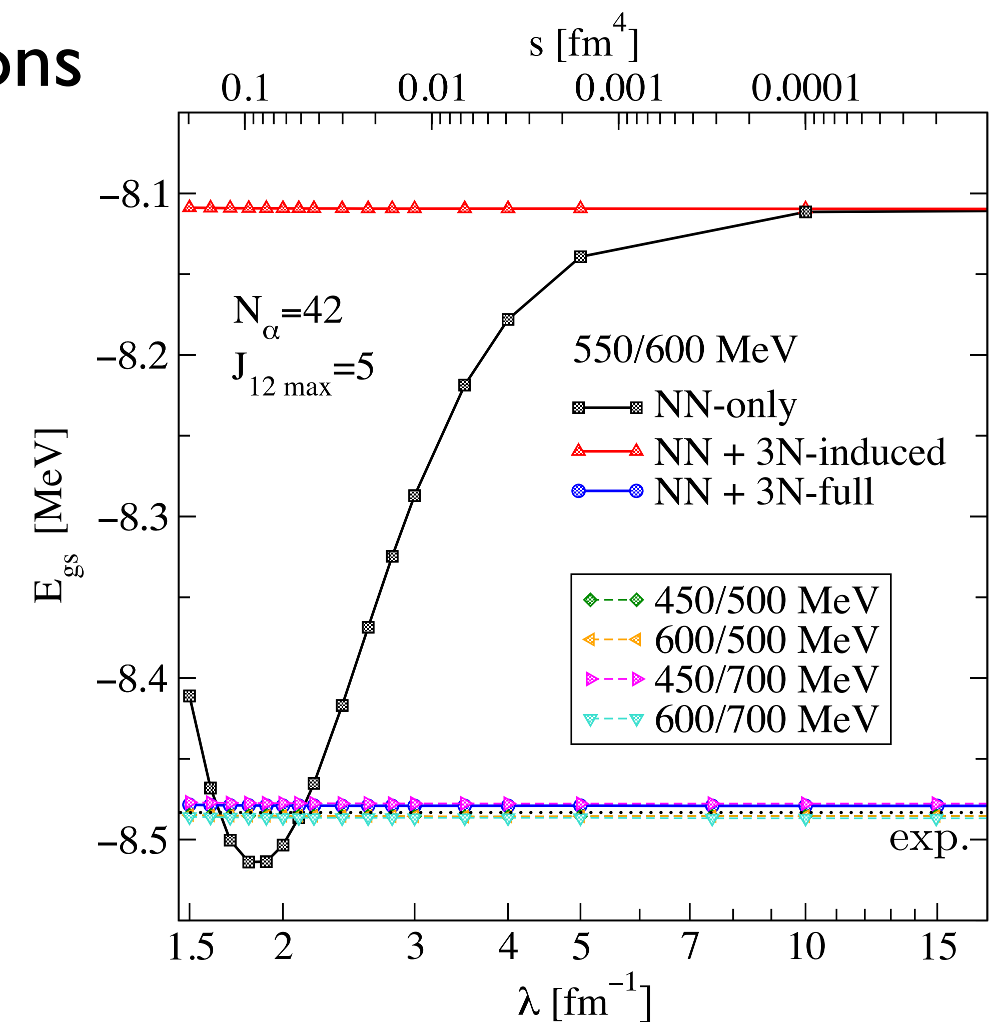
Bogner, Furnstahl, Perry PRC 75, 061001(R) (2007)



Hebeler PRC(R) 85, 021002 (2012)

SRG flow equations of NN and 3N forces in momentum basis

$$\frac{dH_s}{ds} = [\eta_s, H_s] \qquad \eta_s = [T_{\rm rel}, H_s]$$

$$H = T + V_{12} + V_{13} + V_{23} + V_{123}$$

- spectators correspond to delta functions, matrix representation of H_s ill-defined
- solution: explicit separation of NN and 3N flow equations

$$\begin{aligned}
\frac{dV_{ij}}{ds} &= \left[\left[T_{ij}, V_{ij}\right], T_{ij} + V_{ij}\right], \\
\frac{dV_{123}}{ds} &= \left[\left[T_{12}, V_{12}\right], V_{13} + V_{23} + V_{123}\right] \\
&+ \left[\left[T_{13}, V_{13}\right], V_{12} + V_{23} + V_{123}\right] \\
&+ \left[\left[T_{23}, V_{23}\right], V_{12} + V_{13} + V_{123}\right] \\
&+ \left[\left[T_{\rm rel}, V_{123}\right], H_s\right]
\end{aligned}$$

