Calculation of 3N forces at N3LO for novel studies of nuclei and matter

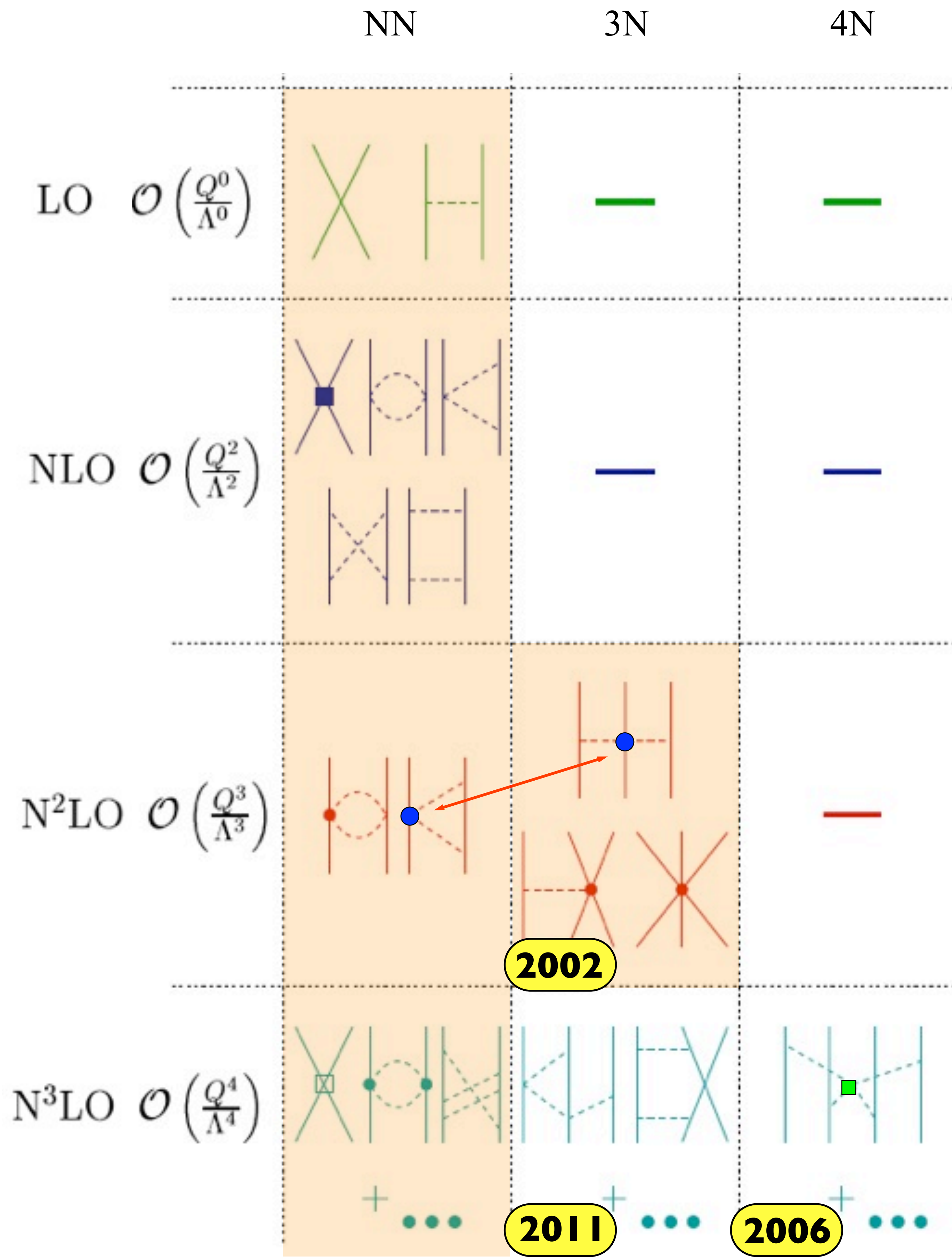
Kai Hebeler

Vancouver, February 20, 2014

Chiral effective field theory for nuclear forces

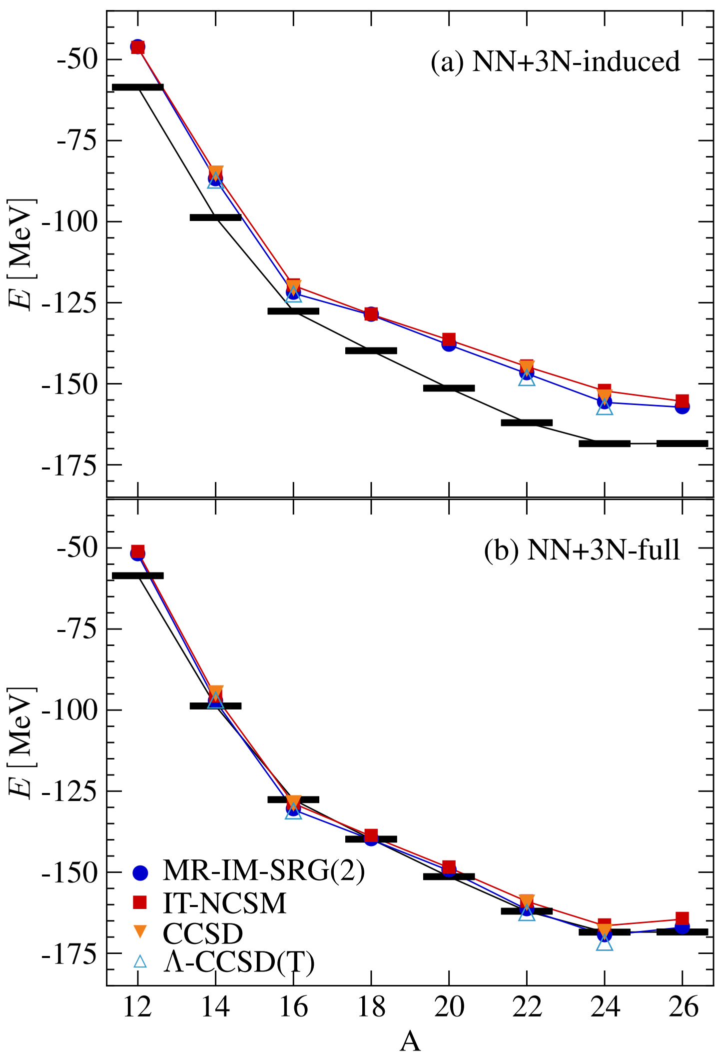
- choose relevant degrees of freedom: here nucleons and pions
- operators constrained by symmetries of QCD
- short-range physics captured in few short-range couplings
- separation of scales: Q << Λ_b, breakdown scale Λ_b~500 MeV
- power-counting: expand in powers Q/Λ_b
- systematic: work to desired accuracy,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

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



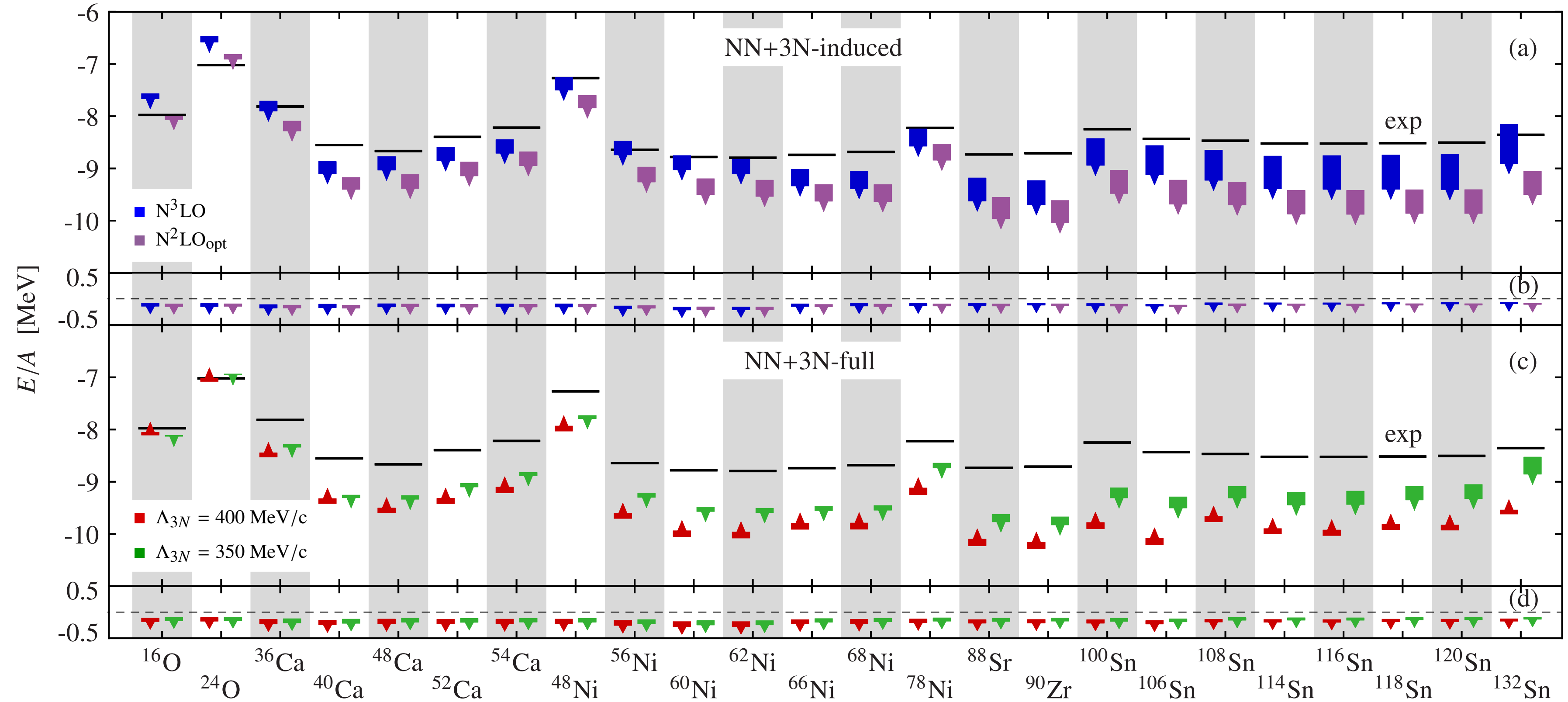
Open issues in nuclear interactions

oxygen chain



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

heavy nuclei



Binder et al., arXiv:1312.5685 (2014)

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

Open issues in nuclear interactions

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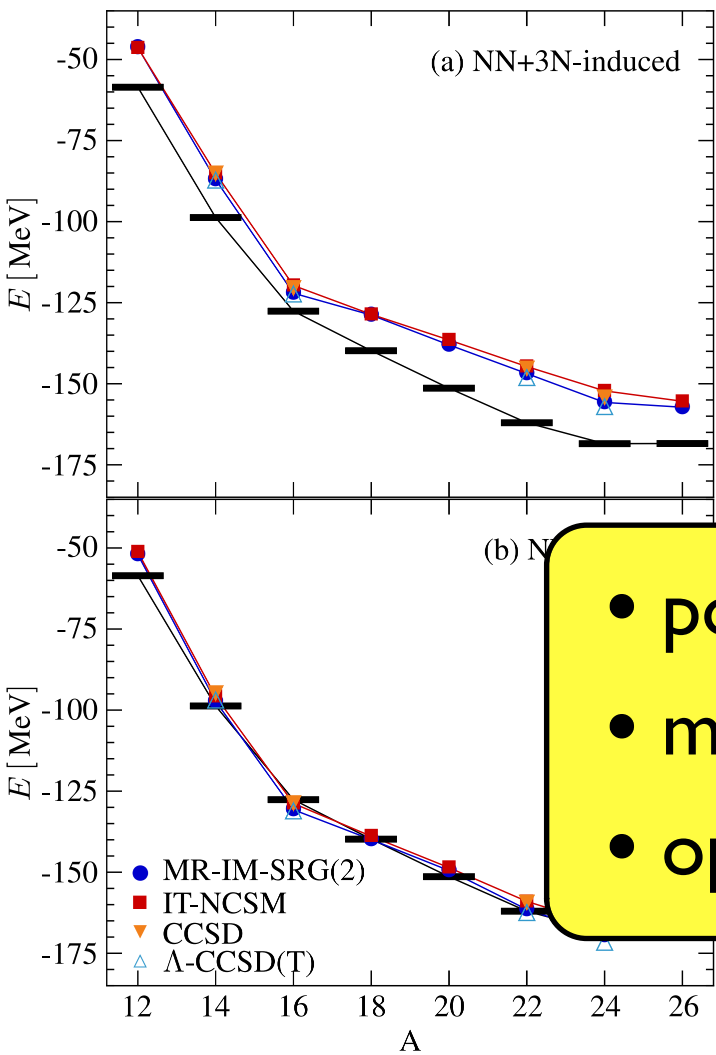

