Calculation of semi-local 3N interactions and first results up to N^3LO

Kai Hebeler

Vancouver, February 23, 2016

TRIUMF workshop on
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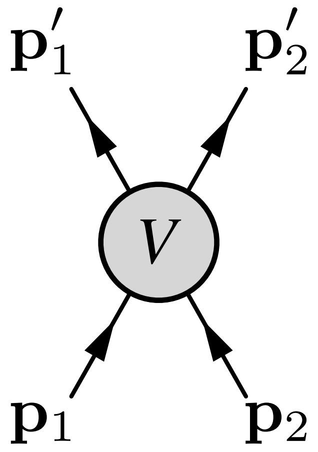
European Research Council
Established by the European Commission

In collaboration with:
Alex Dydalo, Dick Furnstahl, Ingo Tews and LENPIC

Regularization schemes for NN interactions

Separation of long- and short-range physics



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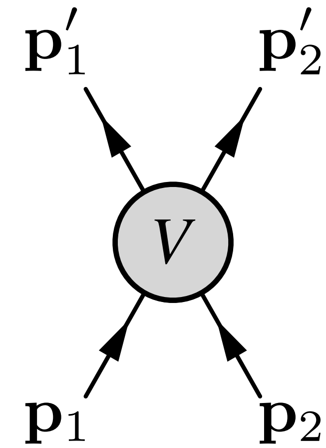

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nonlocal

$$V_{\mathrm{NN}}(\mathbf{p}, \mathbf{p}') \to \exp\left[-\left((p^2 + p'^2)/\Lambda^2\right)^n\right] V_{\mathrm{NN}}(\mathbf{p}, \mathbf{p}')$$

Epelbaum, Glöckle, Meissner, NPA 747, 362 (2005)
Entem, Machleidt, PRC 68, 041001 (2003)

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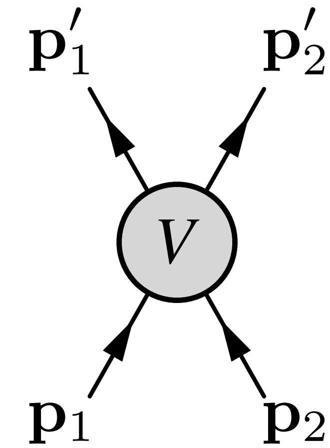

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local (momentum space)

$$V_{\mathrm{NN}}(\mathbf{q}) \rightarrow \exp\left[-\left(q^2/\Lambda^2\right)^n\right] V_{\mathrm{NN}}(\mathbf{q})$$

cf. Navratil, Few-body Systems 41, 117 (2007)

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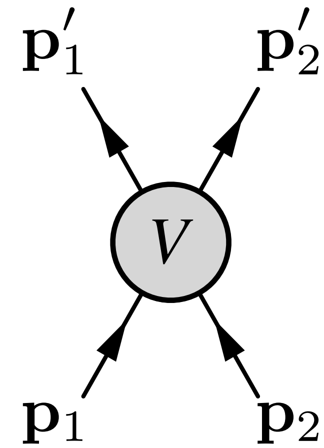

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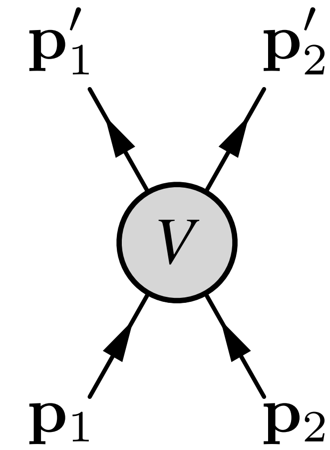
local (coordinate space)

$$V_{\mathrm{NN}}^{\pi}(\mathbf{r}) \to \left(1 - \exp\left[-\left(r^2/R^2\right)^n\right]\right) V_{\mathrm{NN}}^{\pi}(\mathbf{r})$$
$$\delta(\mathbf{r}) \to \alpha_n \exp\left[-(r^2/R^2)^n\right]$$

Gezerlis et. al, PRL, 111, 032501 (2013)

Regularization schemes for NN interactions

Separation of long- and short-range physics



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$$V_{\rm NN}(\mathbf{p}, \mathbf{p}') \to \exp\left[- \left((p^2 + p'^2)/\Lambda^2\right)^n\right] V_{\rm NN}(\mathbf{p}, \mathbf{p}')$$

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semi-local

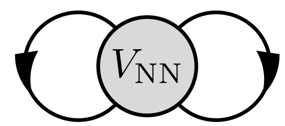
$$V_{\rm NN}^{\pi}(\mathbf{r}) \to \left(1 - \exp\left[- \left(r^2/R^2\right)\right]\right)^n V_{\rm NN}^{\pi}(\mathbf{r})$$
$$\delta(\mathbf{r}) \to C \to \exp\left[- \left((p^2 + p'^2)/\Lambda^2\right)^n\right] C$$

Epelbaum et. al, PRL, 115, 122301 (2015)

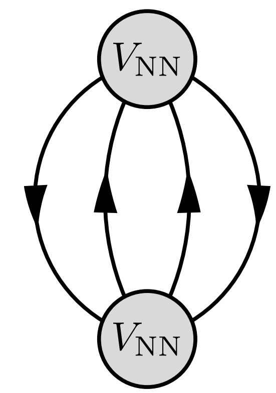
Regulator effects in nuclear matter

Nuclear matter is a clean laboratory to study regulator effects of regulator on the infrared and ultraviolet phase space

Energy per particle:



HF:
IR phase space



2nd order:
IR+UV phase space

Dydalo, Furnstahl, KH, Tews, in preparation

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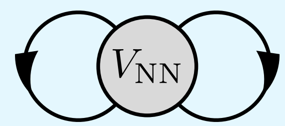

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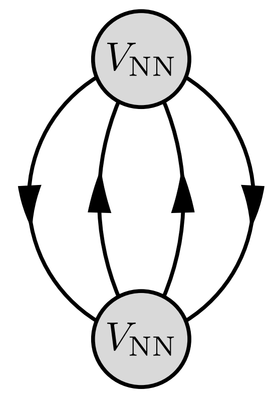

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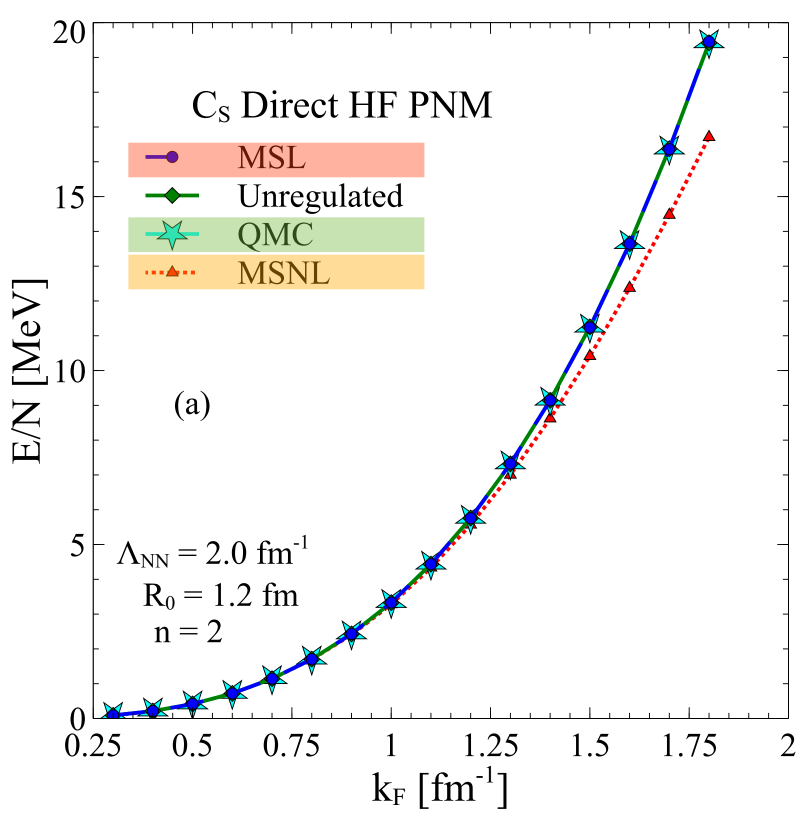

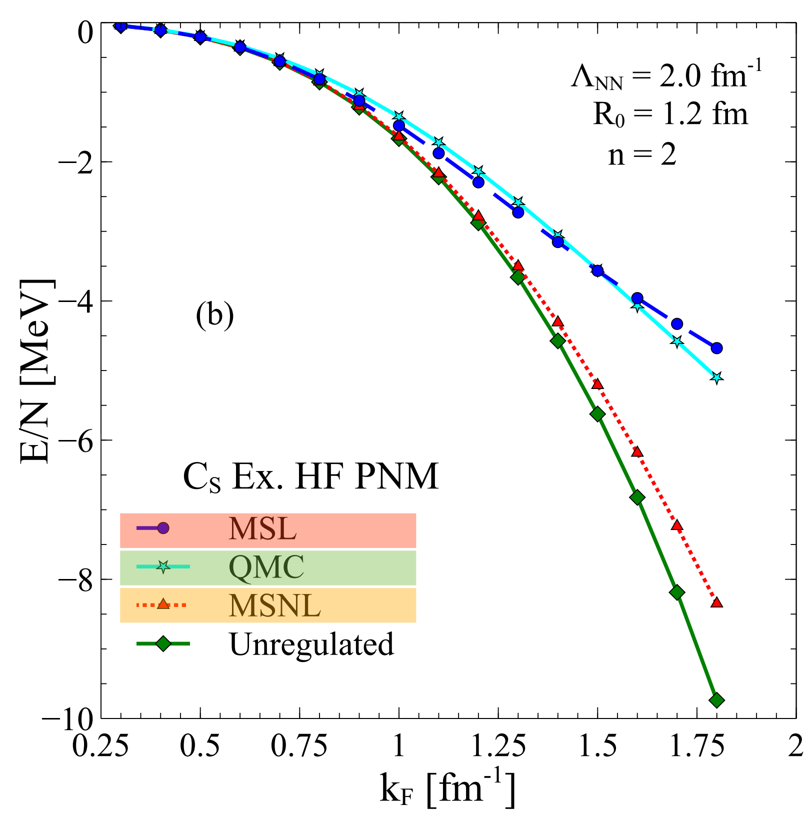

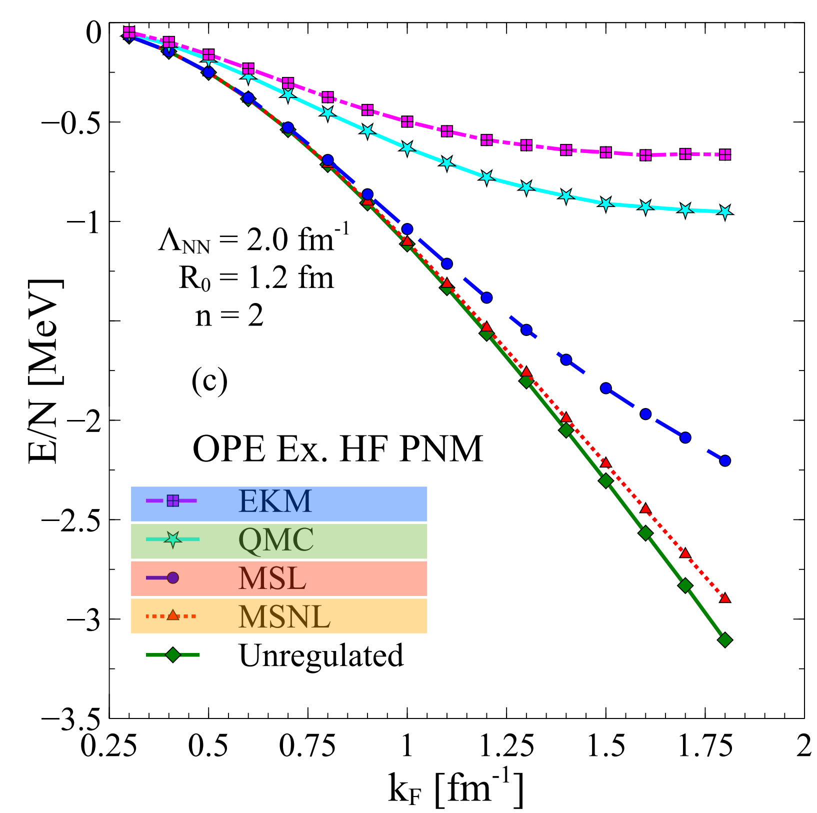

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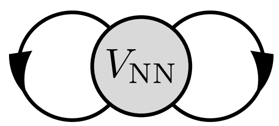