- only connected terms remain in $\frac{dV_{123}}{ds}$,'dangerous' delta functions cancel

see Bogner, Furnstahl, Perry PRC 75, 061001(R) (2007)

SRG evolution in momentum space

- evolve the antisymmetrized 3N interaction

$$\overline{V}_{123} = {}_i\langle pq\alpha| \, (1 + P_{123} + P_{132}) V_{123}^{(i)} (1 + P_{123} + P_{132}) \, |p'q'\alpha'\rangle_i$$

- embed NN interaction in 3N basis:

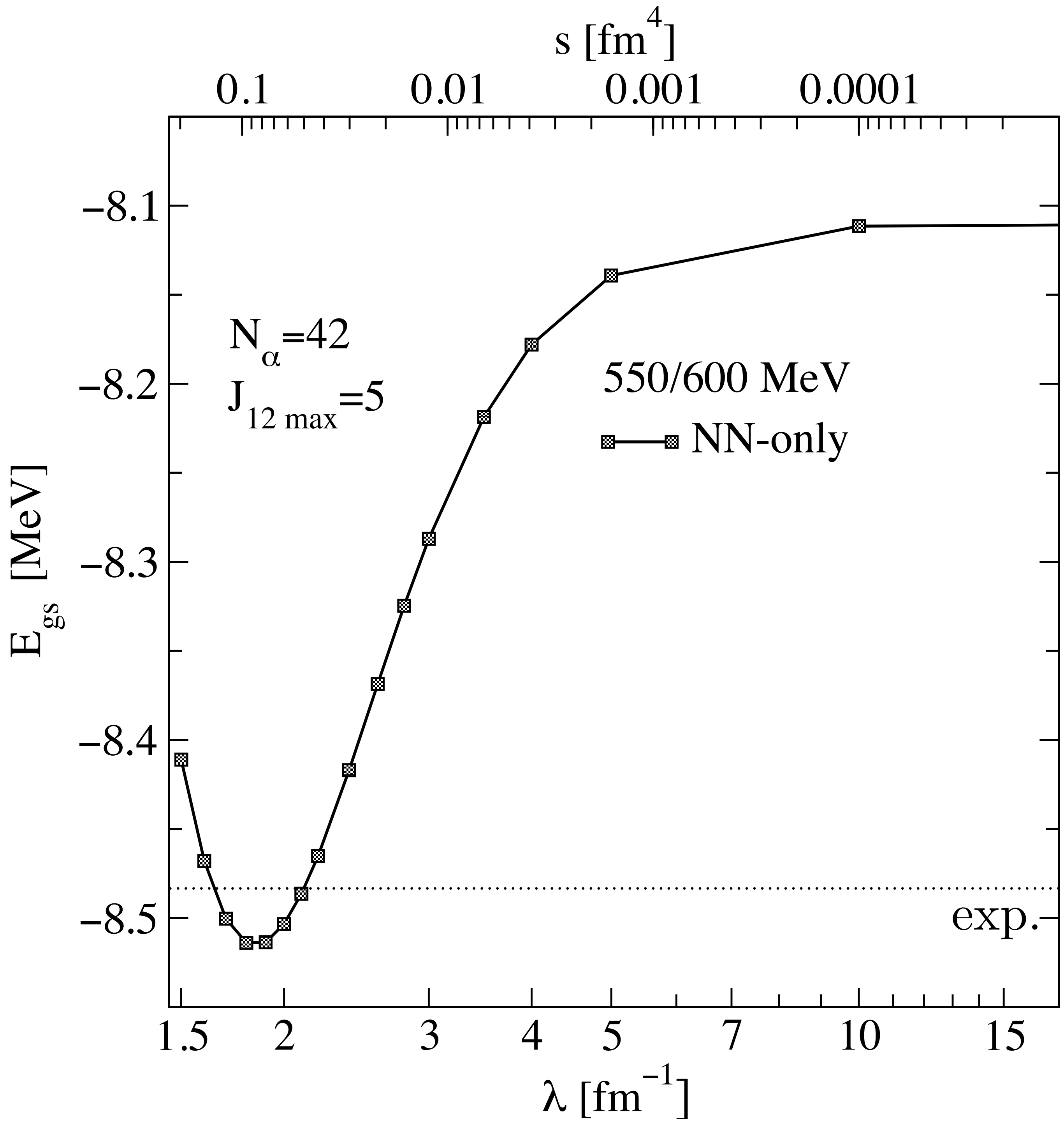
$$V_{13} = P_{123} V_{12} P_{132}, \quad V_{23} = P_{132} V_{12} P_{123}$$

with $${}_3\langle pq\alpha|V_{12}|p'q'\alpha'\rangle_3 = \langle p\tilde{\alpha}|V_{\rm NN}|p'\tilde{\alpha}'\rangle \, \delta(q-q')/q^2$$