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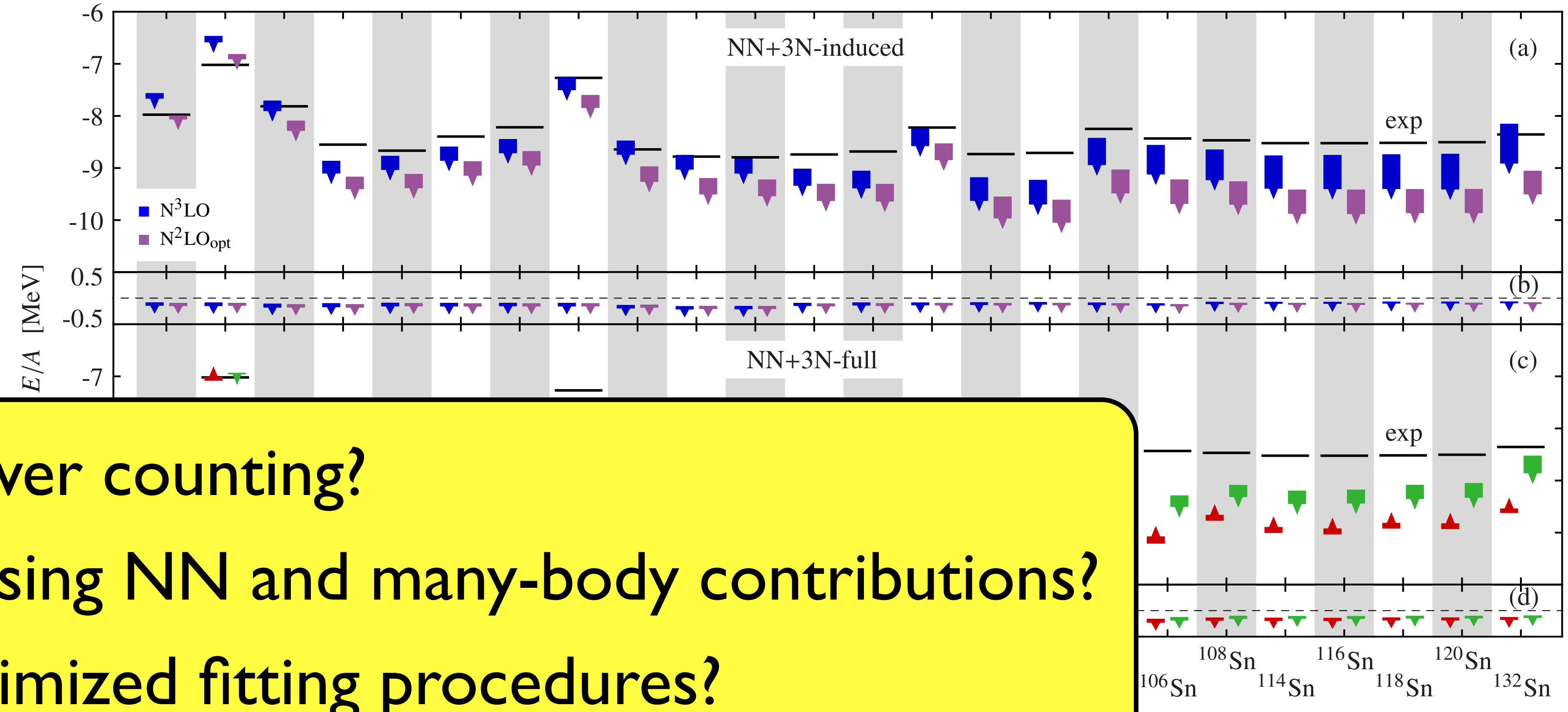
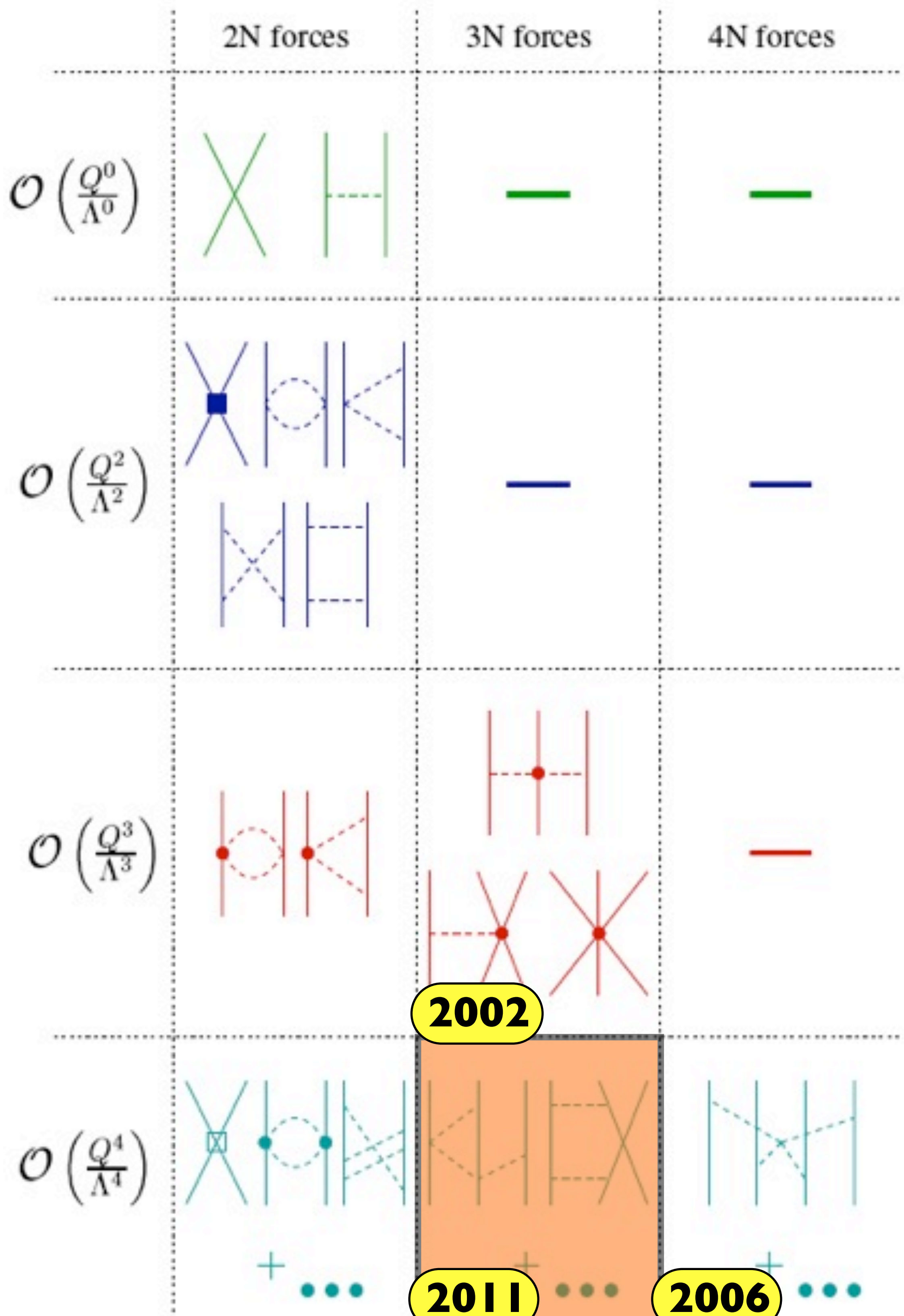
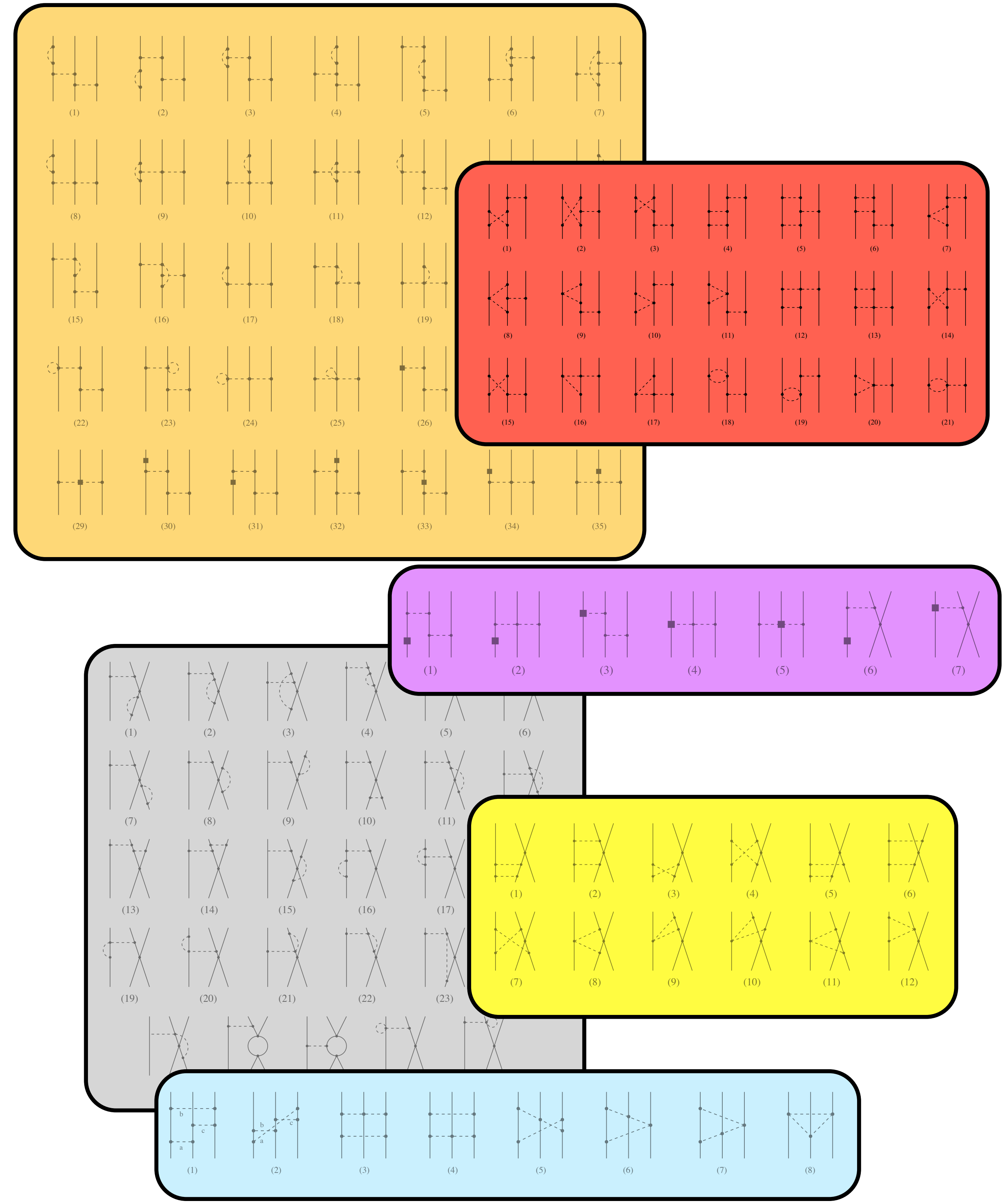


- power counting?
- missing NN and many-body contributions?
- optimized fitting procedures?

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

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





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)

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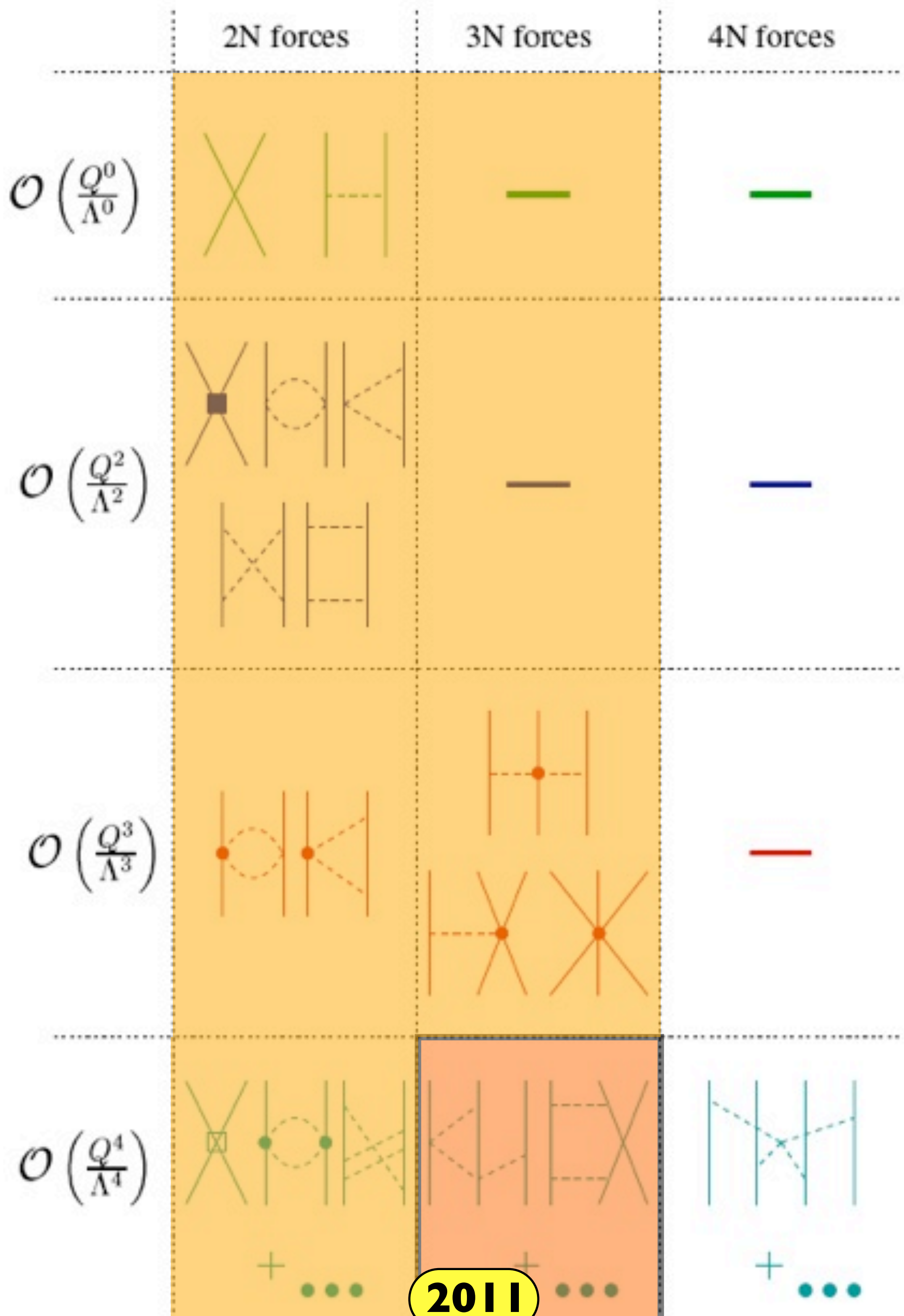

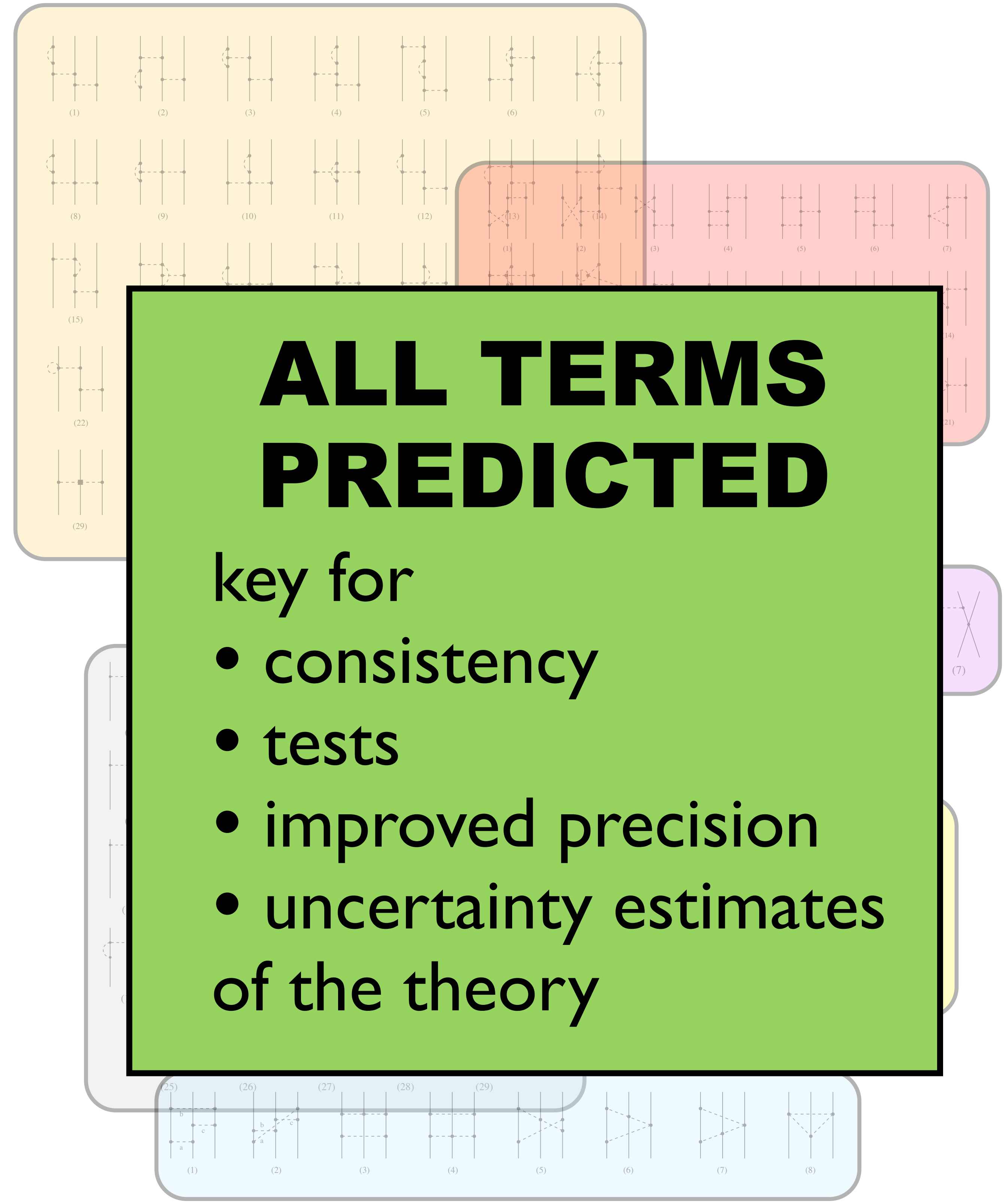

ALL TERMS PREDICTED

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)