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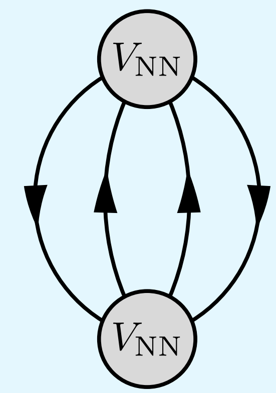

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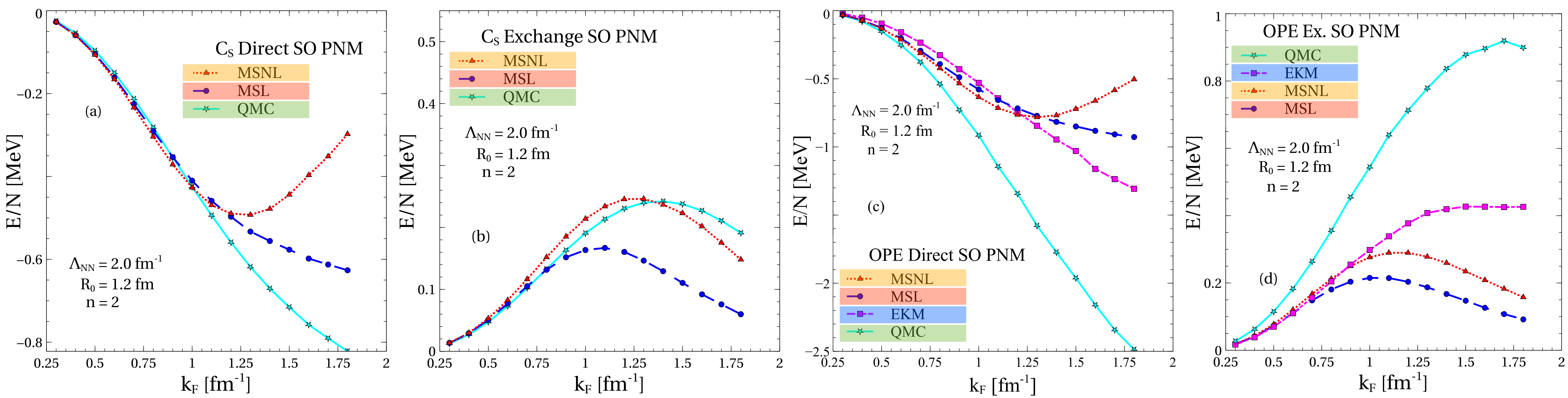

→ for more details see talk by Ingo Tews

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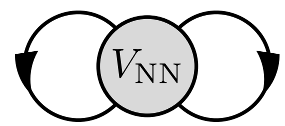

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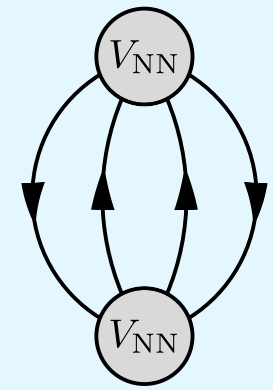

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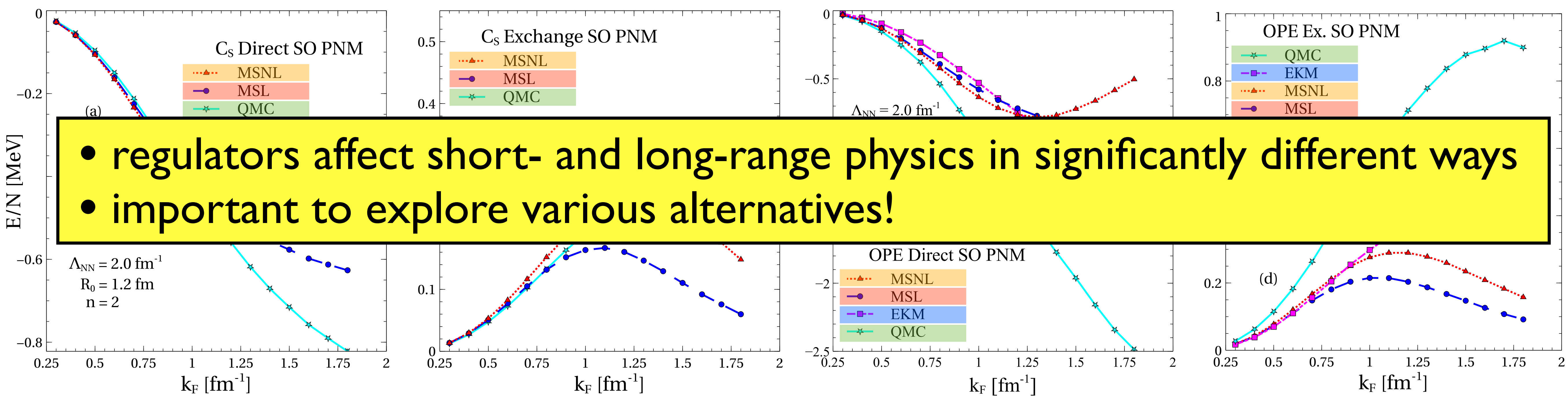


- regulators affect short- and long-range physics in significantly different ways
- important to explore various alternatives!

⟶ for more details see talk by Ingo Tews

Calculation of 3N interactions

1. non-local regularization:

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

- multiplicative, trivial to apply to unregularized interactions

2. semi-local regularization (long-range part):

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

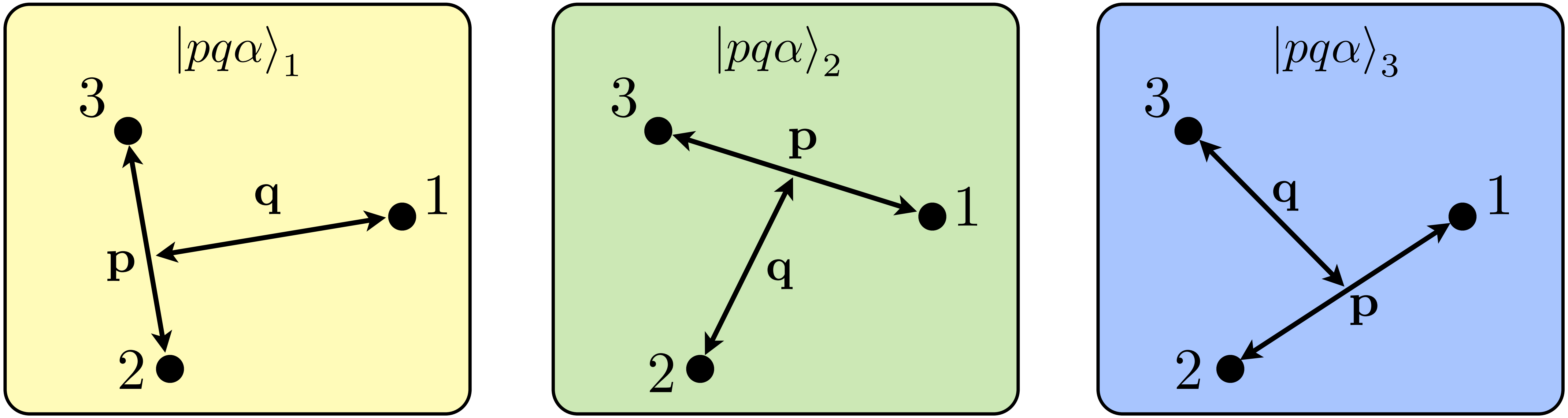
$$= \prod_{ij} f(r_{ij})V_{3\mathrm{N}}(\mathbf{r}_{12},\mathbf{r}_{23},\mathbf{r}_{13})$$

- partial wave mixing: application of regulator non-trivial in partial-wave basis
- Fourier transform regulator and perform convolution integrals:

$$V_{3\mathrm{N}}(\mathbf{p},\mathbf{q},\mathbf{p}',\mathbf{q}') \to \int d\tilde{\mathbf{p}}\int d\tilde{\mathbf{q}}\, V_{3\mathrm{N}}(\mathbf{p},\mathbf{q},\tilde{\mathbf{p}},\tilde{\mathbf{q}})f(\tilde{\mathbf{p}},\tilde{\mathbf{q}},\mathbf{p}',\mathbf{q}')$$

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.

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

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

Calculation of 3N forces in momentum partial-wave representation

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

traditional method:

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

much more efficient 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 for 3 integrals analytically

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

3NF matrix elements

- 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

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

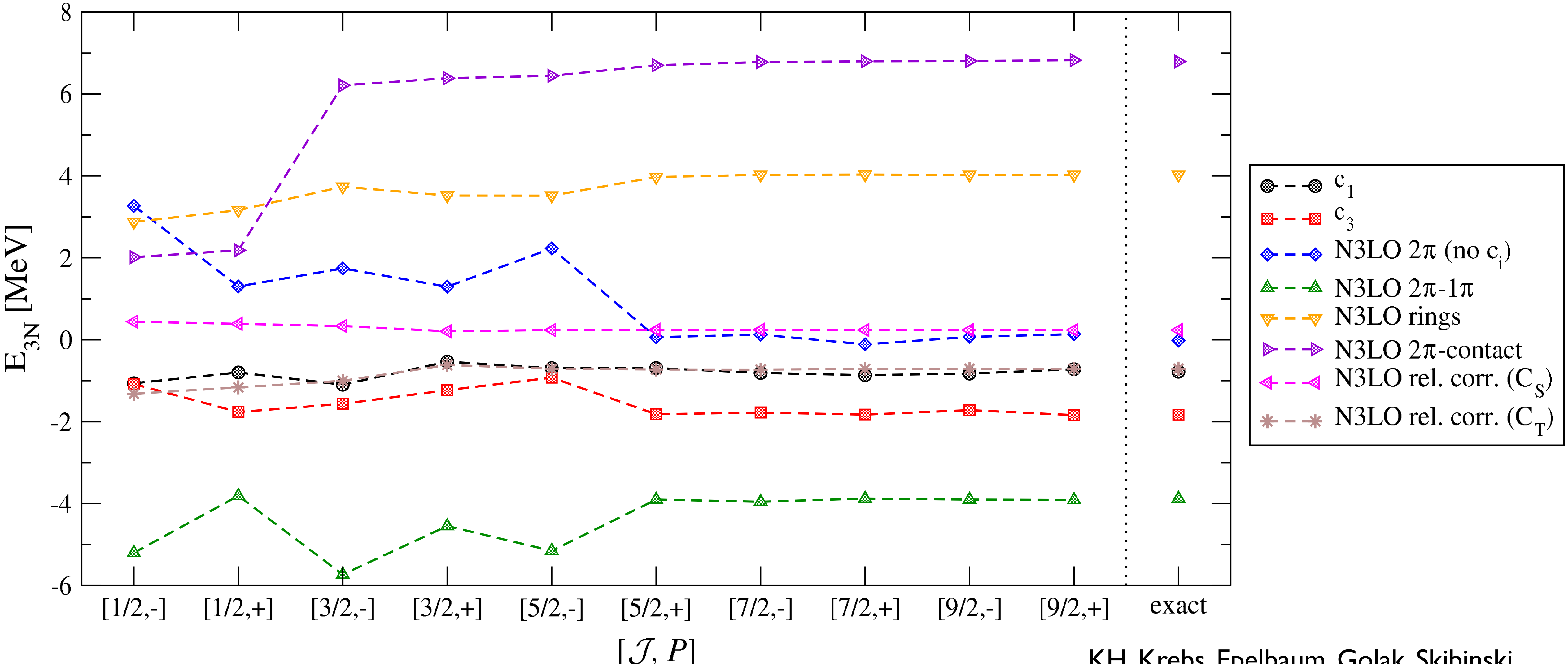
- HDF5 file format for efficient I/O   *http://www.hdfgroup.org*