- use $P_{123}\overline{V}_{123} = P_{132}\overline{V}_{123} = \overline{V}_{123}$

$$\Rightarrow \quad \begin{aligned} d\overline{V}_{123}/ds = & \, C_1(s, T, V_{\rm NN}, P) \\ & + C_2(s, T, V_{\rm NN}, \overline{V}_{123}, P) \\ & + C_3(s, T, \overline{V}_{123}) \end{aligned}$$

SRG evolution of 3N interactions in momentum space: Results for the Triton



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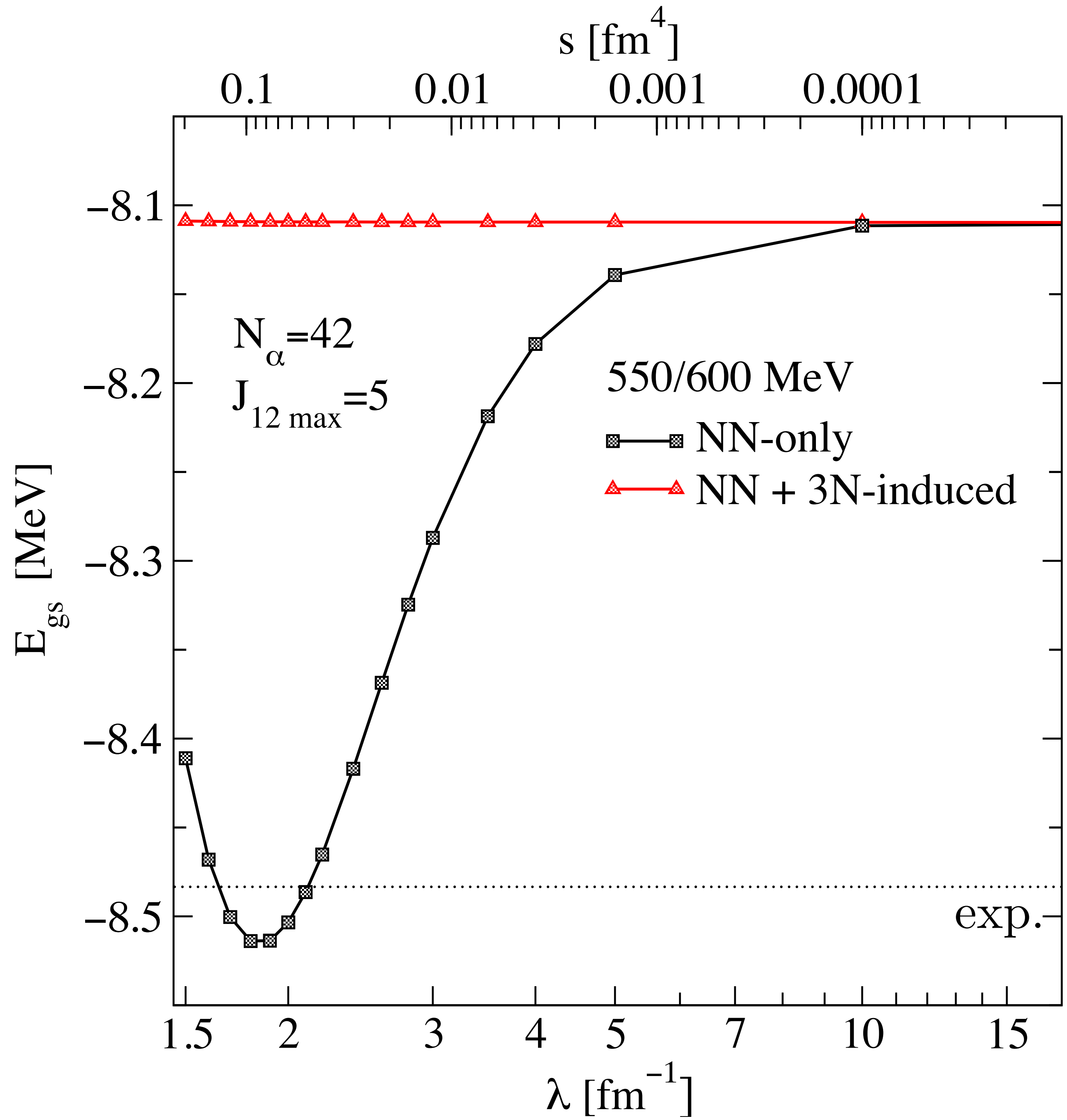
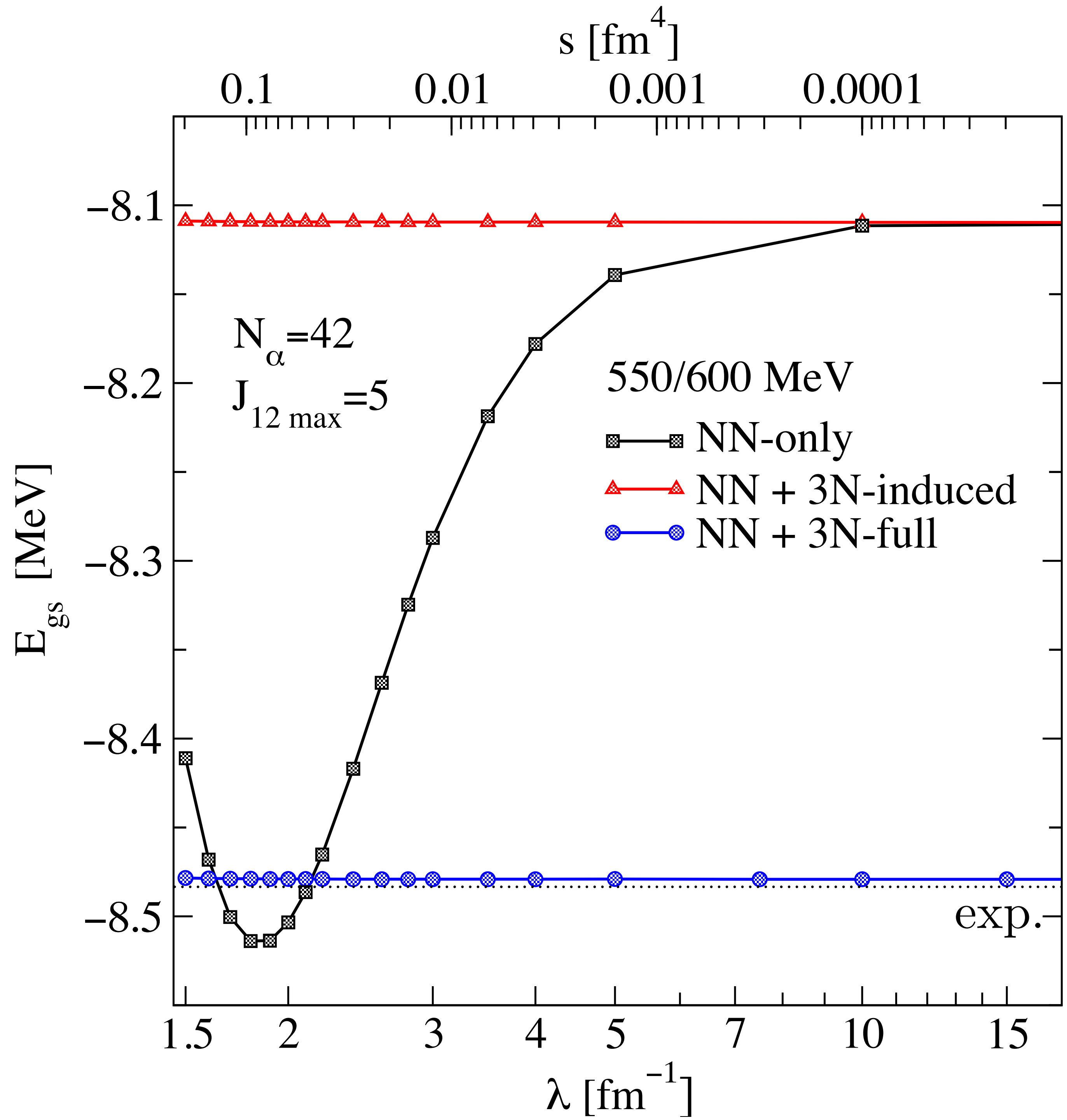