Calculation of many-body forces

Low
Energy
Nuclear
Physics
International
Collaboration

J. Golak, R. Skibinski, K. Tolponicki, H. Witala

E. Epelbaum, H. Krebs

A. Nogga

R. Furnstahl

S. Binder, A. Calci, K. Hebeler, J. Langhammer, R. Roth

P. Maris, J. Vary

H. Kamada

Goal

Calculate matrix elements of 3NF in a partial-wave decomposed form which is suitable for different few- and many-body frameworks

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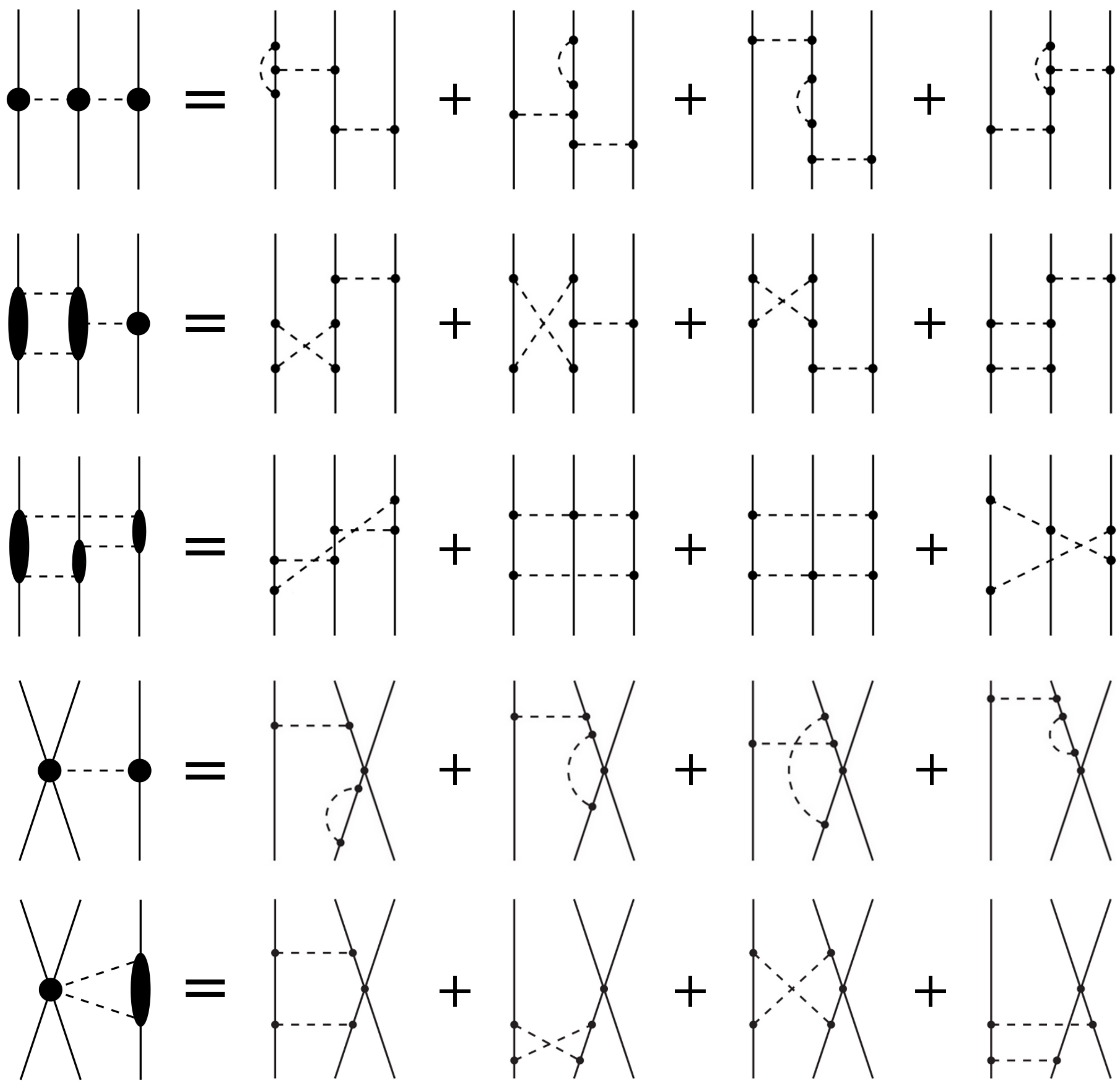
Challenge

Due to the large number of matrix elements, the calculation is extremely expensive.

Strategy

Develop an efficient framework that allows to treat arbitrary 3N interactions.
(Krebs and Hebeler)

Three-nucleon force contributions at N^{3}LO



2pi exchange

2pi-1pi exchange

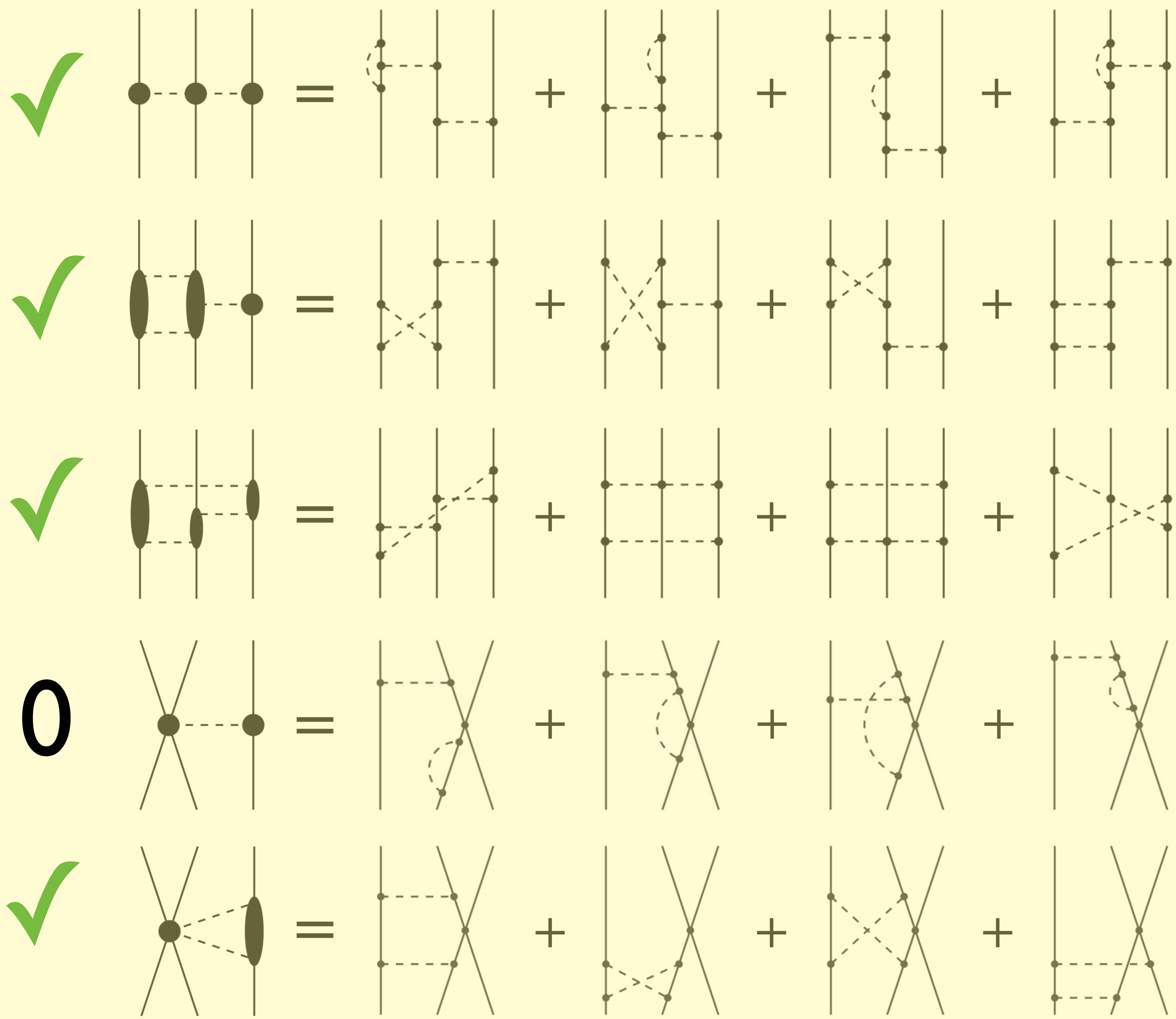
pion rings

1pi-contact

2pi-contact

rel. corrections

Three-nucleon force contributions at N^{3}LO



2pi exchange

2pi-1pi exchange

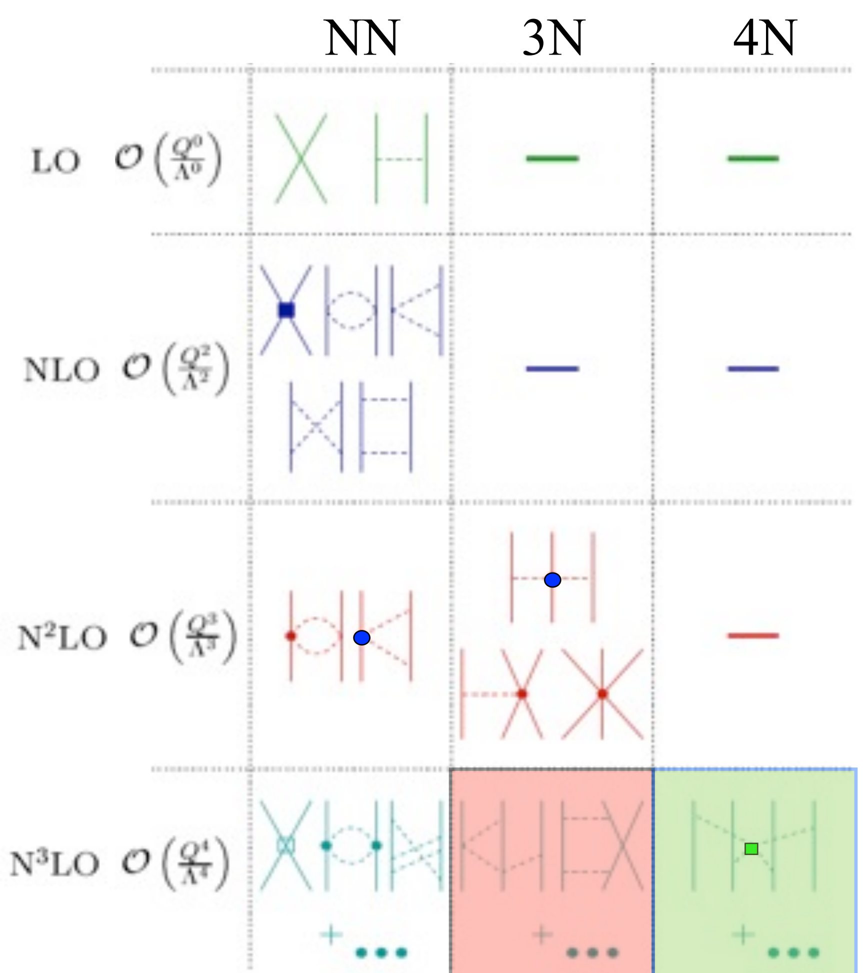
pion rings

1pi-contact

2pi-contact

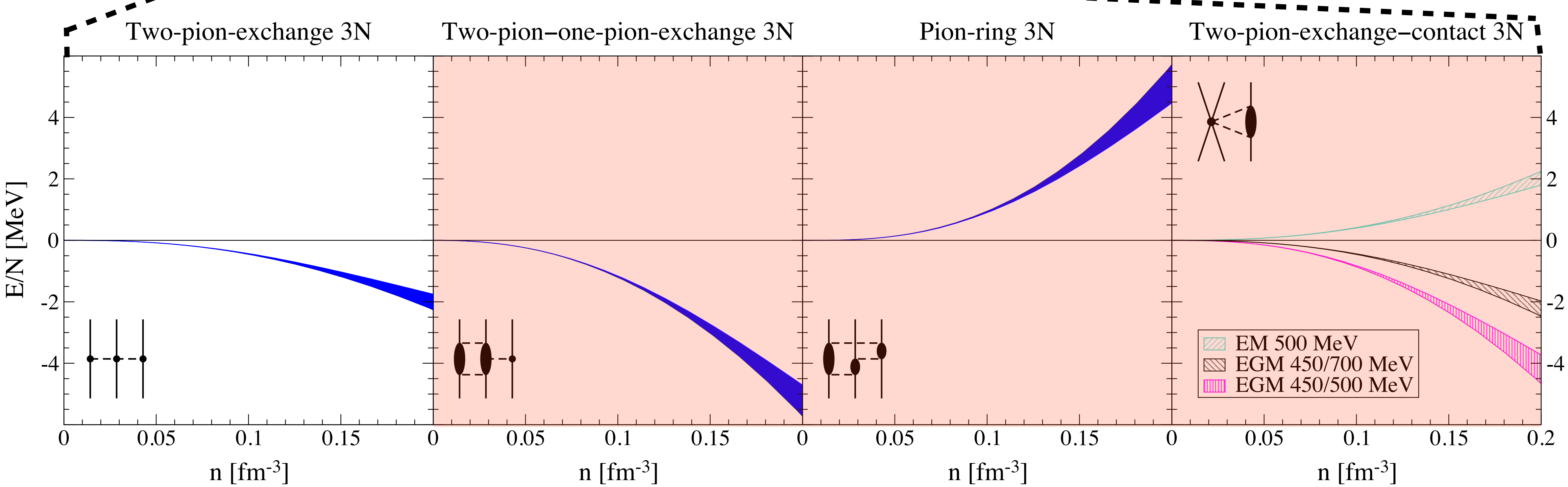
non-local, can also be calculated efficiently, stay tuned! rel. corrections