- current model space limits:

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

Hartree-Fock energy of infinite matter (unregularized 3NF)

neutron matter:

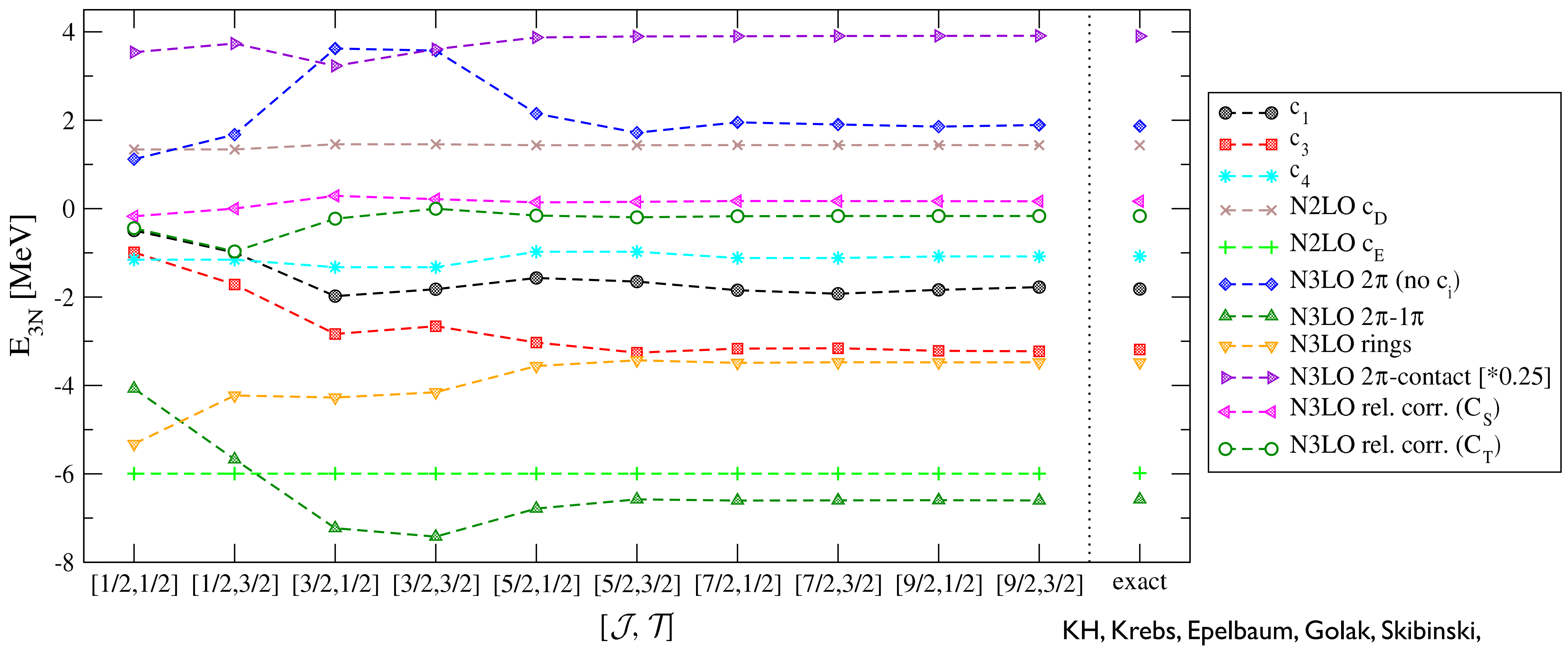


KH, Krebs, Epelbaum, Golak, Skibinski, PRC 91, 044001 (2015)

- 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)

Hartree-Fock energy of infinite matter (unregularized 3NF)

symmetric nuclear matter:



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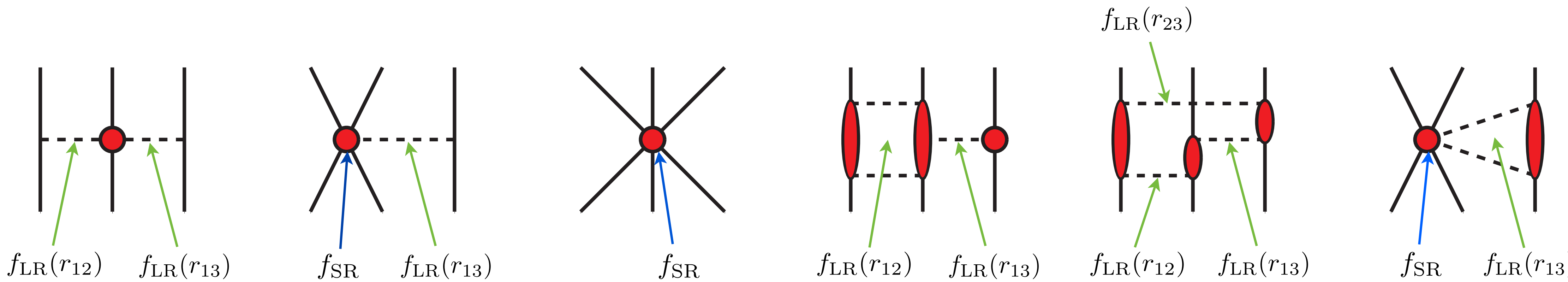
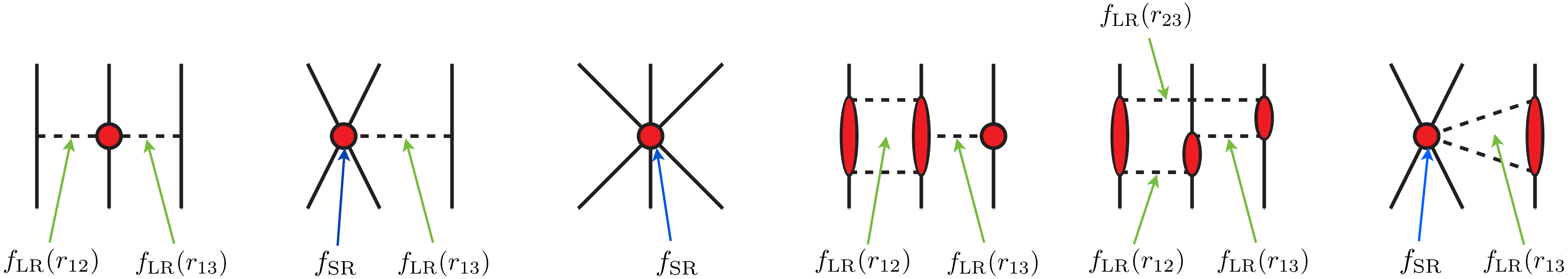
Semi-local regularization of 3NF up to N^{3}LO



$1/m$

Semi-local regularization of 3NF up to N^{3}LO



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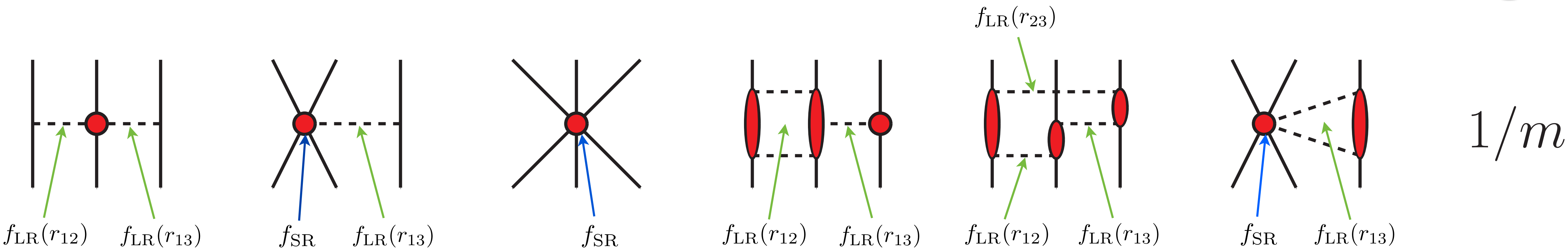
Computational strategy:

(1) calculate unregularized 3NF in sufficiently large partial-wave basis

Semi-local regularization of 3NF up to N^3LO



Computational strategy:

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(2) fourier transform coordinate space regulator to momentum space

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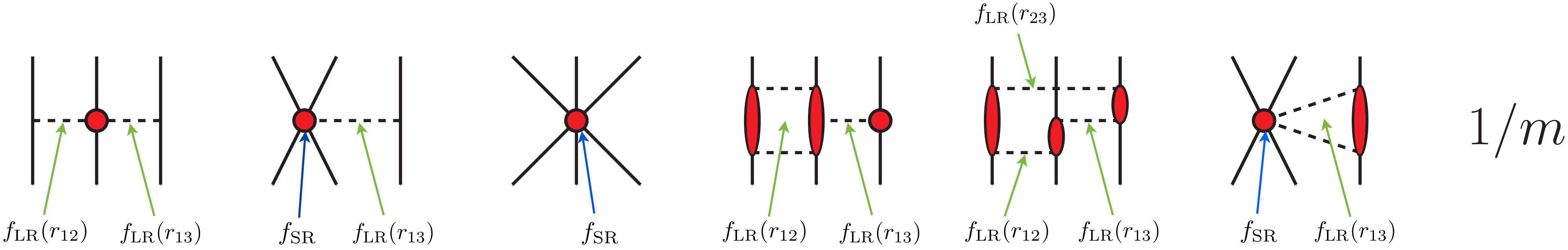

Computational strategy:

(1) calculate unregularized 3NF in sufficiently large partial-wave basis

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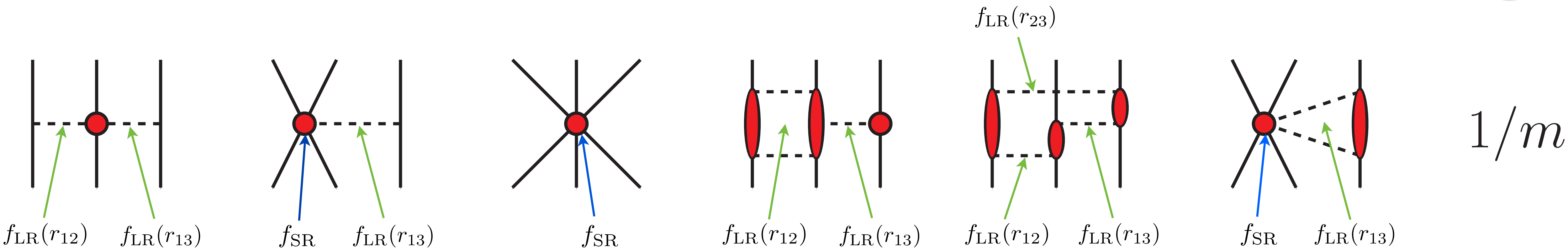
(3) decompose regulator f_{LR} in partial wave momentum basis