Hebeler PRC(R) 85, 021002 (2012)

It works:

Invariance of $E_{\rm gs}^{^3H}$ within $\leq 1\,\mathrm{eV}$ for consistent chiral interactions at $\mathrm{N^2LO}$

SRG evolution of 3N interactions in momentum space: Results for the Triton



Hebeler PRC(R) 85, 021002 (2012)

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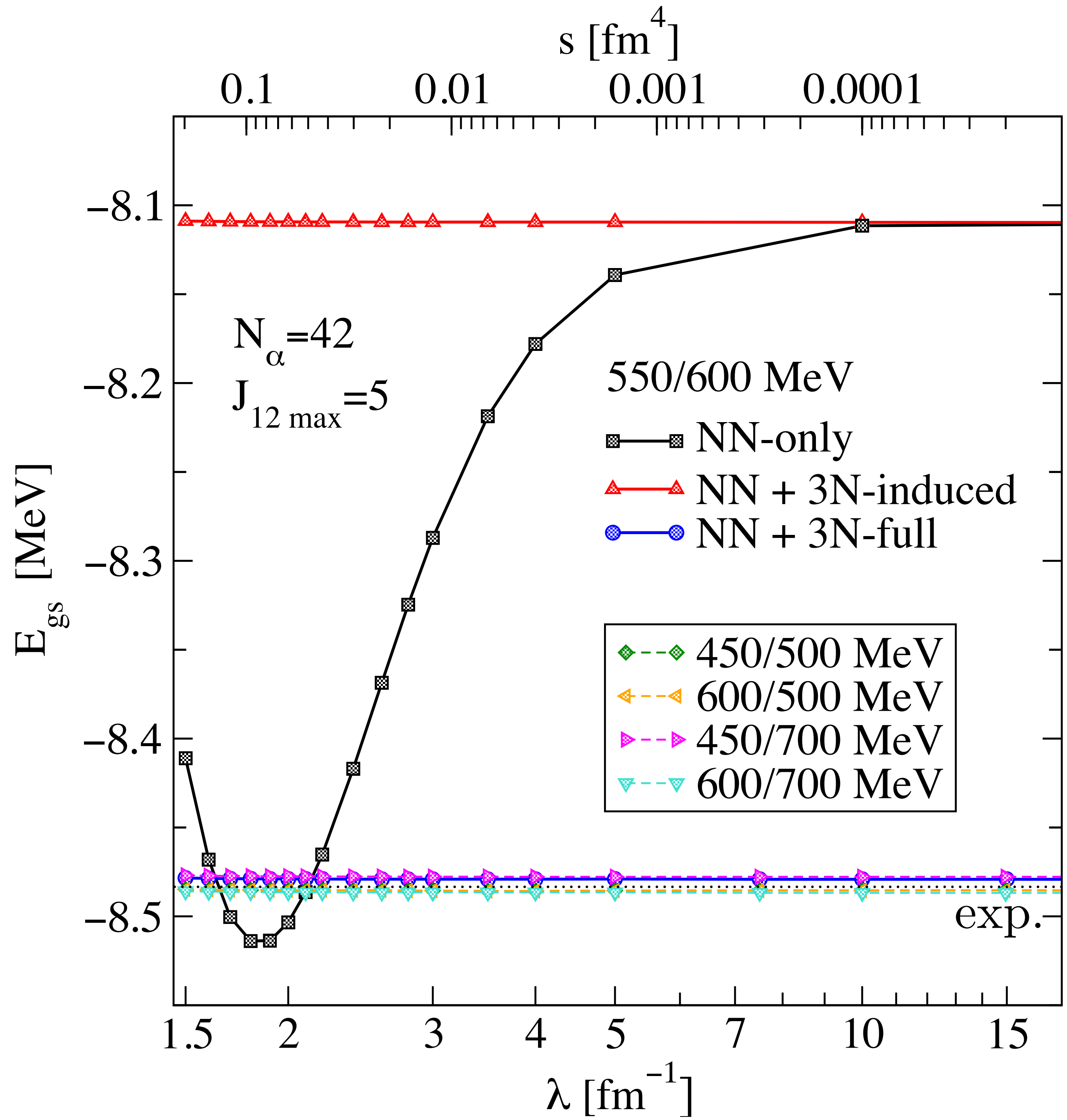

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