Contributions of many-body forces at N³LO in neutron matter



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

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



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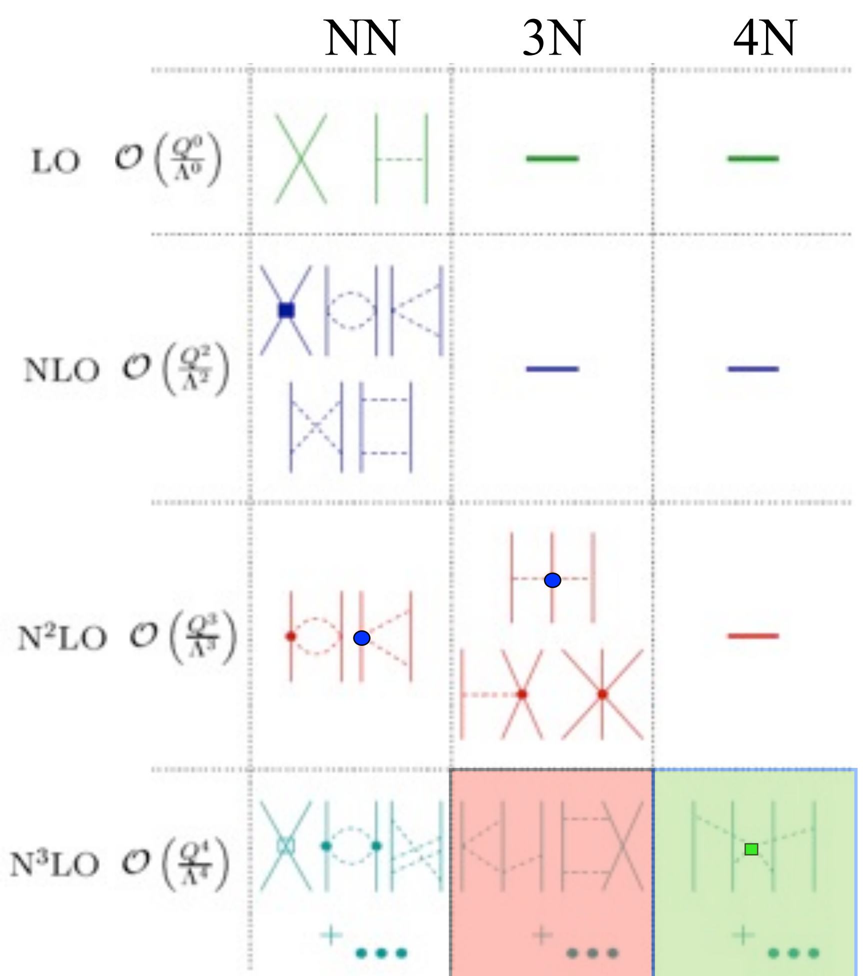

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- 4NF contributions small

Tews, Krueger, KH, Schwenk
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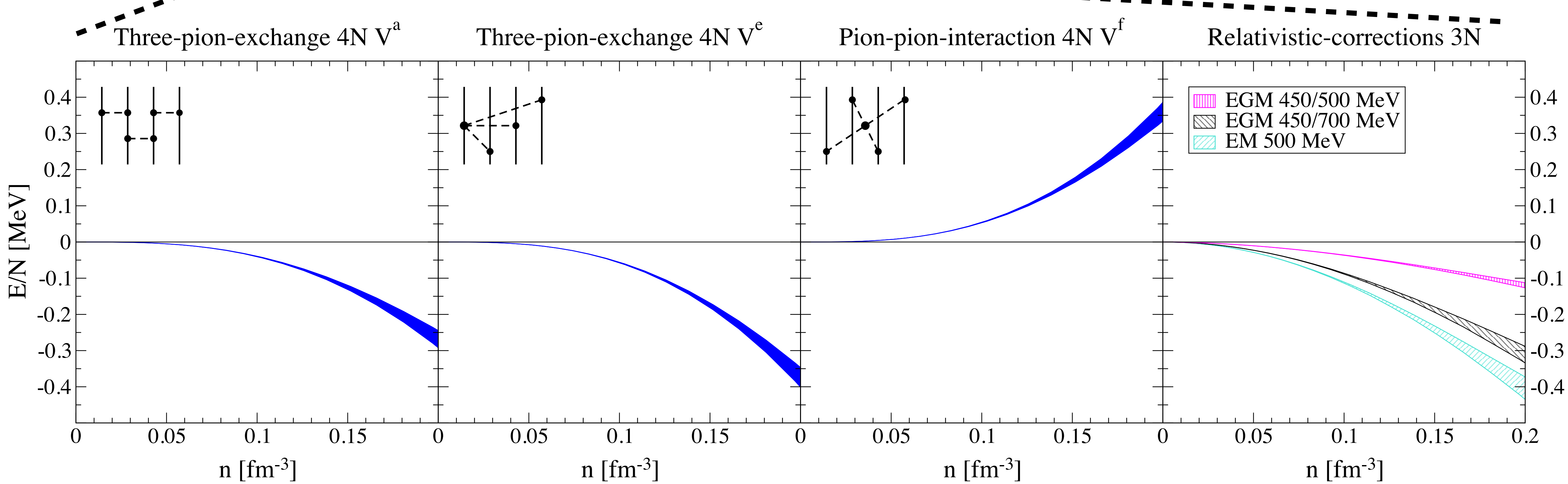
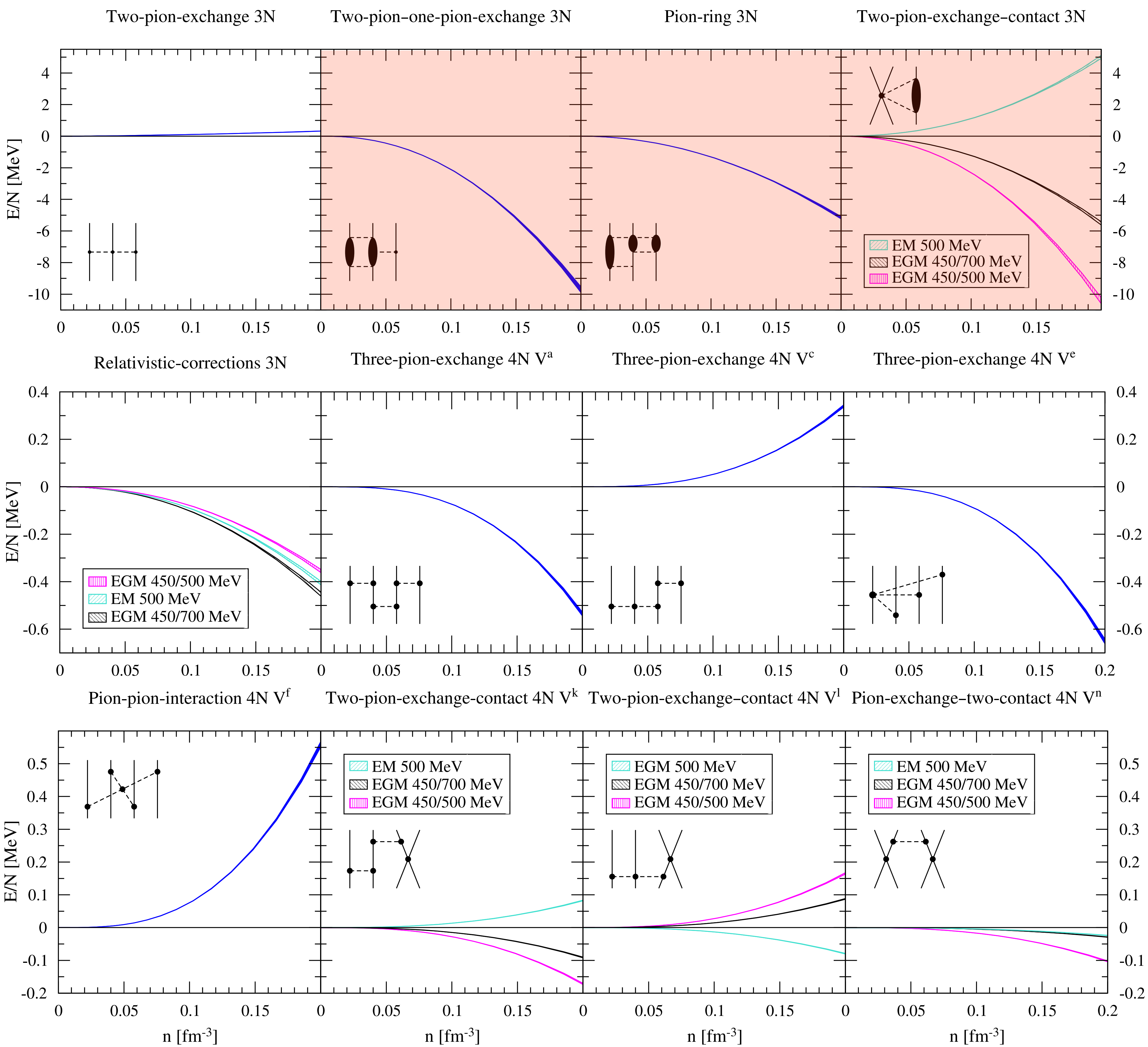
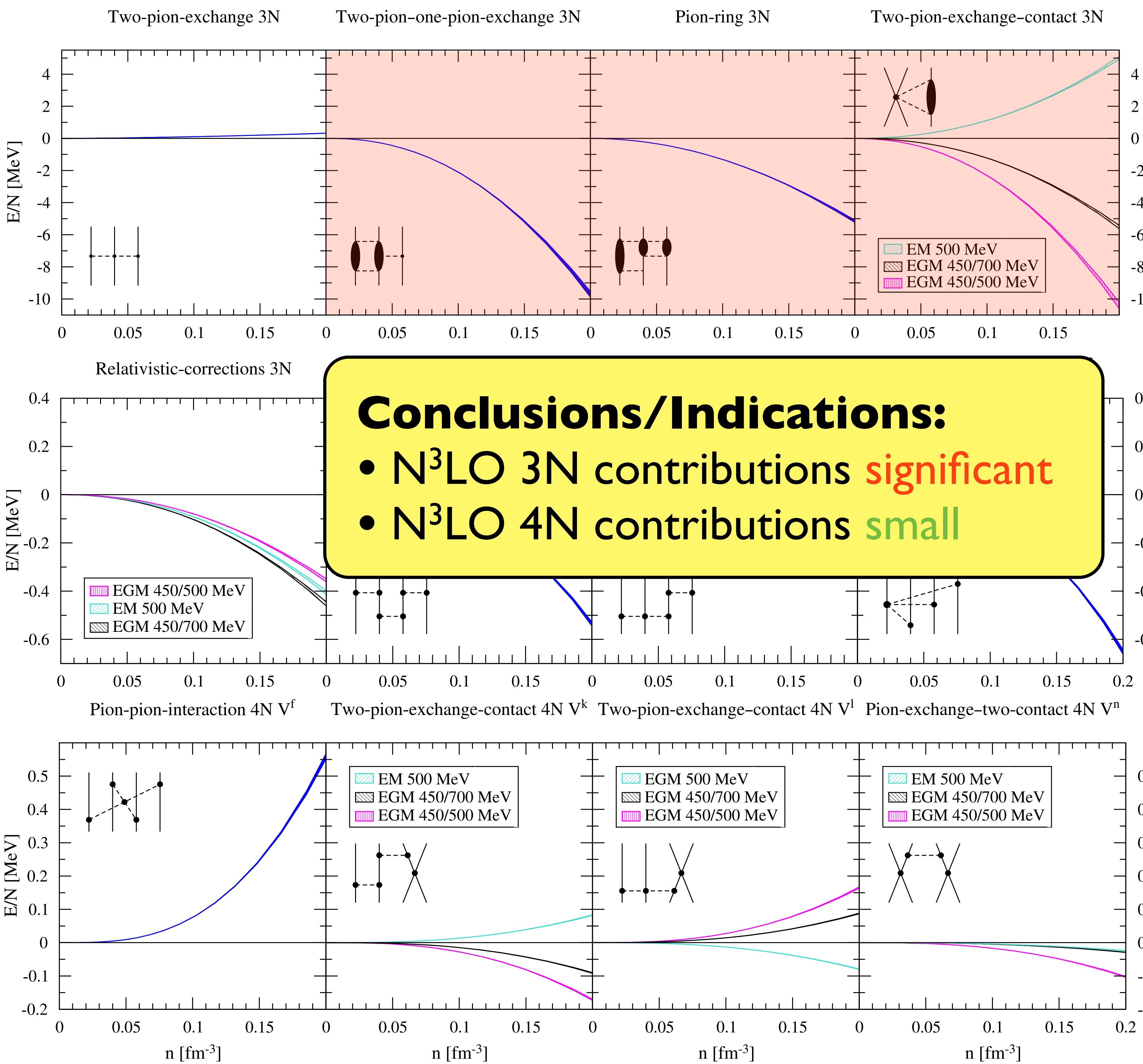


N^3LO contributions in nuclear matter (Hartree Fock)



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

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



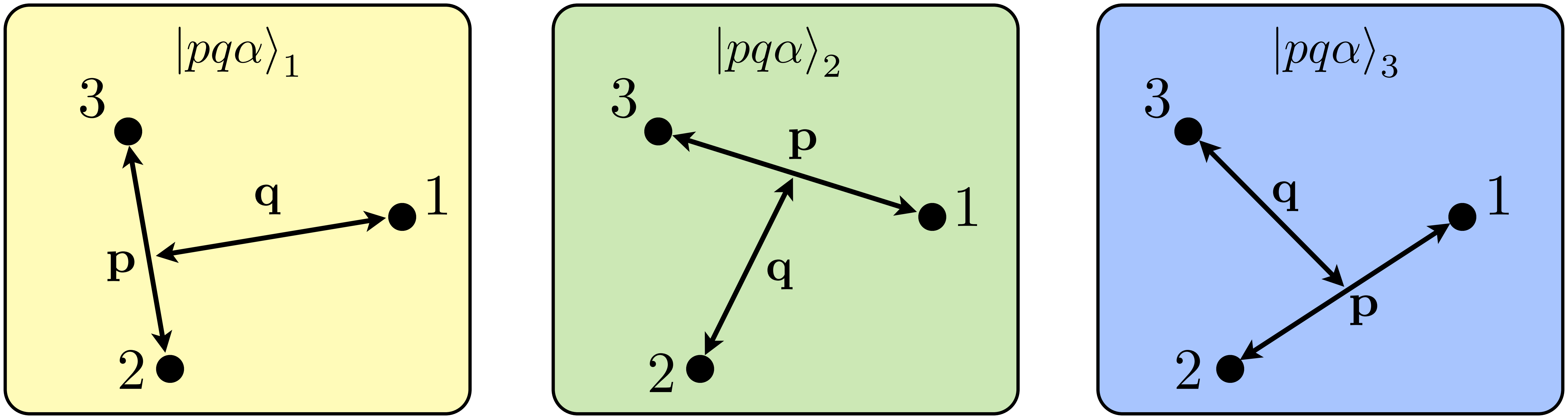
Conclusions/Indications:

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

Krueger, 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.

$$N_p \simeq N_q \simeq 15$$
$$N_\alpha \simeq 30 - 180$$

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

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

Calculation of 3N forces in partial-wave decomposed 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:

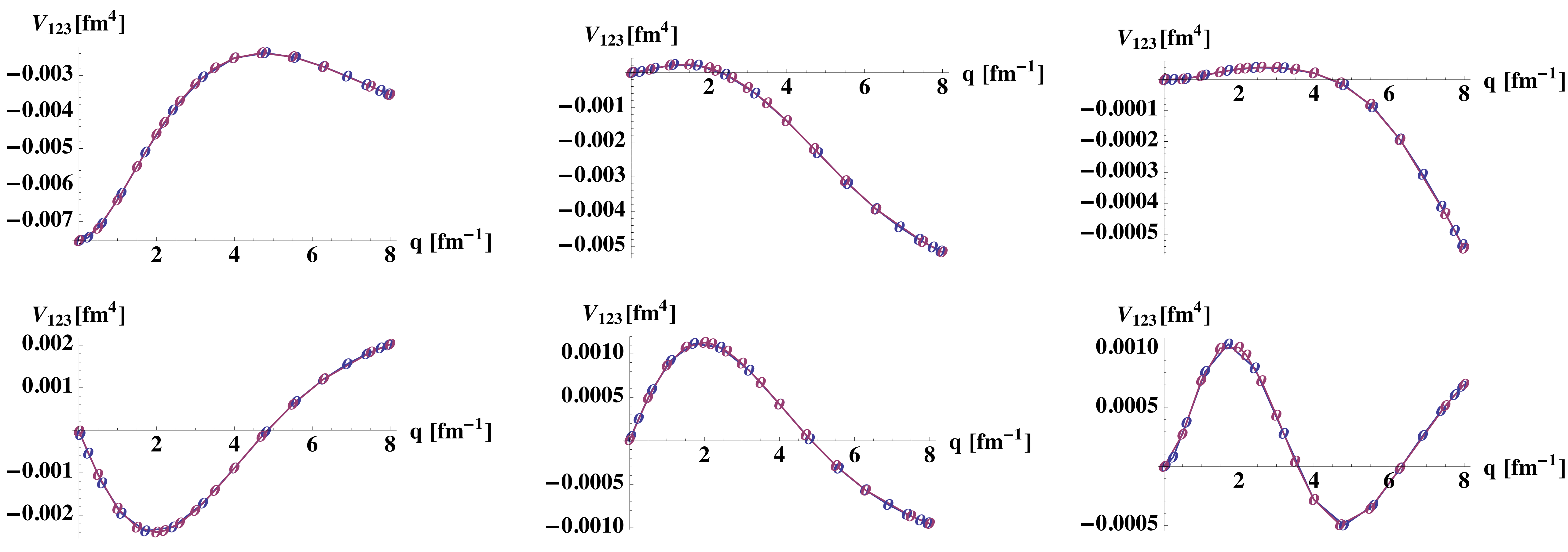
- use that all interaction contributions (except rel. corr.) are local:

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

$\longrightarrow$ allows to perform 3 integrals analytically

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

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



- **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

$$\langle pq\alpha | V^i_{123} | p'q'\alpha' \rangle$$

  as well as antisymmetrized matrix elements

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

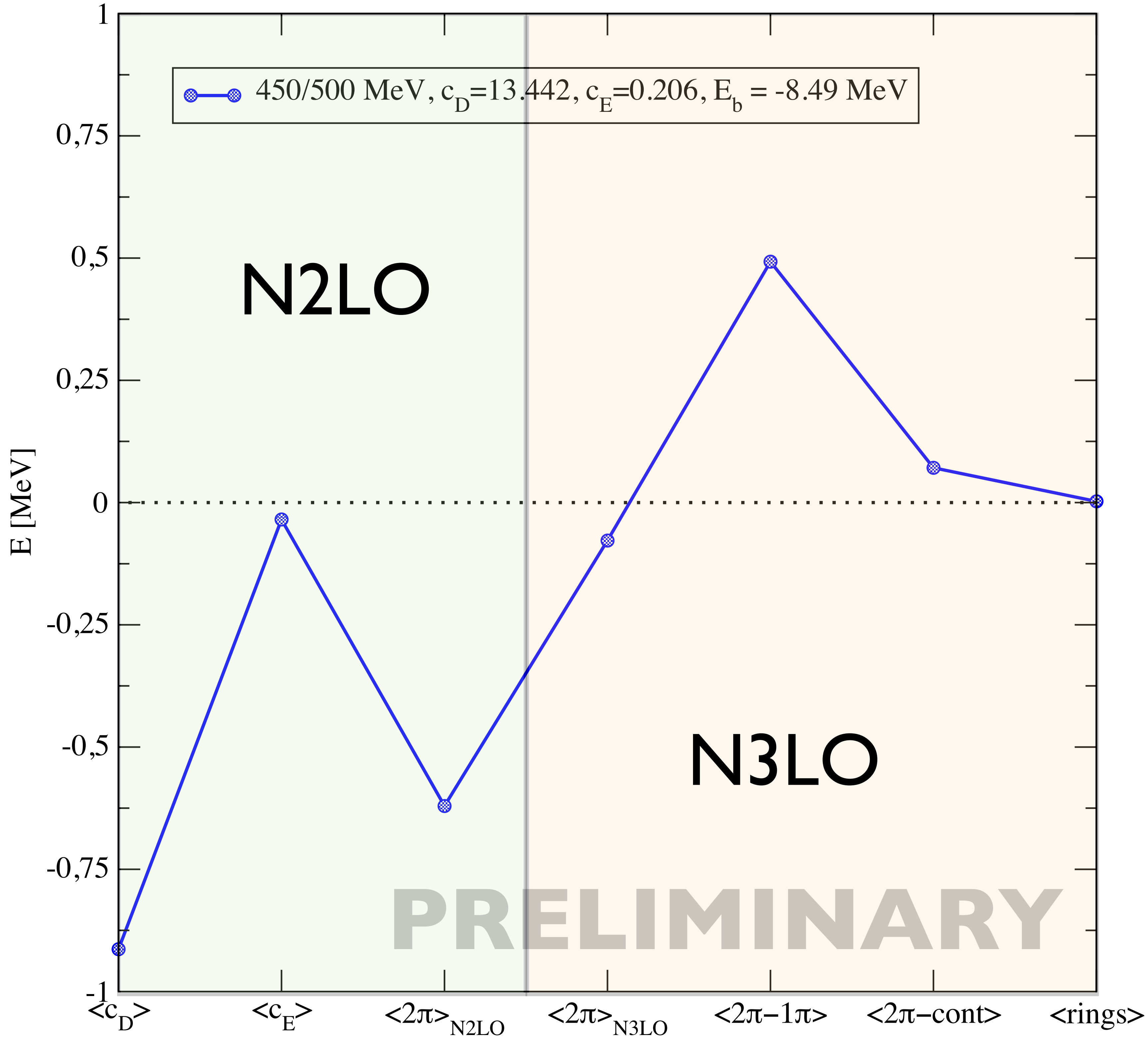
- HDF5 file format for efficient I/O

http://www.hdfgroup.org

- current model space limits: (all elements calculated on a single node of a local cluster at OSU)

$\mathcal{J}$	$\mathcal{T}$	J^{12}_{max}	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

Contributions of separate 3NFs in light nuclei: ^{3}H



see also Skibinski et al., Few-Body Syst. 54, 1315 (2013)

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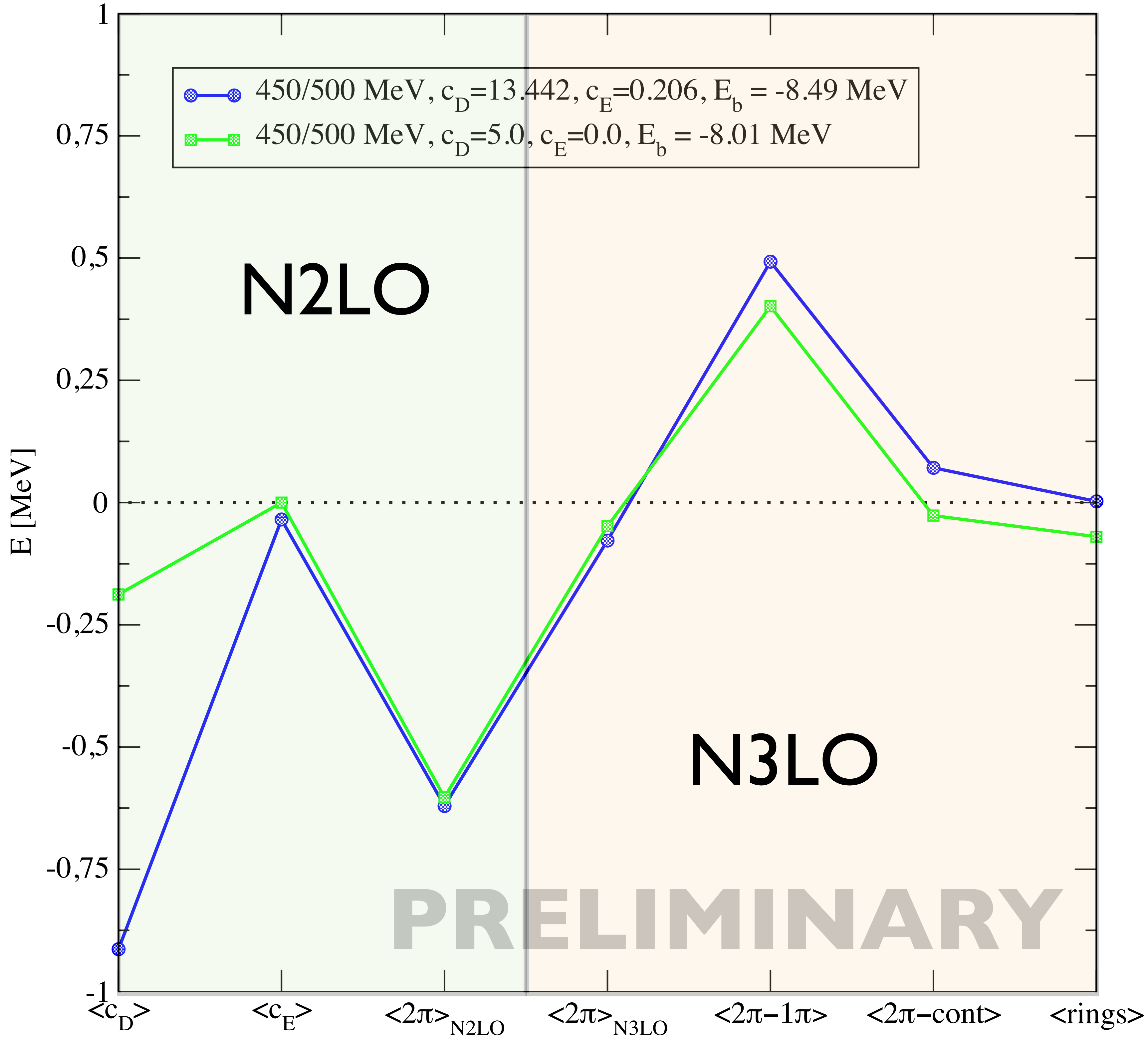

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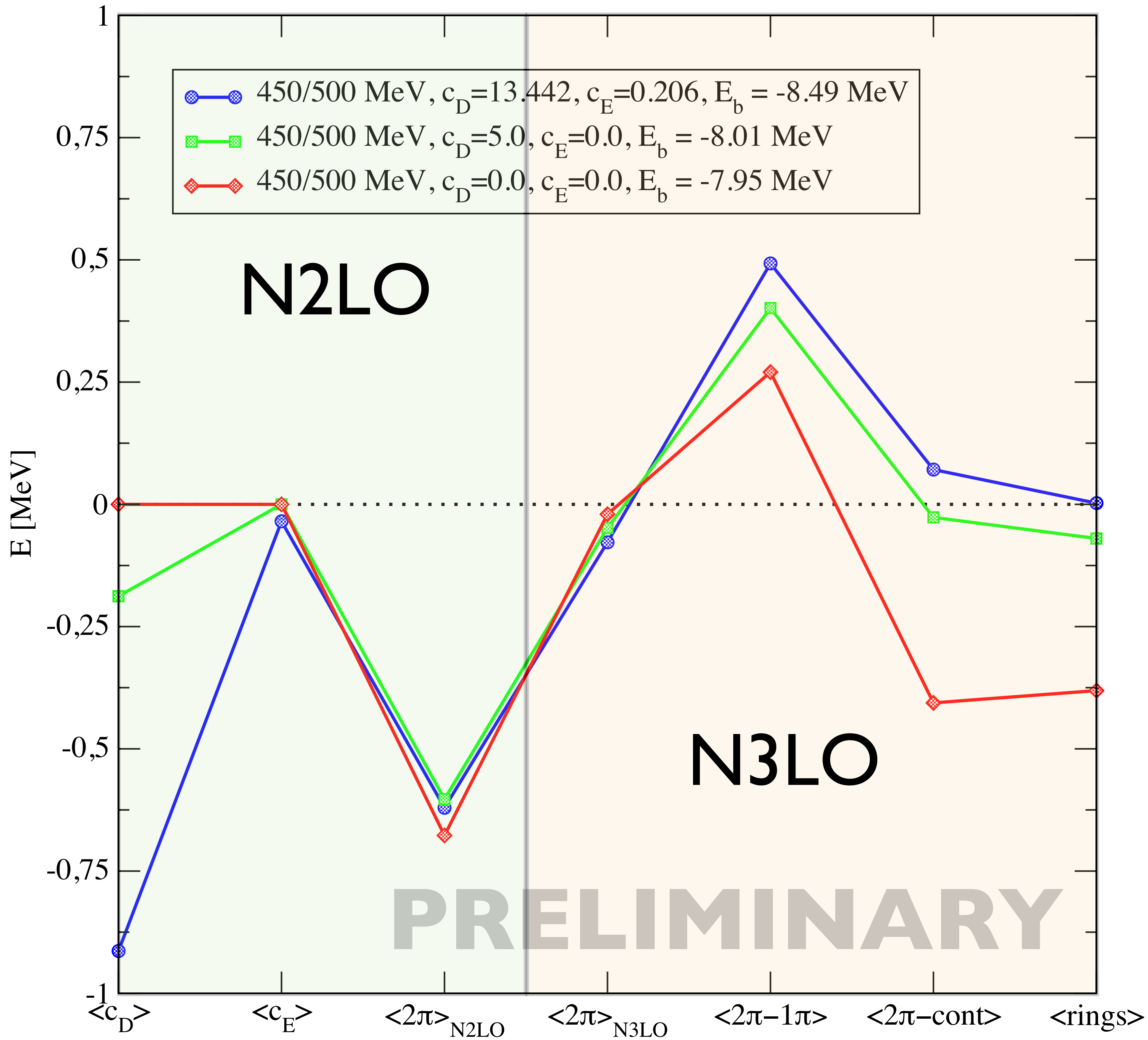