Semi-local regularization of 3NF up to N^{3}LO



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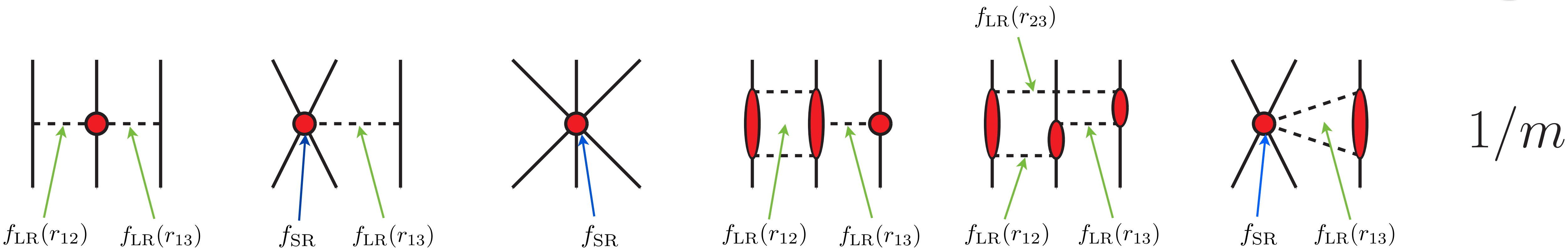
(4) perform convolution integrals:

$$\langle pq\alpha | V_{123}^{\rm reg} | p'q'\alpha' \rangle = \int d\tilde{q}\, \tilde{q}^2 \int d\tilde{p}\, \tilde{p}^2 \sum_{\tilde{\alpha}} \langle pq\alpha | V_{123} | \tilde{p}\tilde{q}\tilde{\alpha} \rangle \, \langle \tilde{p}\tilde{q}\tilde{\alpha} | f_{LR} | p'q'\alpha' \rangle$$

Semi-local regularization of 3NF up to N^{3}LO



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(5) regularize short-range parts in interactions with non-local regulator

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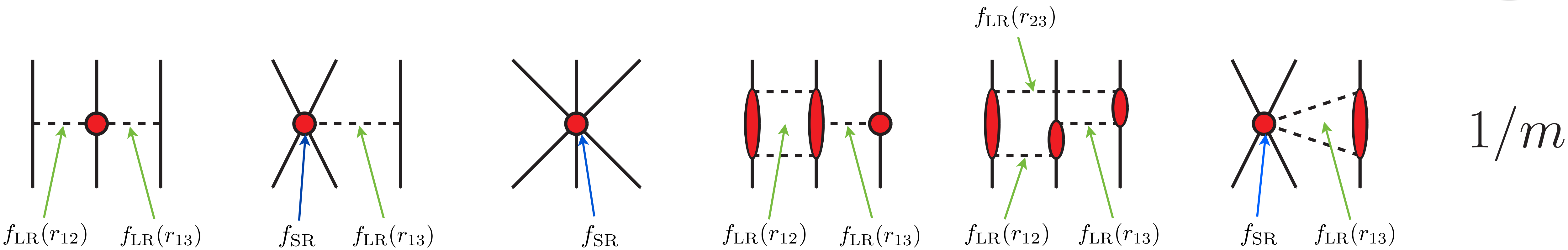

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(5) regularize short-range parts in interactions with non-local regulator

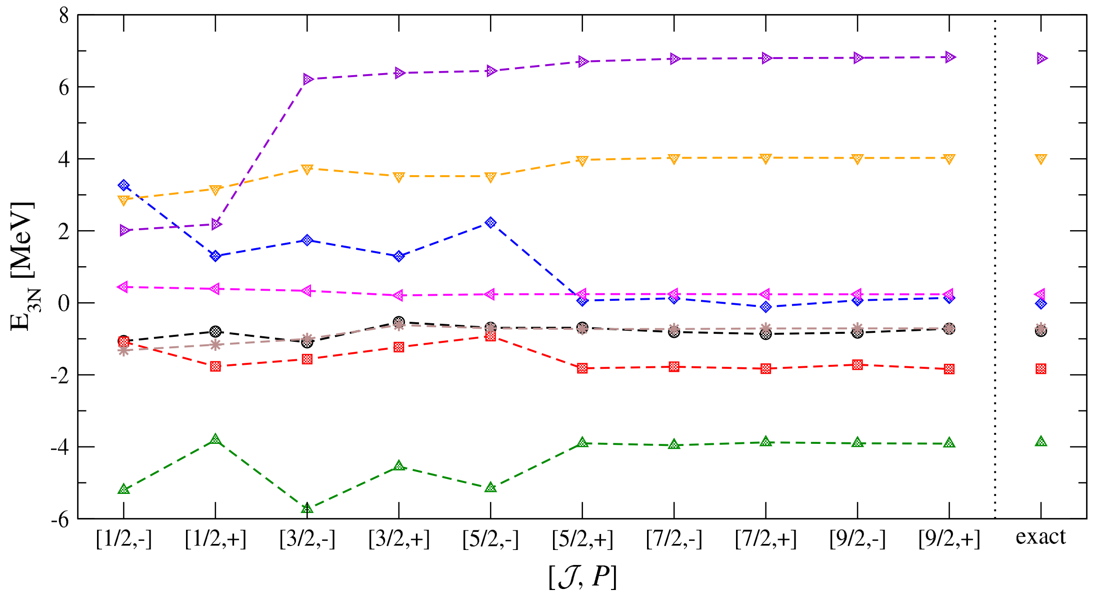
(6) antisymmetrize interactions (optional)

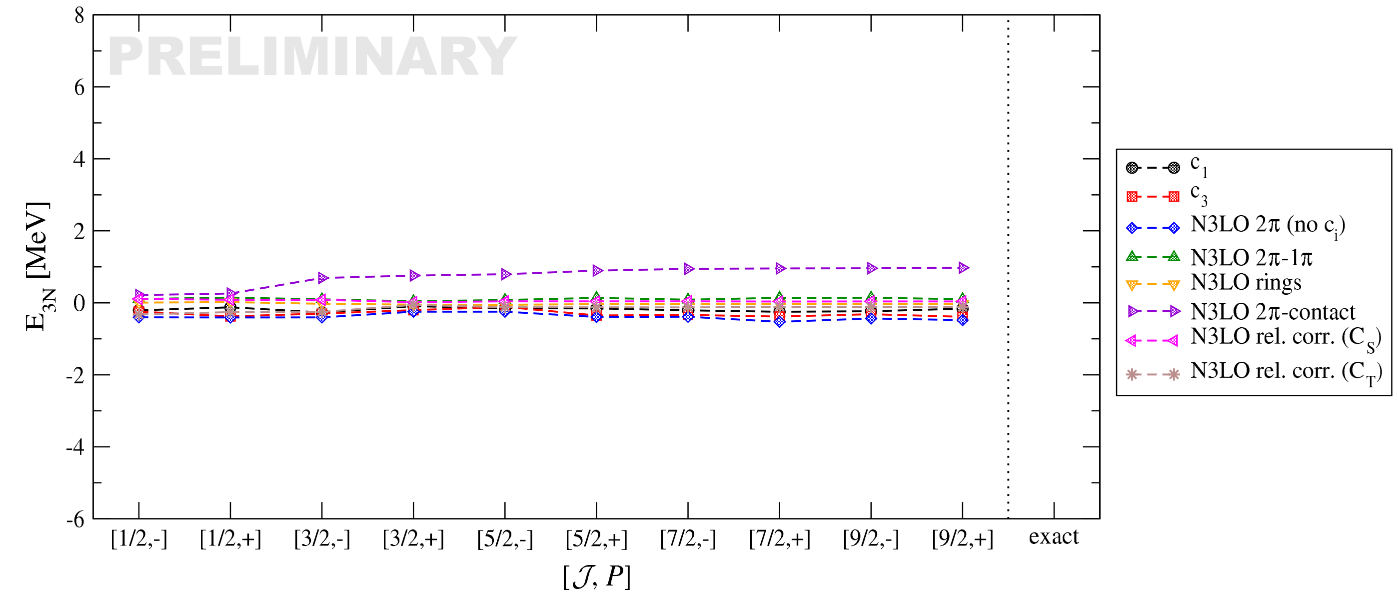
Hartree-Fock energy of infinite matter

nonlocal

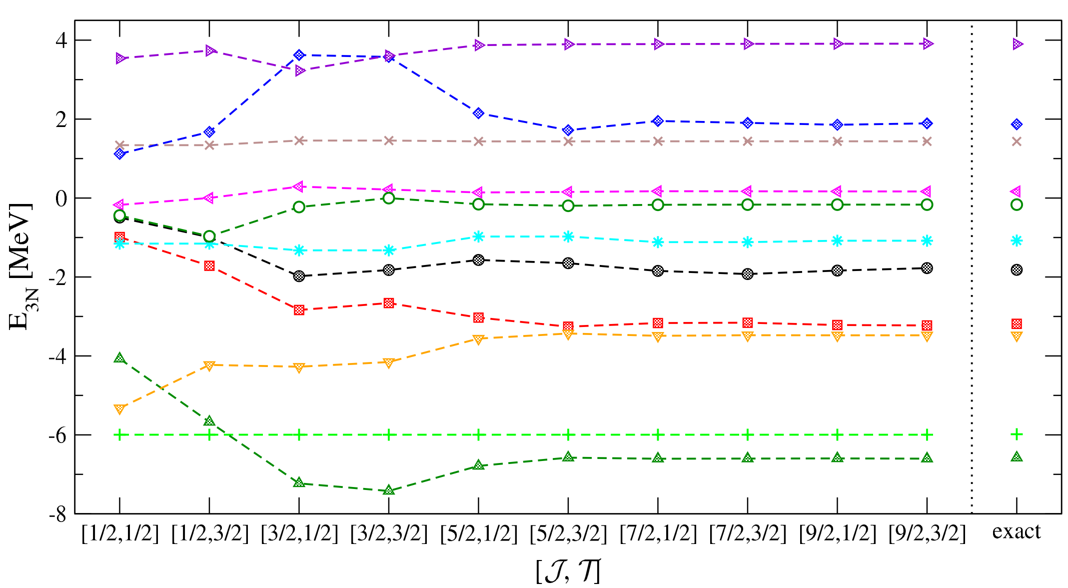
semi-local

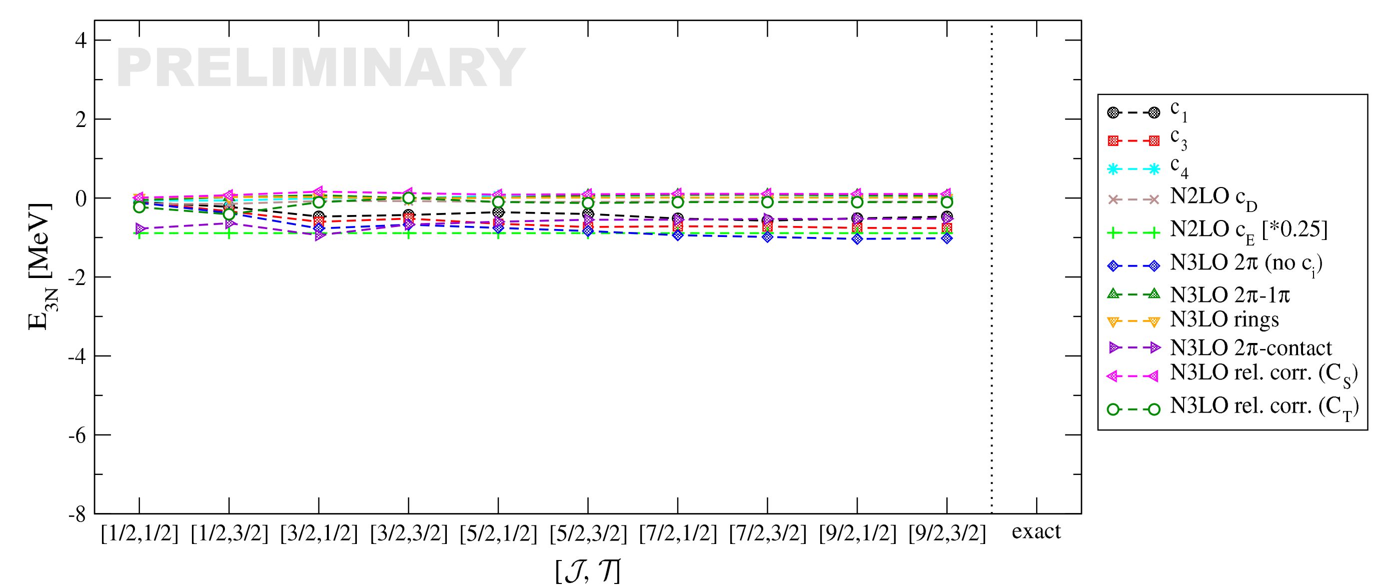
PNM





SNM





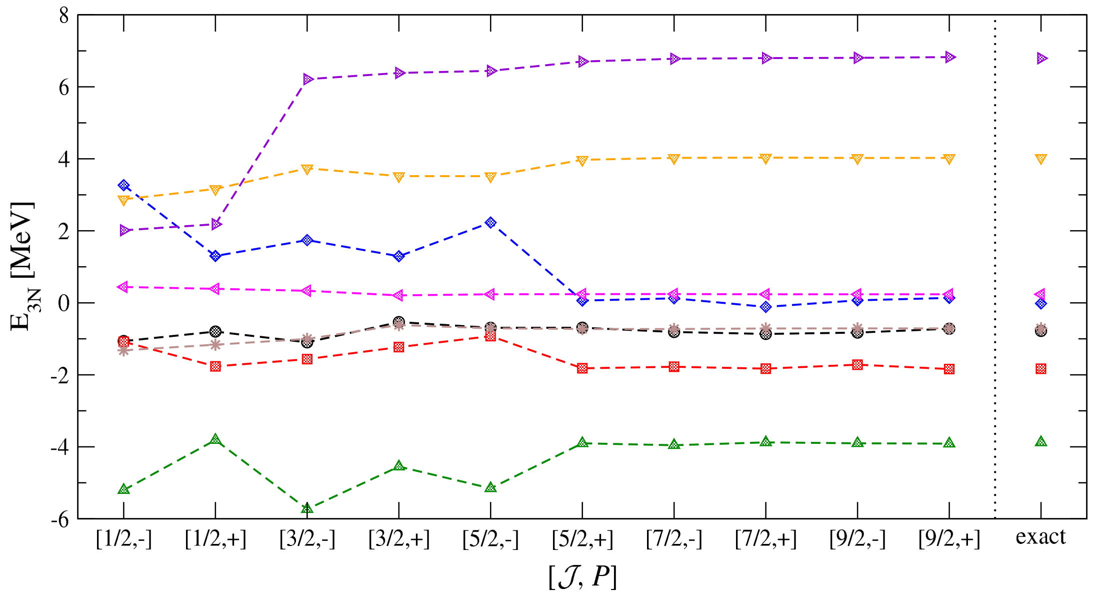
- contributions from semi-local 3NF significantly smaller
- partial wave-convergence comparable for both regulators

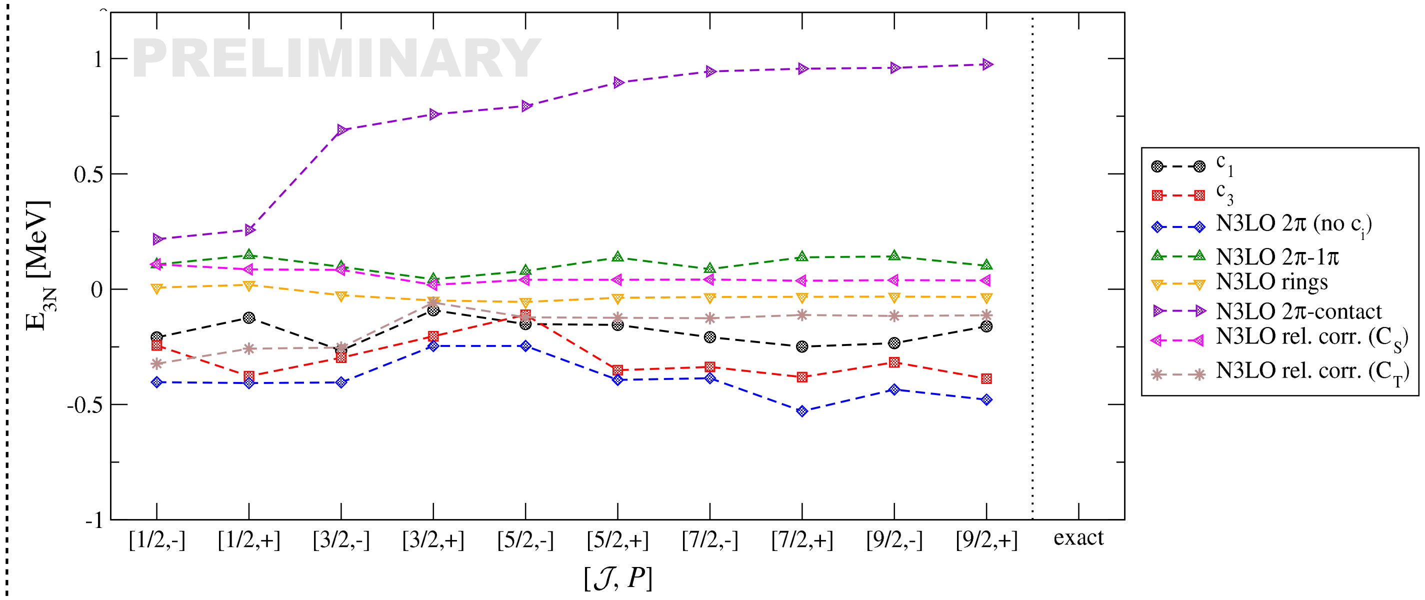
Hartree-Fock energy of infinite matter

nonlocal

semi-local

PNM





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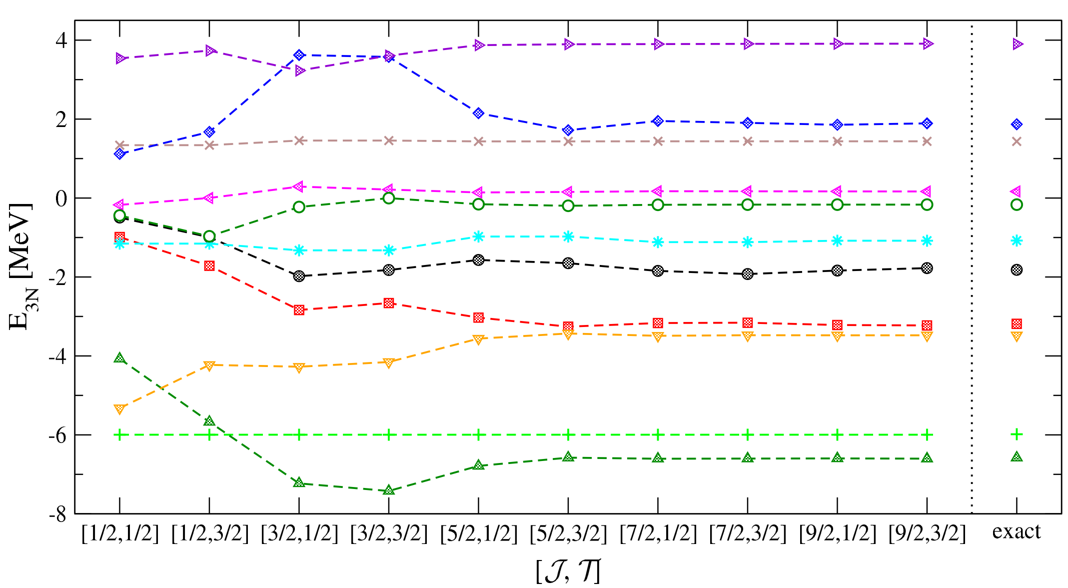