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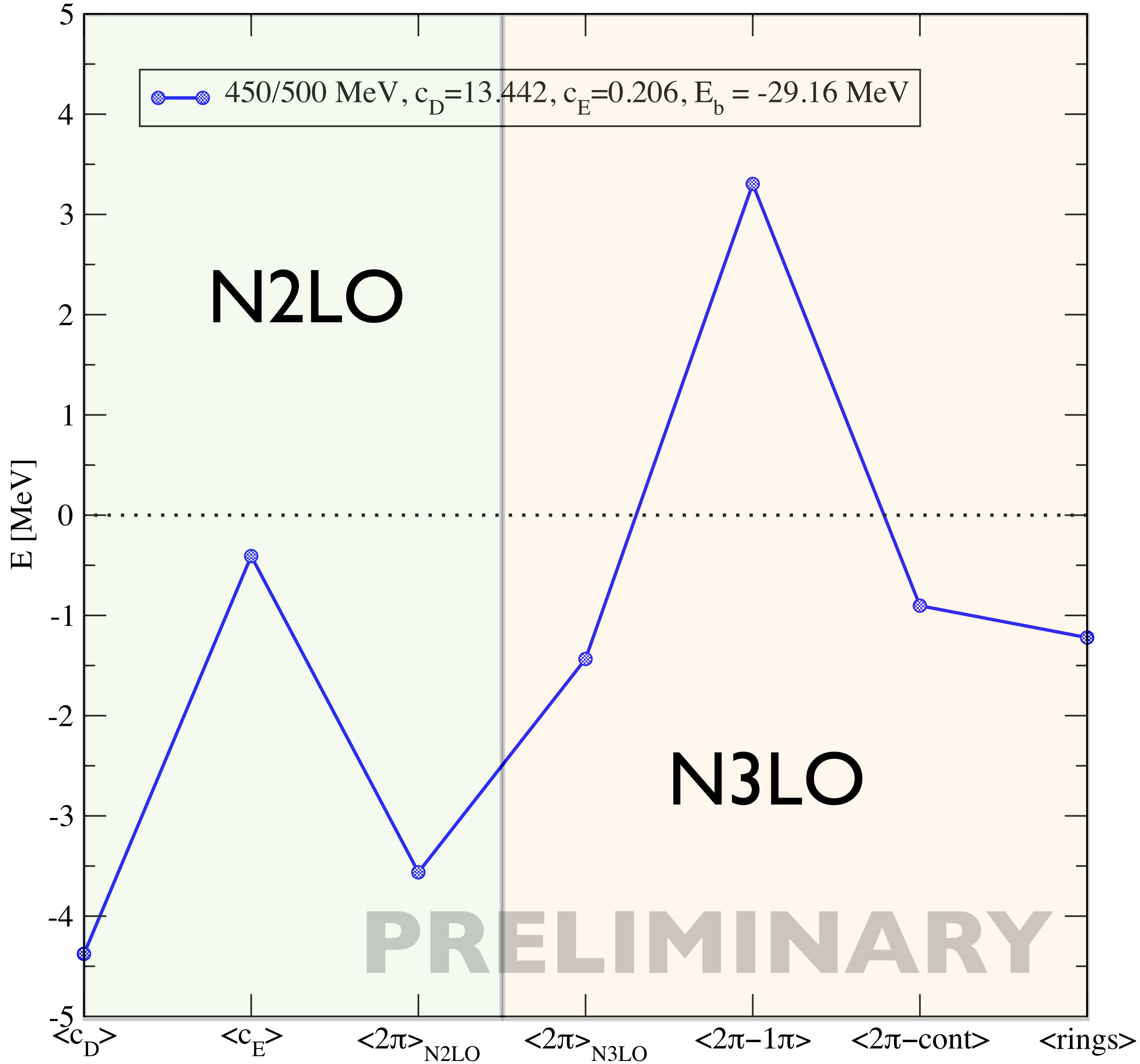


Applications of chiral 3N forces at N^{3}LO

Hyperspherical harmonics

Bacca (TRIUMF), Barnea (Hebrew U.),
Wendt (Oak Ridge)

Faddeev, Faddeev-Yakubovski

Nogga (Juelich), Witala (Kracow)

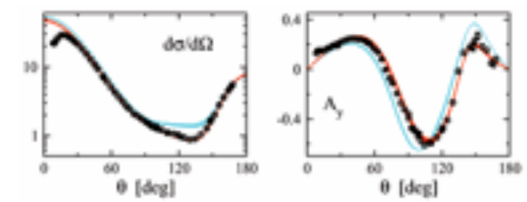


FIG. 4: Nd elastic observables at 65 MeV.

no-core shell model

Roth, Calci, Langhammer, Binder (TU Darmstadt)
Navratil (TRIUMF), Vary (Iowa)

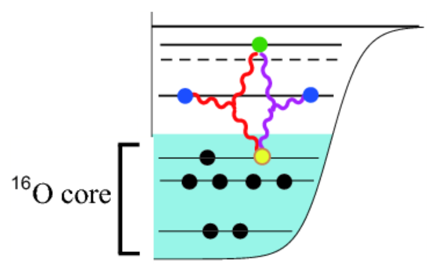
coupled cluster method

Ekstroem, Hagen, Papenbrock (Oak Ridge)
Binder, Roth (TU Darmstadt)

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

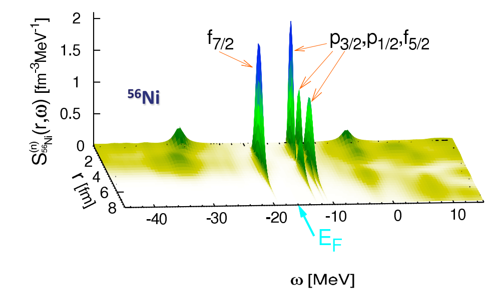
valence shell model

Holt, Menendez, Schwenk
(TU Darmstadt)

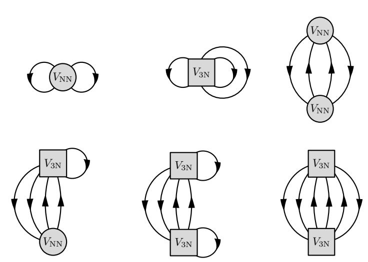


Self-consistent Greens function

Barbieri (Surrey), Soma (TU Darmstadt)

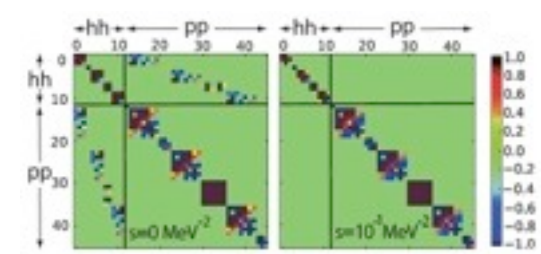


Many-body perturbation theory



In-medium SRG

Bogner (MSU), Hergert (OSU)



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

Inclusion of chiral 3N forces in many-body frameworks

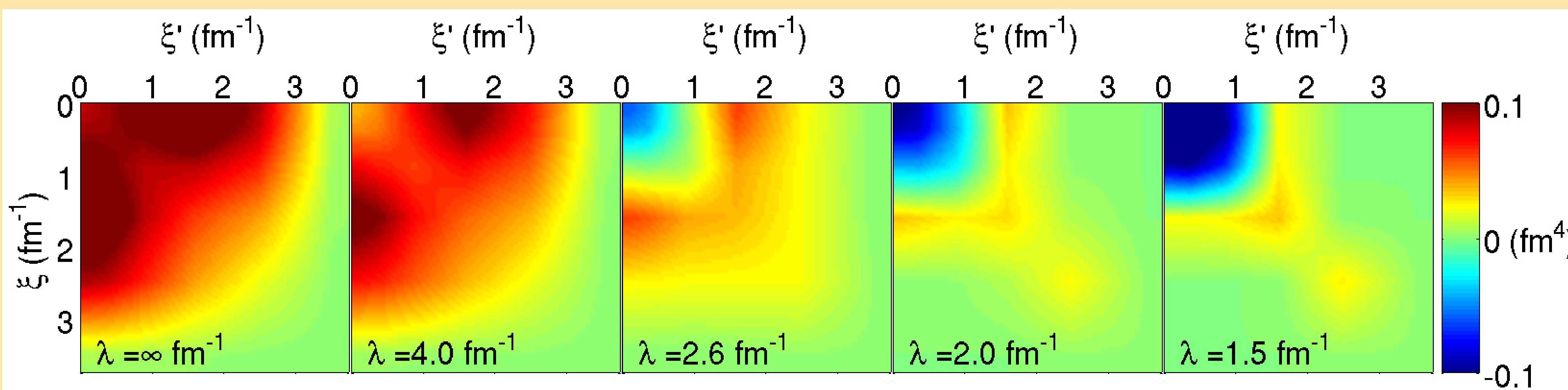
Problem:

Basis size for converged results of ab initio calculations including 3N forces grows rapidly with the number of particles.
Calculations limited to light nuclei.

Use SRG transformations to **decouple** low- and high momentum states.
Required basis size decreases drastically.

⟶ *see also talks by Angelo Calci and Kyle Wendt*

Implementation of SRG evolution of 3NF in a momentum basis:

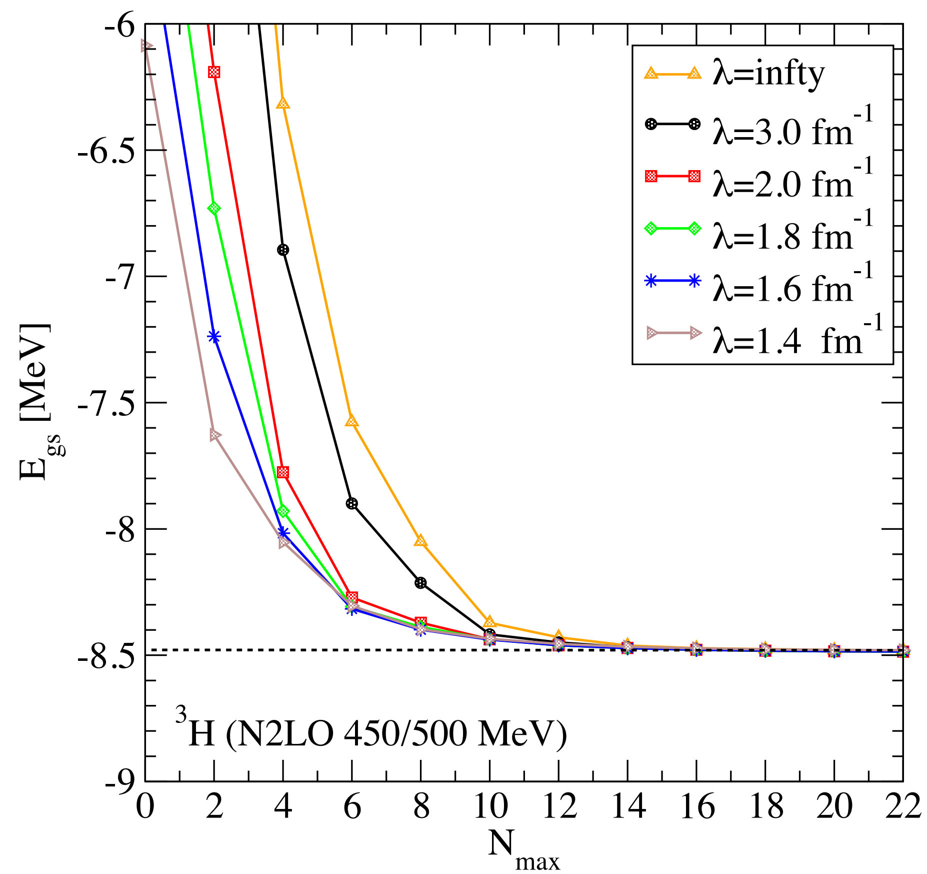


Hebeler PRC(R) 85, 021002 (2012)

Inclusion of chiral 3N forces in many-body frameworks

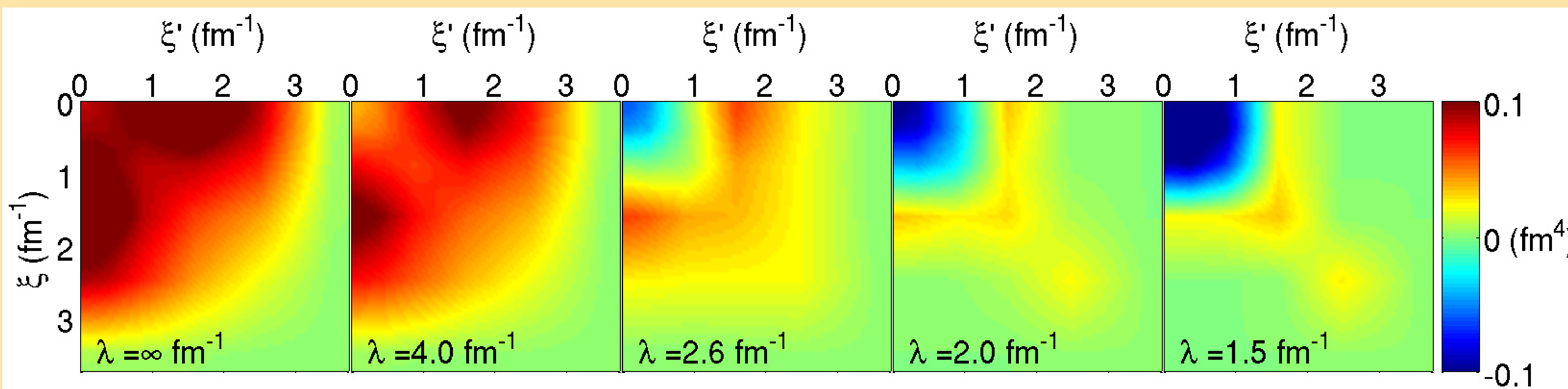
Basis size for conve… …tions including
3N forces gro… …particles.
Calc…

Transformation to HO basis:



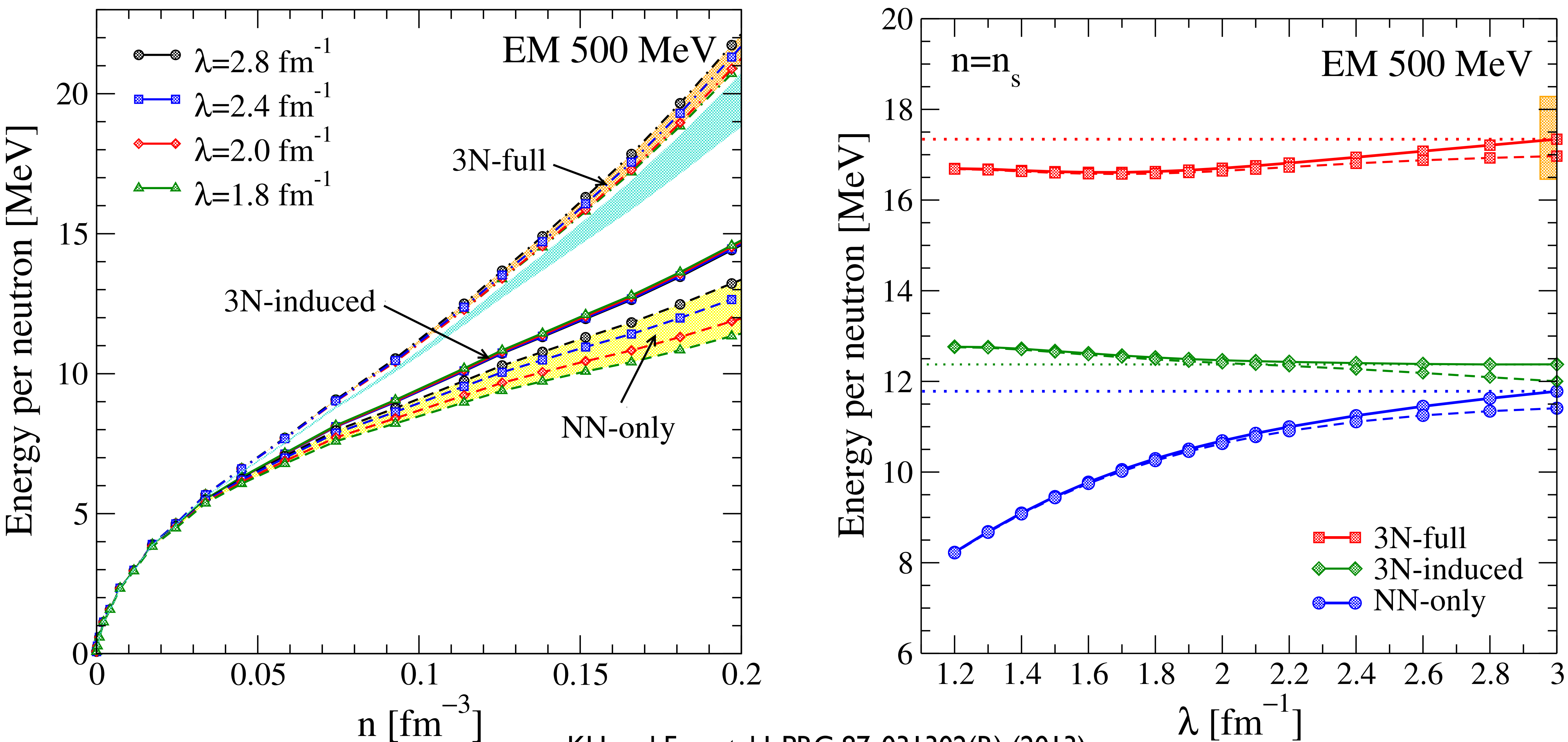
Use SRG transformati… …gh momentum states.
Requ… …cally.

Implementation … …omentum basis:



Hebeler PRC(R) 85, 021002 (2012)

Results for neutron matter based on consistently evolved forces (N2LO)



KH and Furnstahl, PRC 87, 031302(R) (2013)

- so far 3NF treated in Hartree-Fock approximation
- no indications for unnaturally large 4N force contributions

Ab initio nuclear structure calculations: Current developments and future directions

- application to finite nuclei and infinite matter
  - equation of state
  - systematic study of induced many-body contributions, scaling behavior
  - include initial N3LO 3N interactions, study power counting
    (delta-full EFT, N4LO, incorporation and calculation of consistent currents)

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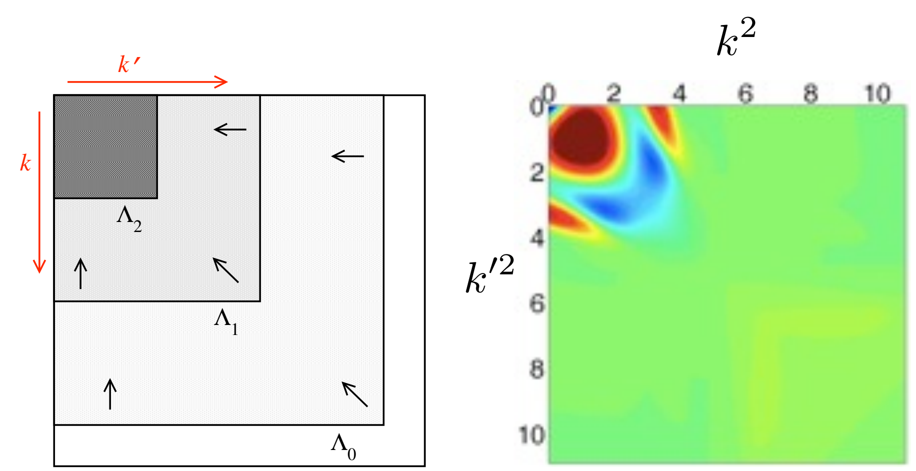
- study of various generators
  - different decoupling patterns (e.g. $V_{\text{low } k}$)
  - improved efficiency of evolution
  - suppression of many-body forces?



Anderson et al., PRC 77, 037001 (2008)

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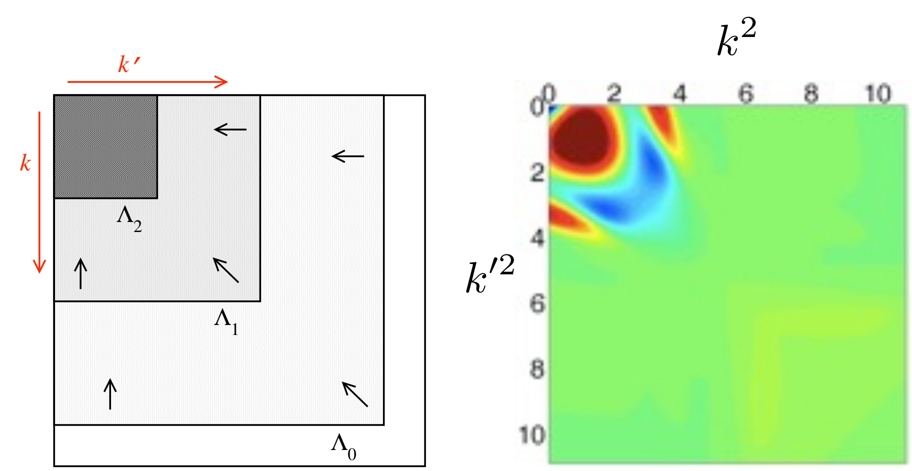


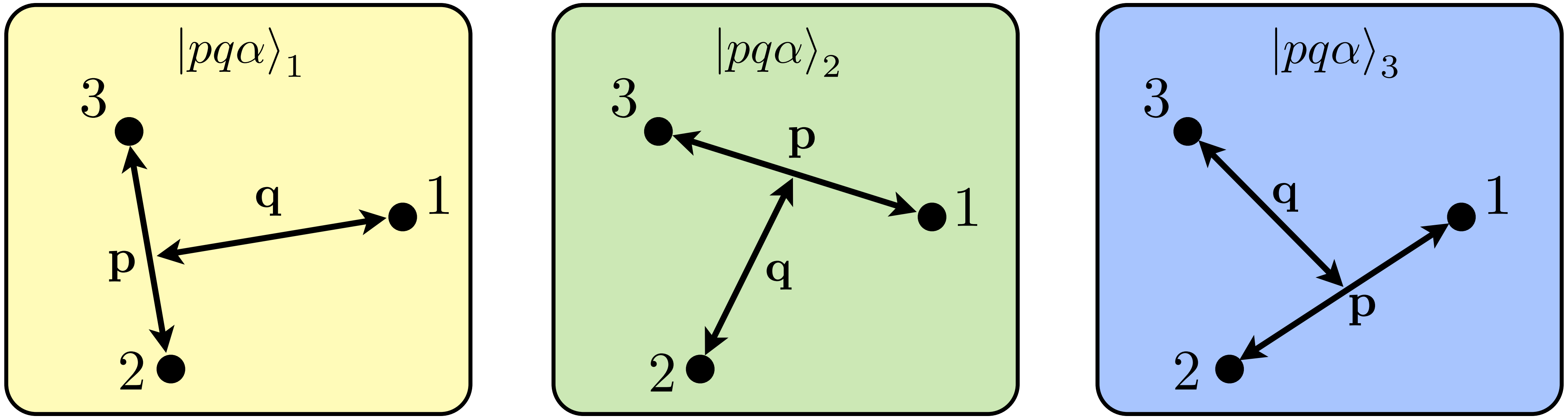
Anderson et al., PRC 77, 037001 (2008)

- explicit calculation of unitary transformation
  - RG evolution of operators
  - study of correlations in nuclear systems, 'factorization'

  ⟶ see talk by Dick Furnstahl

Thank you!

RG evolution of 3N interactions in momentum space

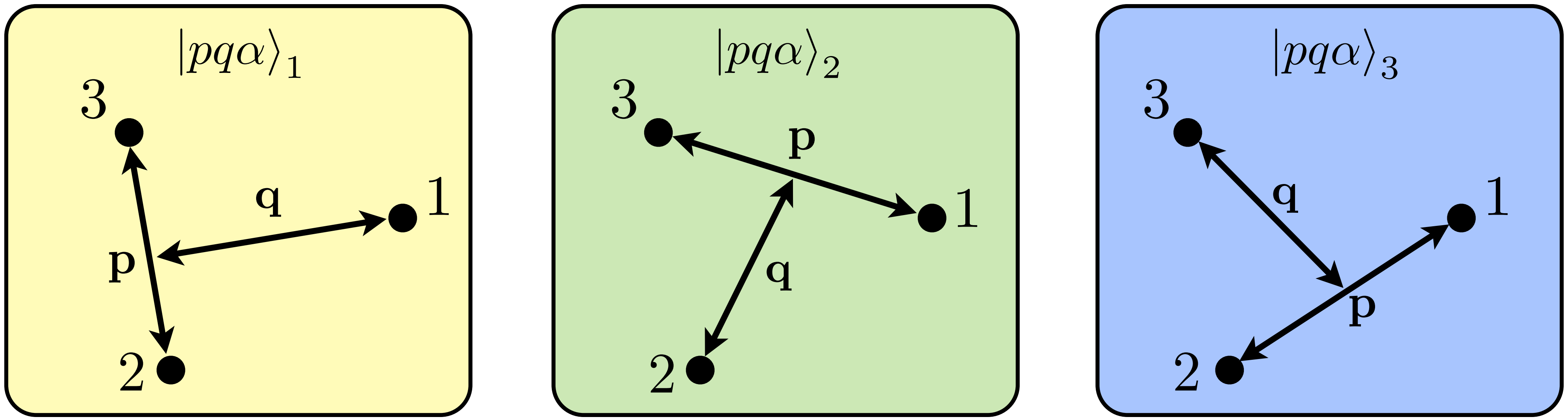


- represent interaction in basis $|pq\alpha\rangle_i \equiv |p_i q_i; [(LS)J(ls_i)j]\,\mathcal{J}\mathcal{J}_z(Tt_i)\mathcal{T}\mathcal{T}_z\rangle$
- explicit equations for NN and 3N flow equations

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

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

RG evolution of 3N interactions in momentum space



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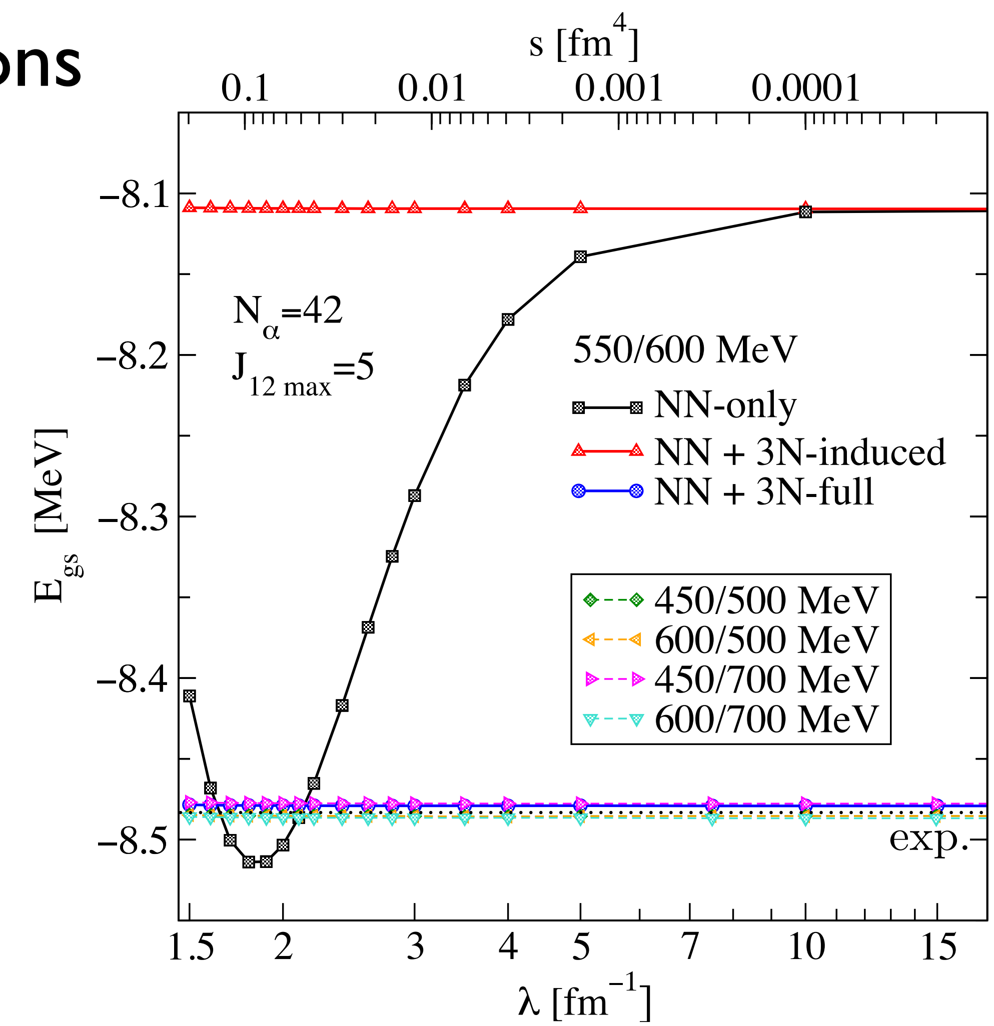


Hebeler PRC(R) 85, 021002 (2012)

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

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

- 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

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

- embed NN interaction in 3N basis:

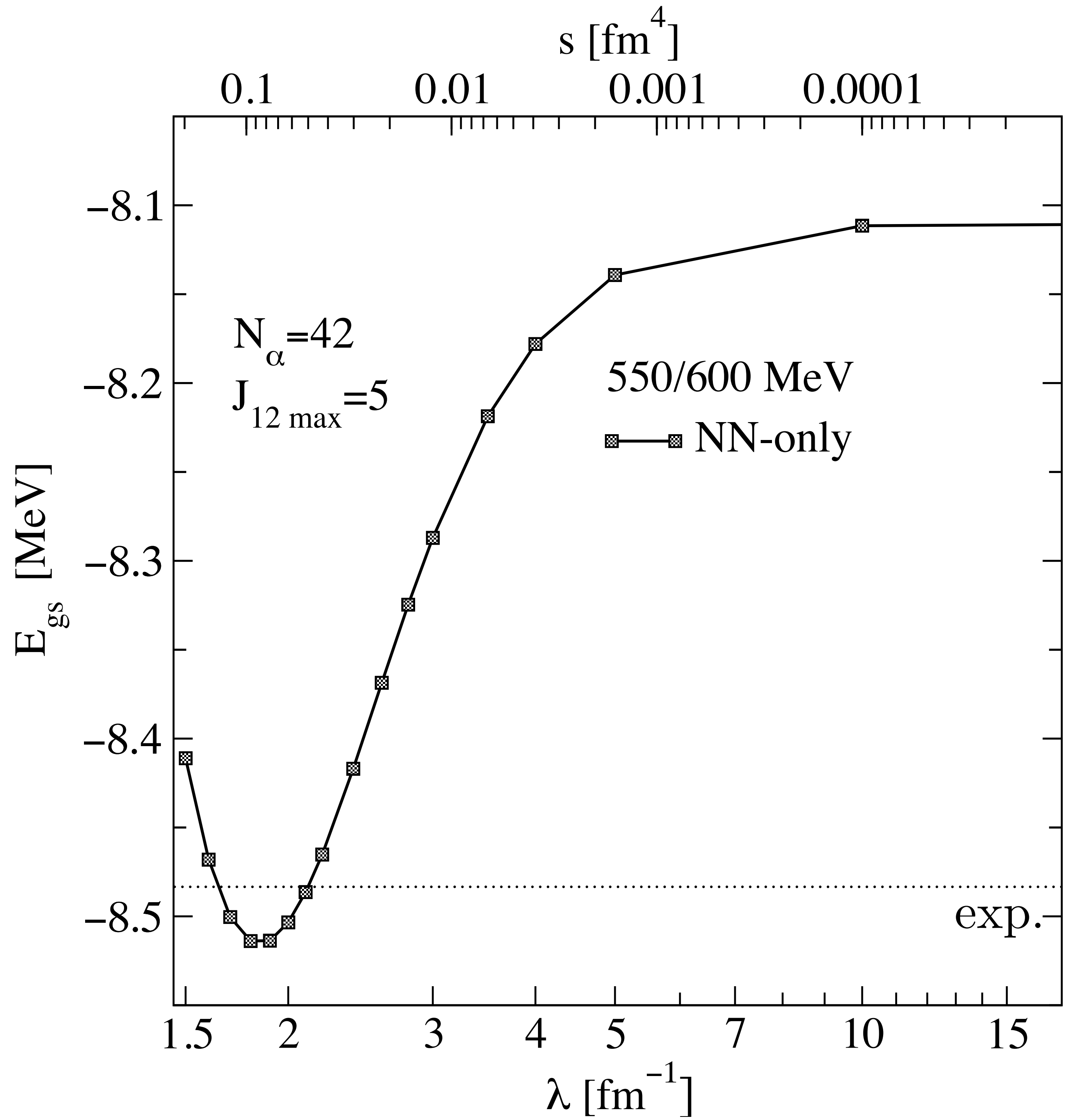
$$V_{13} = P_{123}V_{12}P_{132}, \quad V_{23} = P_{132}V_{12}P_{123}$$

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

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

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

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



Hebeler PRC(R) 85, 021002 (2012)

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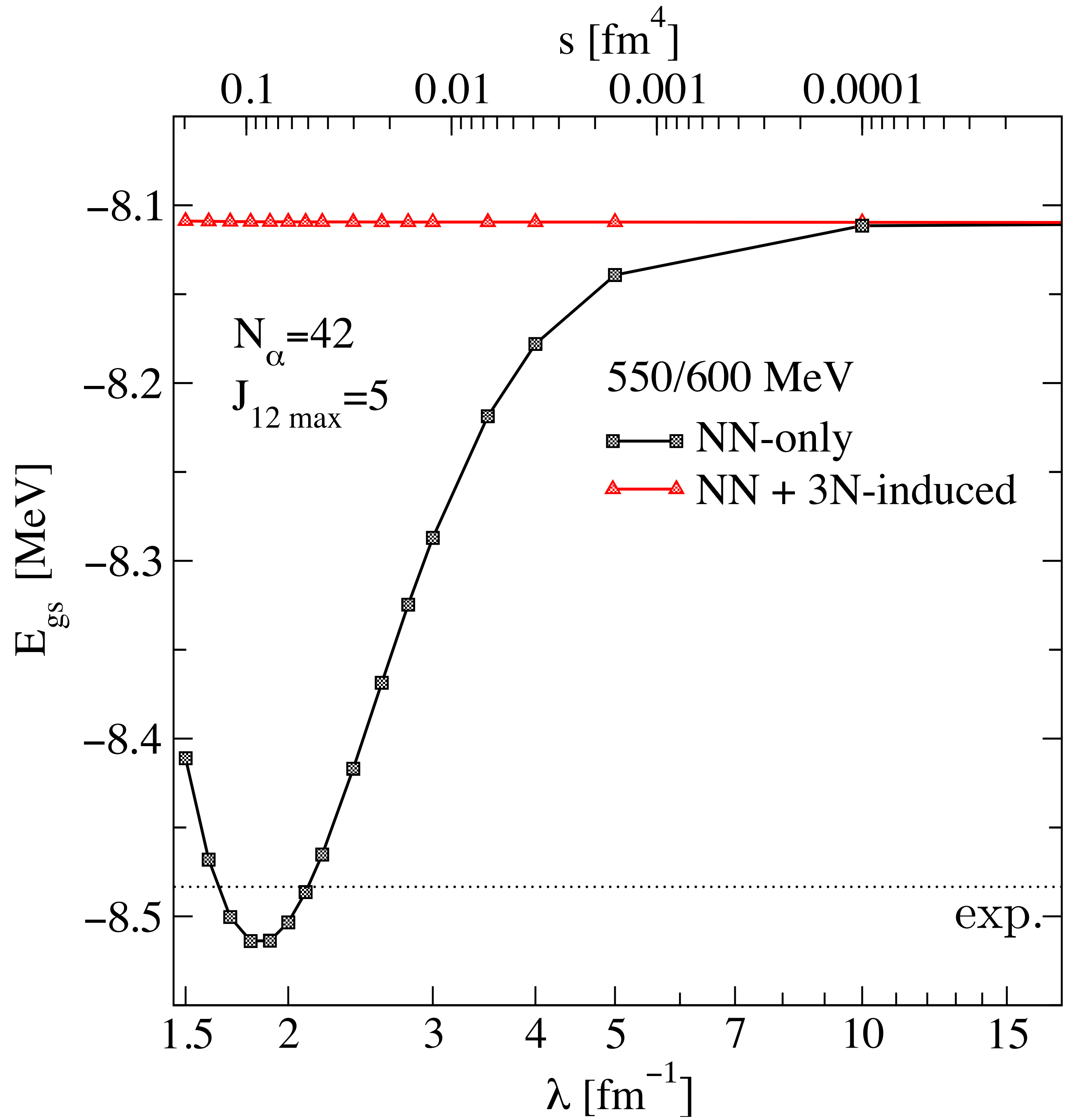

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It works:

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

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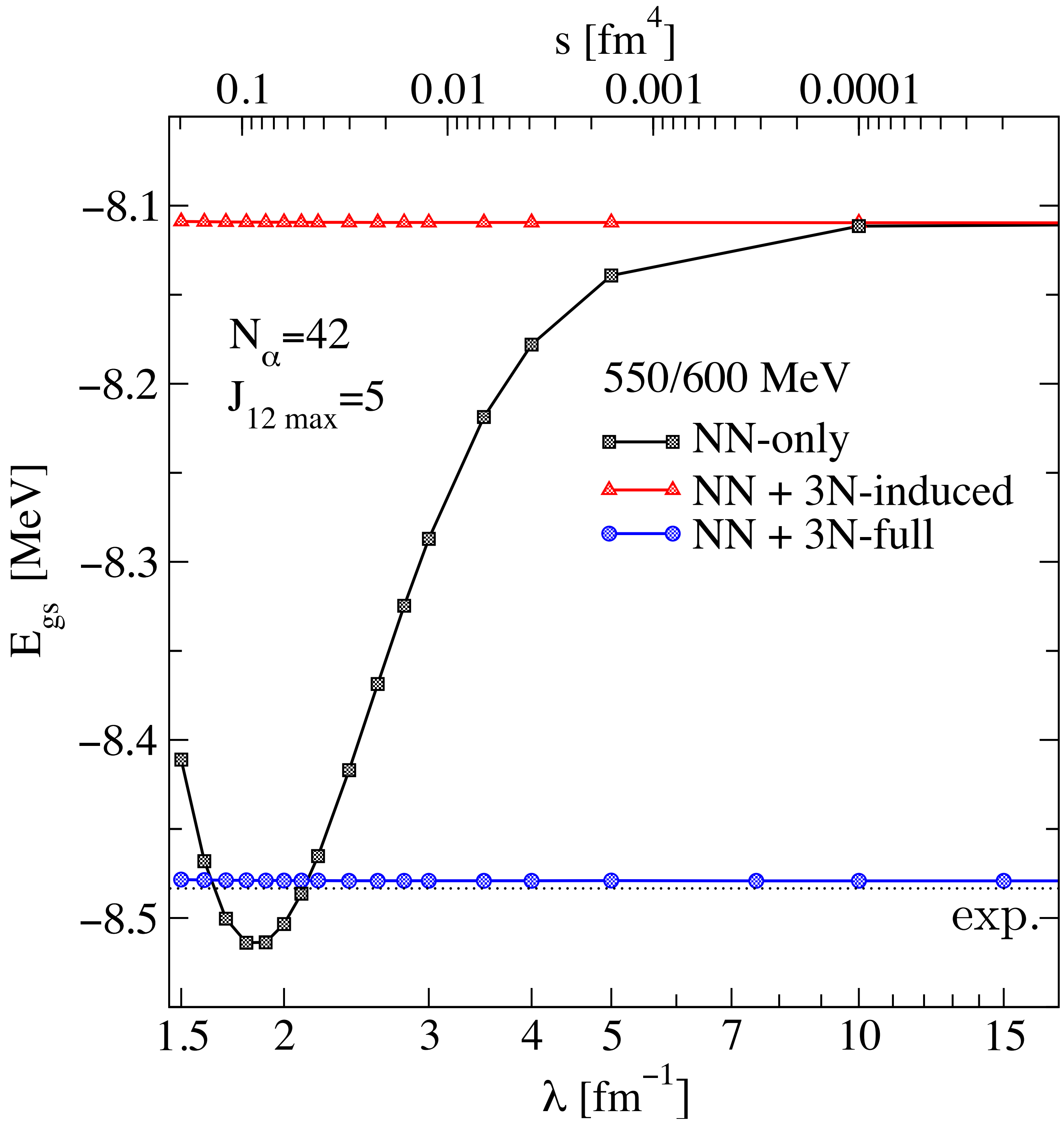

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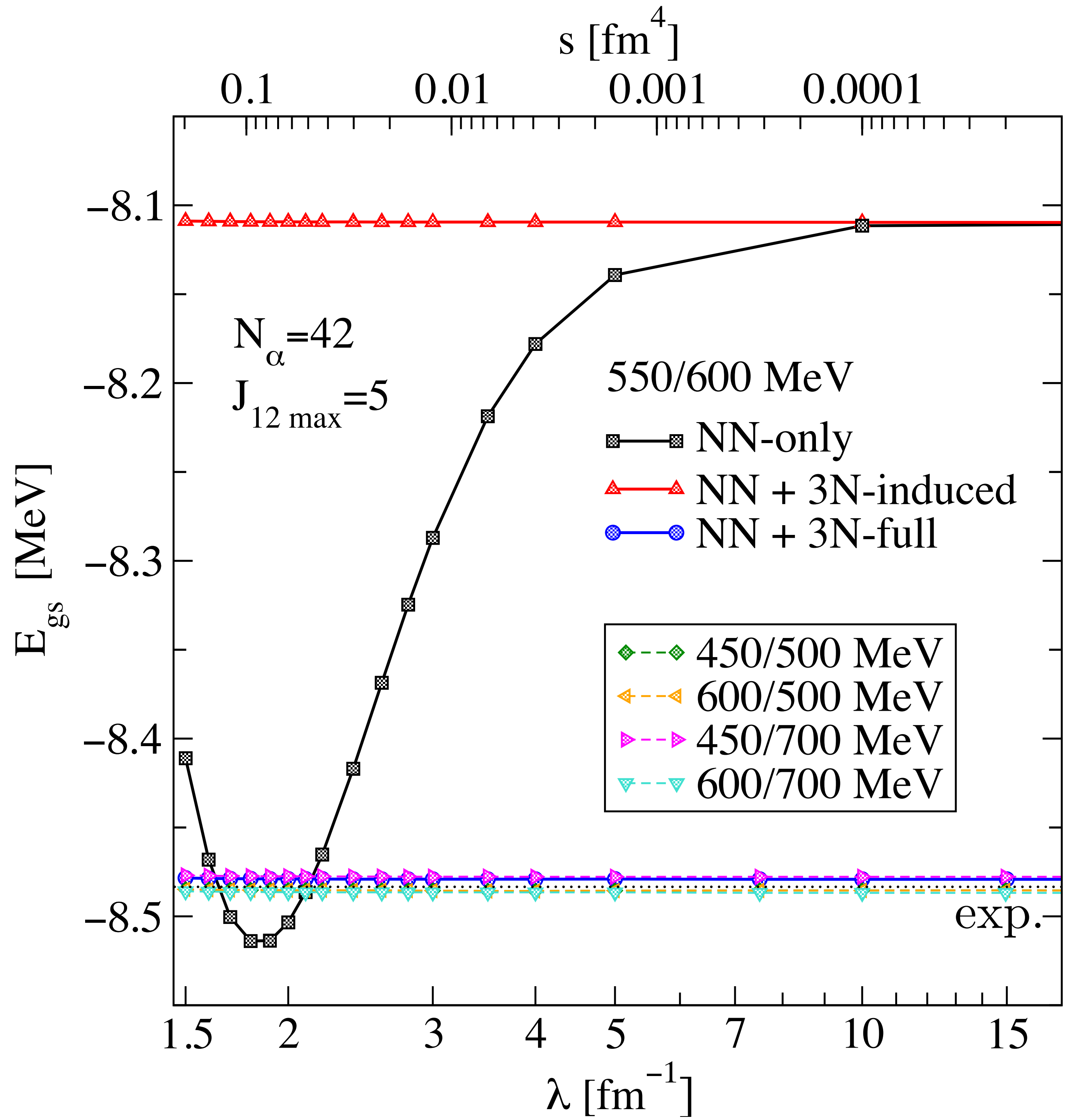

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