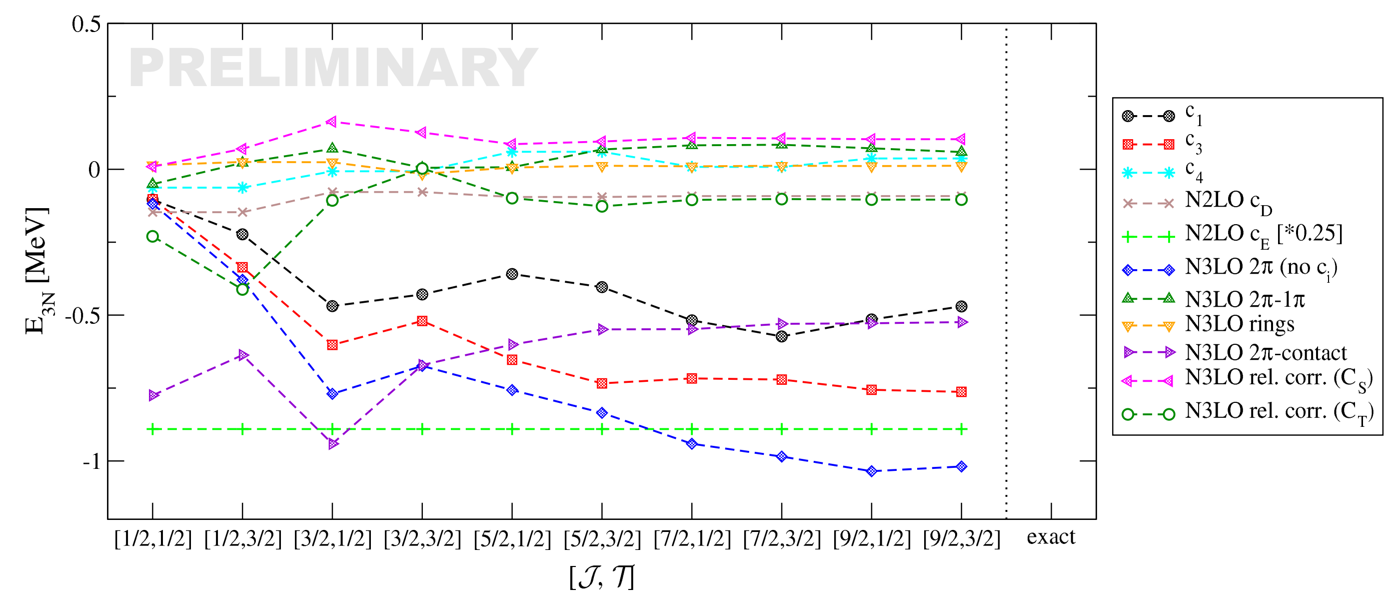

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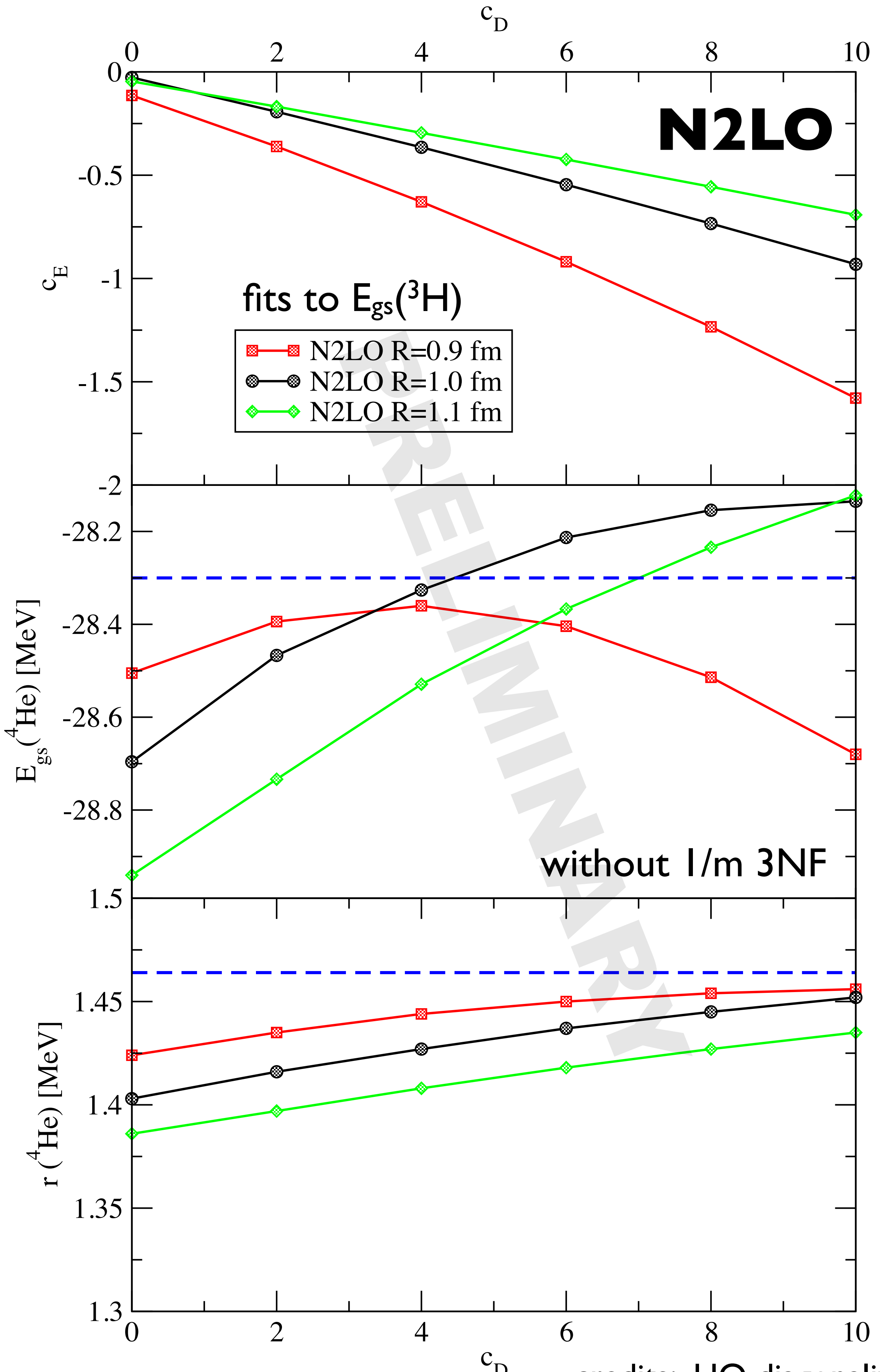
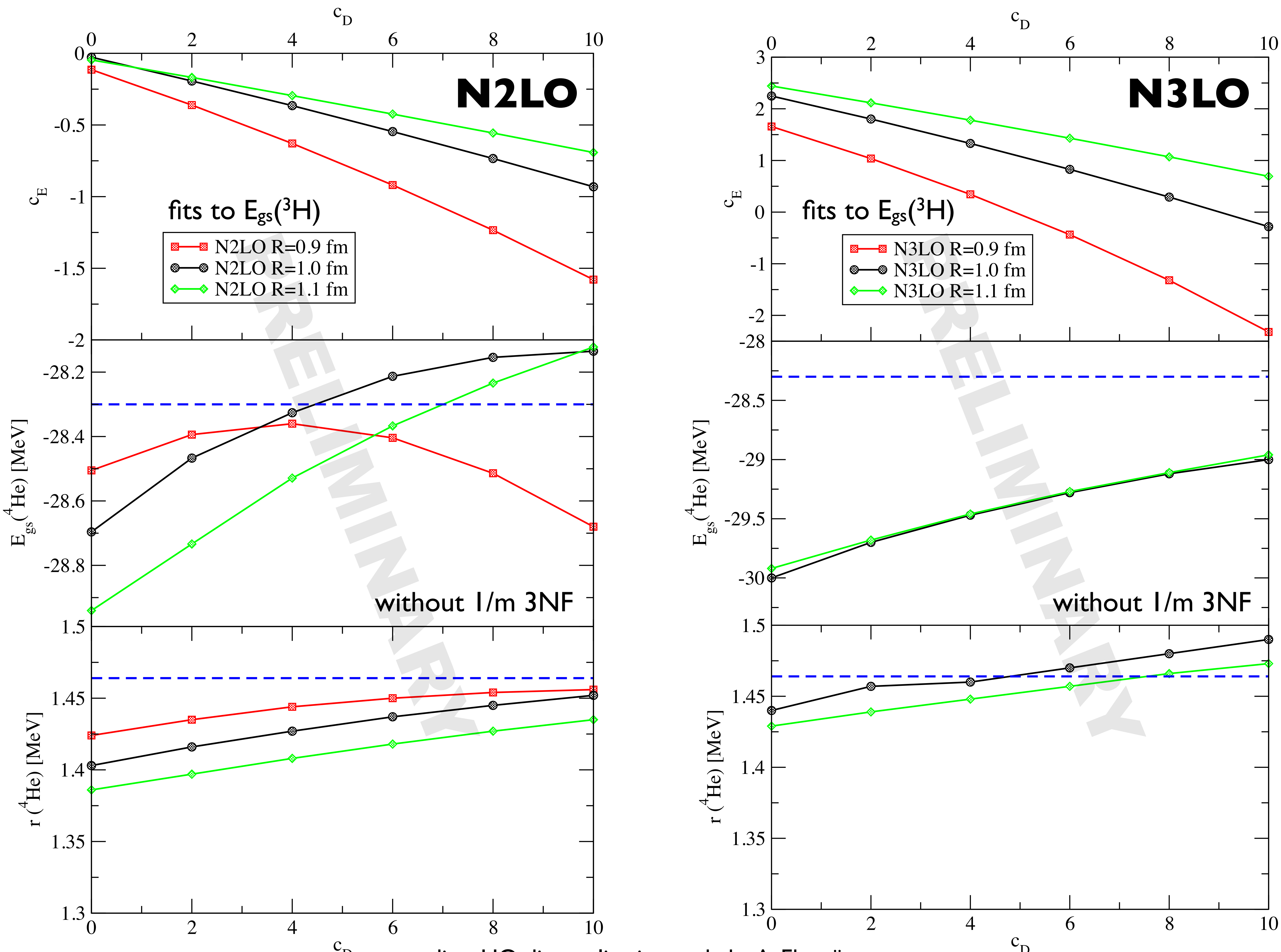
- partial wave-convergence comparable for both regulators

Few-body results based on semi-local NN+3N interactions



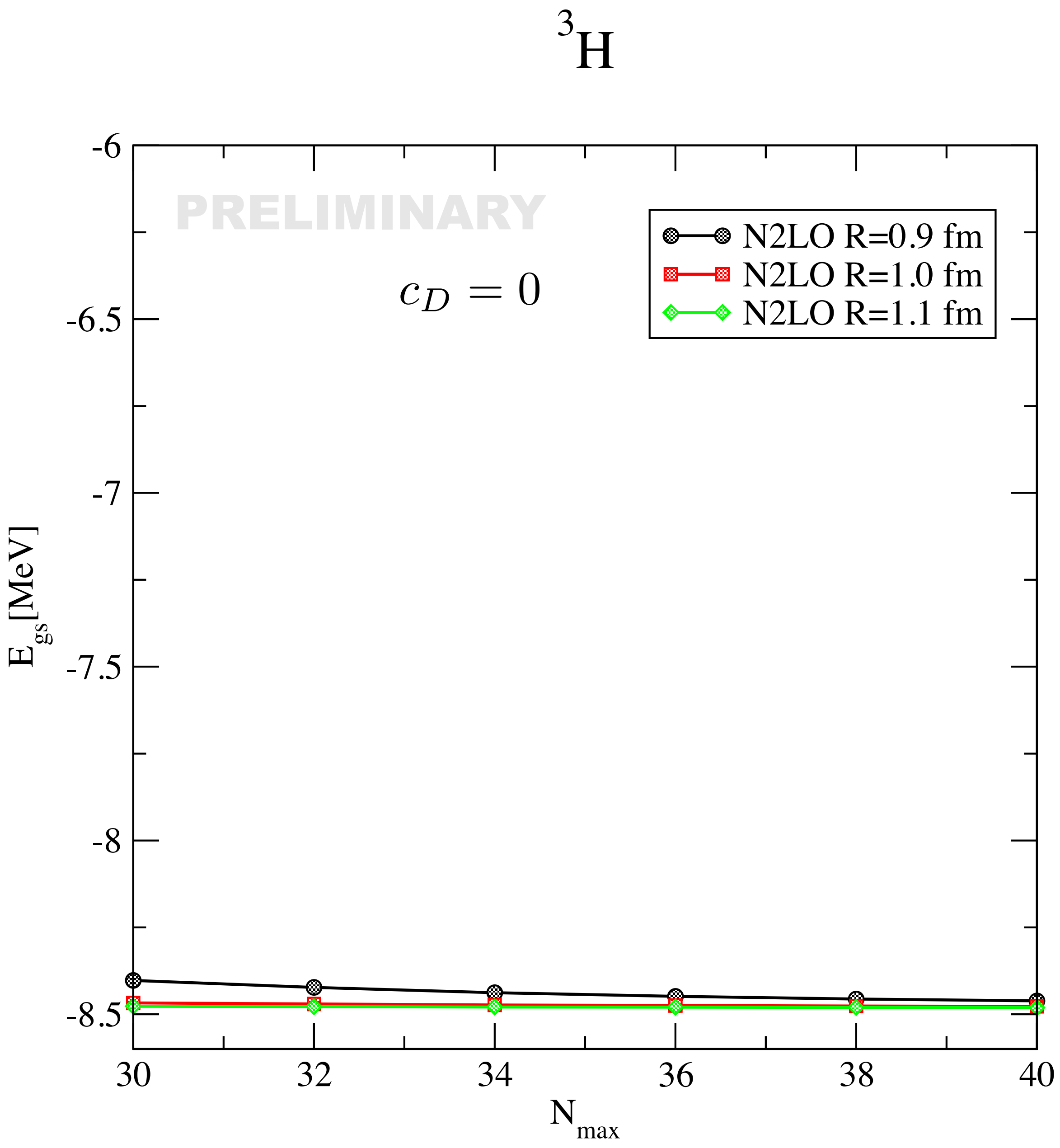
credits: HO diagonalization code by A. Ekström

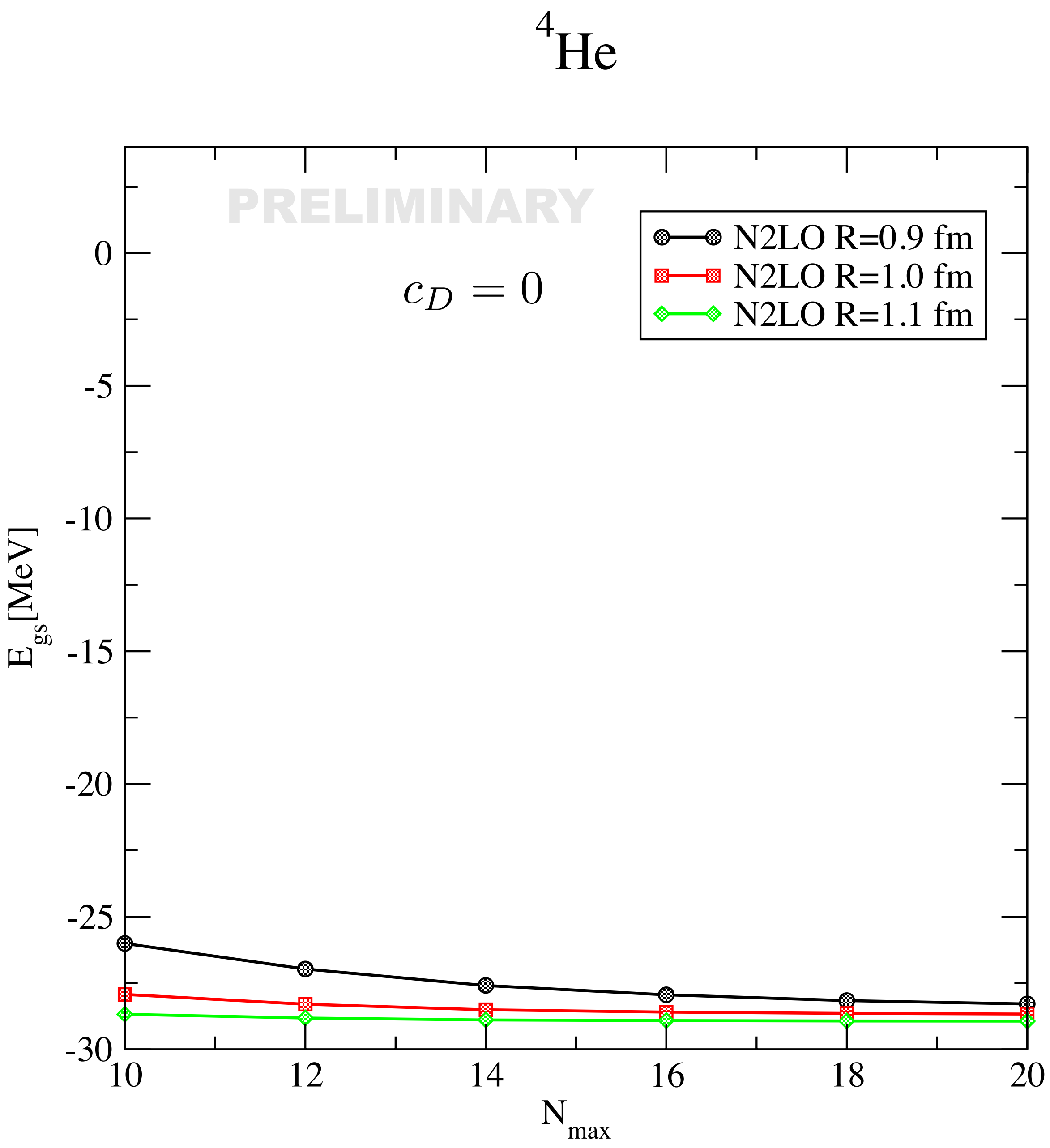
Few-body results based on semi-local NN+3N interactions



credits: HO diagonalization code by A. Ekström

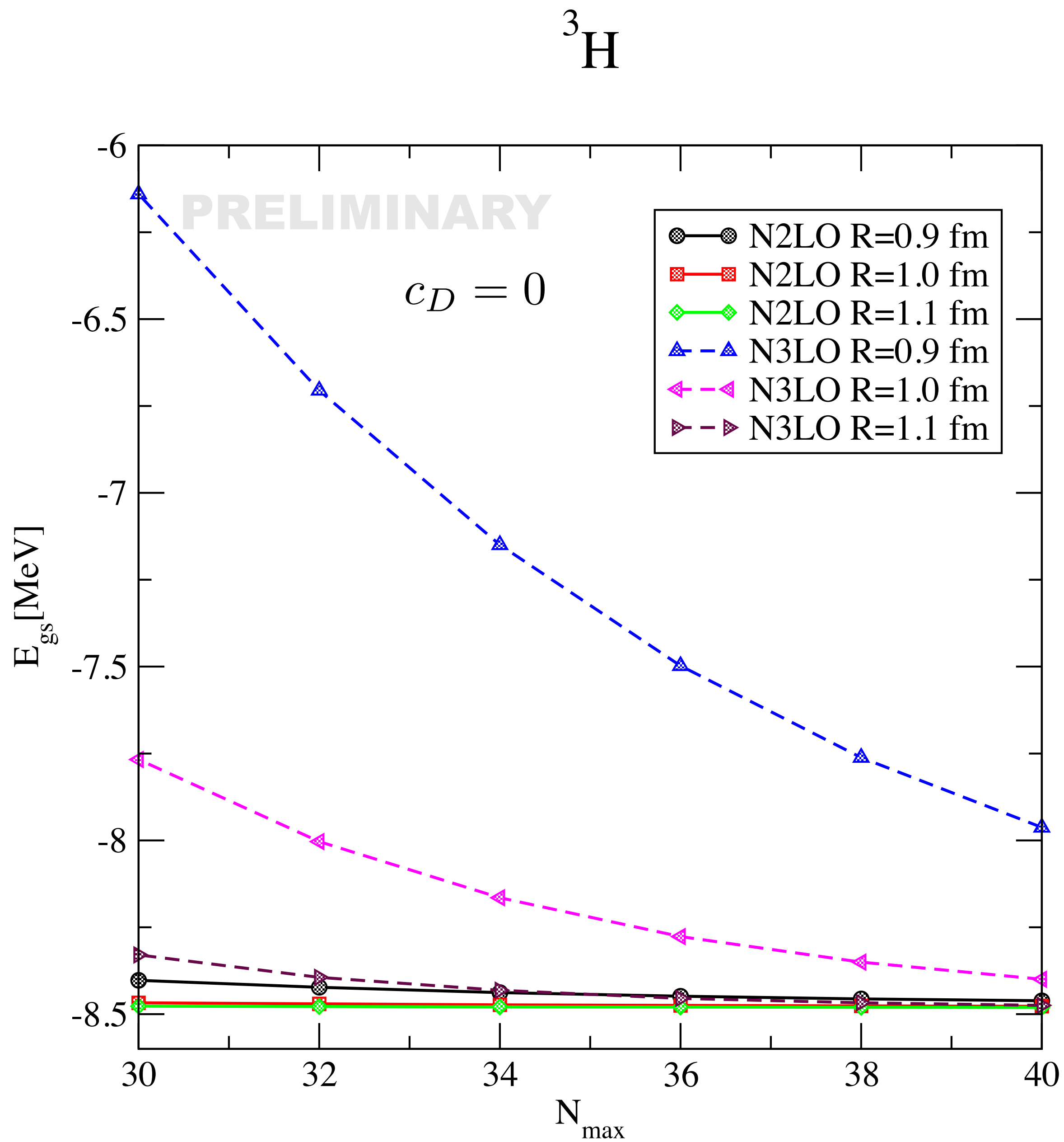
Convergence in harmonic oscillator basis

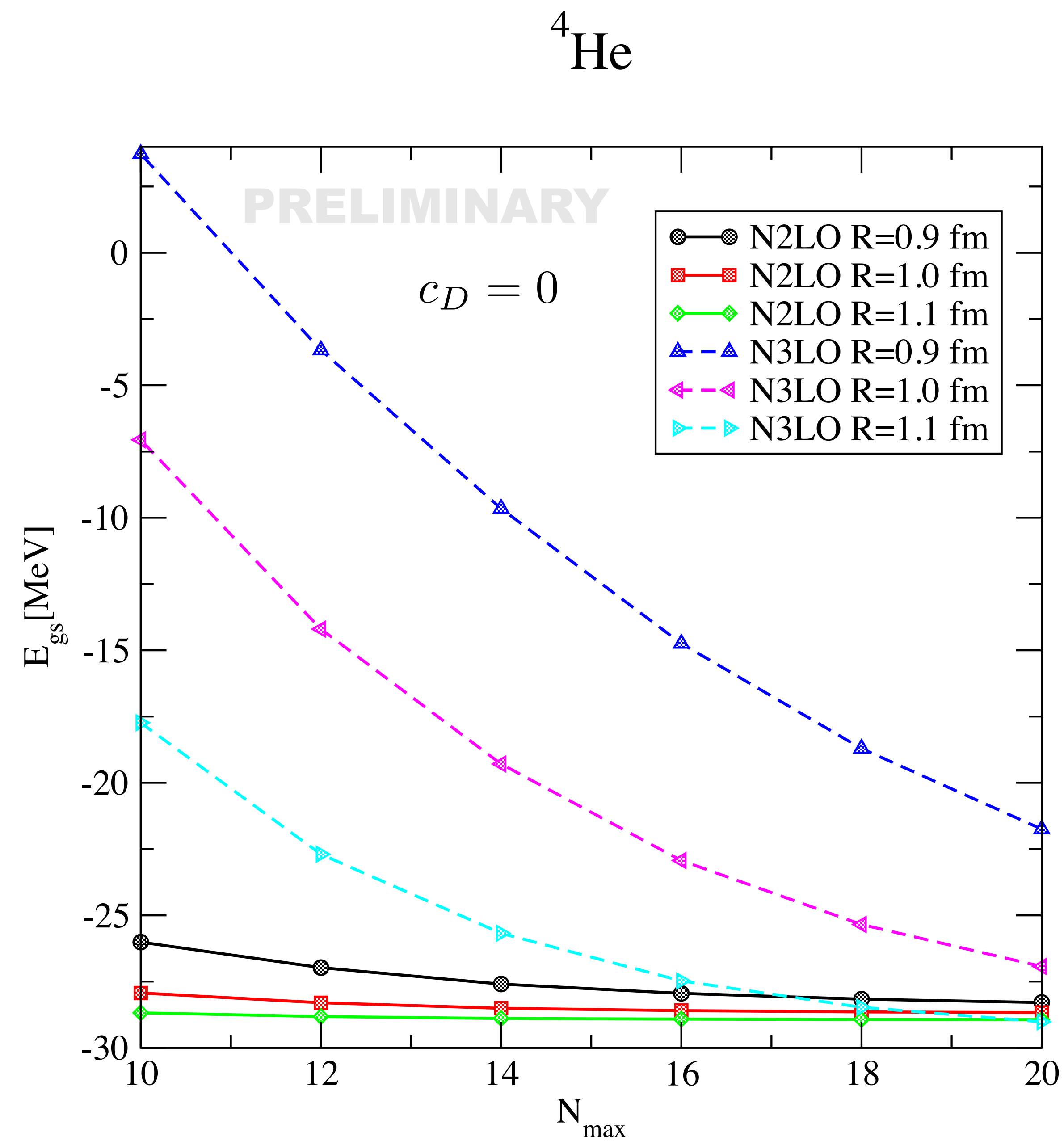




credits: HO diagonalization code by A. Ekström

Convergence in harmonic oscillator basis

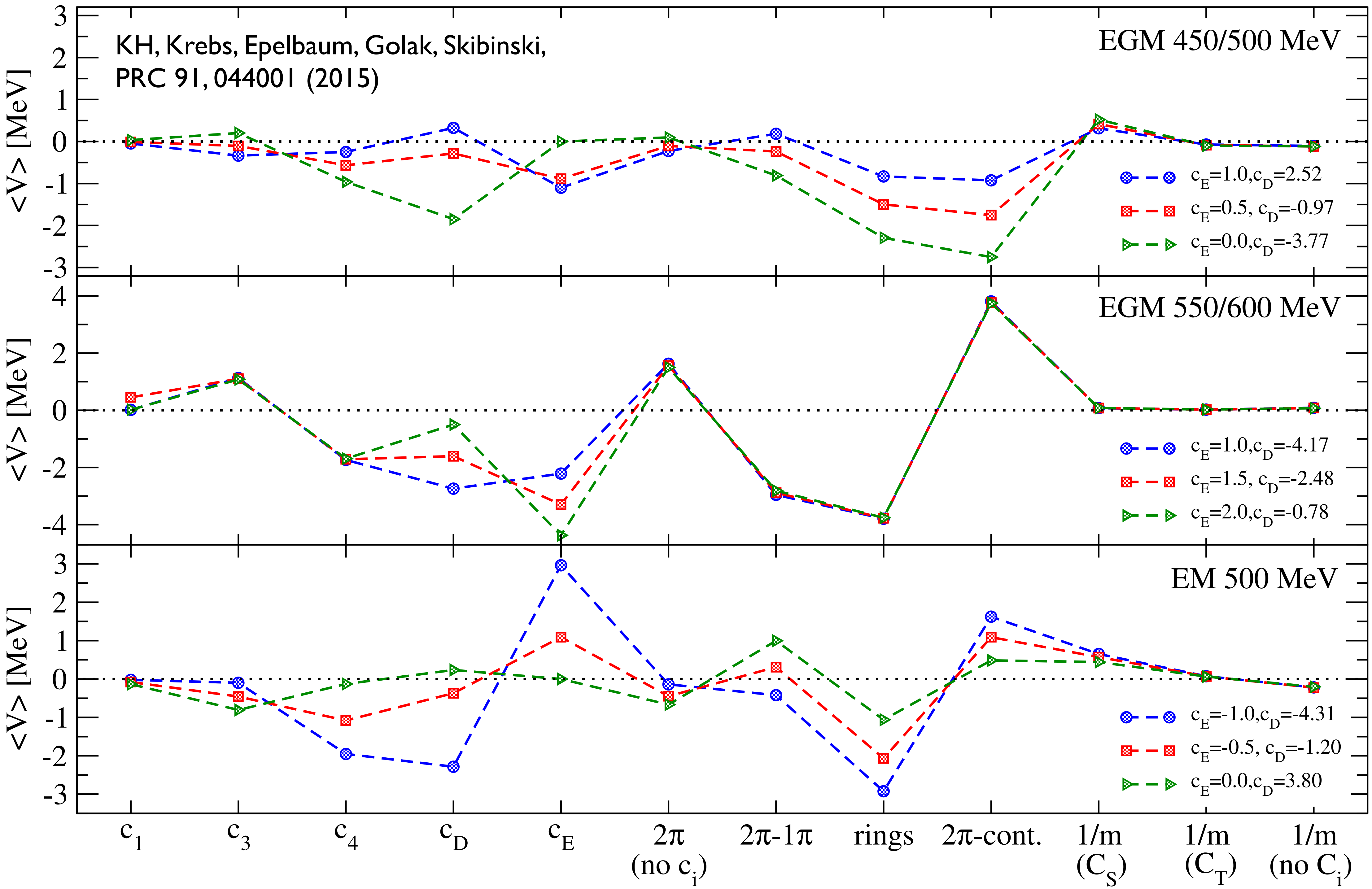




credits: HO diagonalization code by A. Ekström

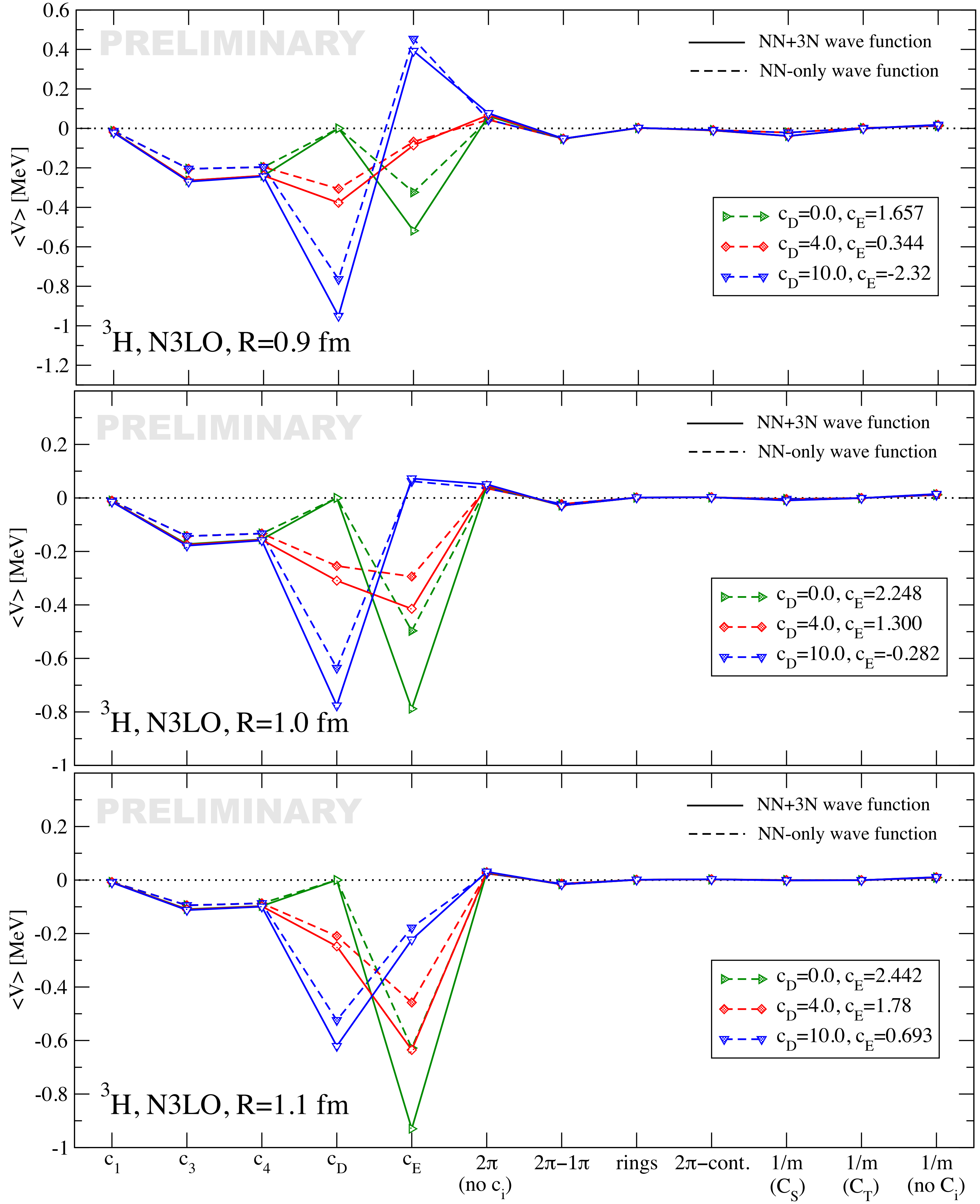
- systematic improvement of convergence for larger cutoffs R
- significantly slower convergence for N^2LO compared to N^3LO
- SRG evolution most likely required for A > 4 (see talk by Klaus Vobig)

Contributions of individual topologies in ^3H (nonlocal)



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

Contributions of individual topologies in ^{3}H (semi-local)



- contributions of individual topologies very similar for all cutoffs R at N3LO
- N3LO contributions significantly suppressed compared to N2LO!
- 3NF behaves perturbatively

Summary

- nuclear matter results at HF at second order in MBPT depend sensitively on regularization scheme of NN and 3N interactions
- development of framework to efficiently calculate 3N interaction up to N3LO
  $\longrightarrow$ generalized framework for calculation of semi-local regularization for 3NF
- contributions of N3LO 3NF topologies in 3H:
  - not suppressed for non-local NN+3N interactions
  - suppressed for semi-local NN+3N interactions

Outlook and open questions

- understanding of chiral power counting for different regularization schemes
- fitting of LECs in chiral EFT interactions (talk by Andreas Ekström)
- explore few-body scattering observables based on NN+3N interactions
- explore semi-local interactions in heavier nuclei (talk by Klaus Vobig)

Backup slides

Future directions: Incorporation in different many-body frameworks

Hyperspherical harmonics

Faddeev, Faddeev-Yakubovski

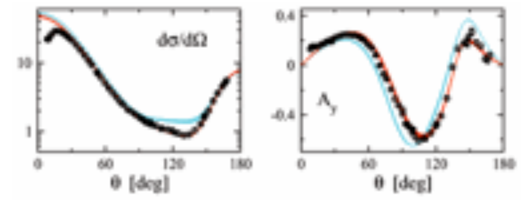


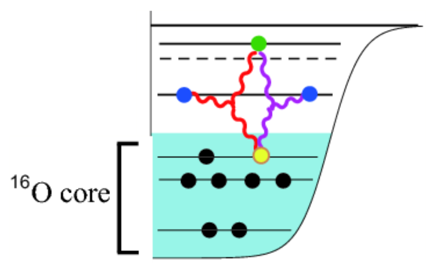
FIG. 4: Nd elastic observables at 65 MeV.

no-core shell model

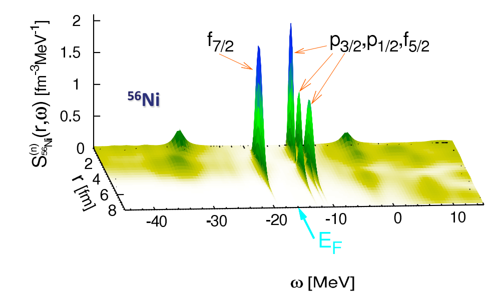
coupled cluster method

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

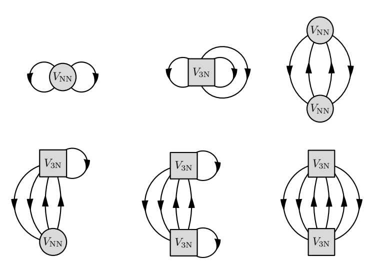
valence shell model



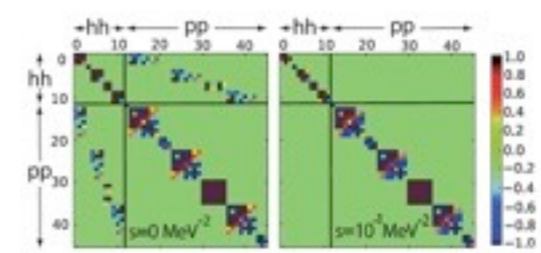
Self-consistent Greens function



Many-body perturbation theory



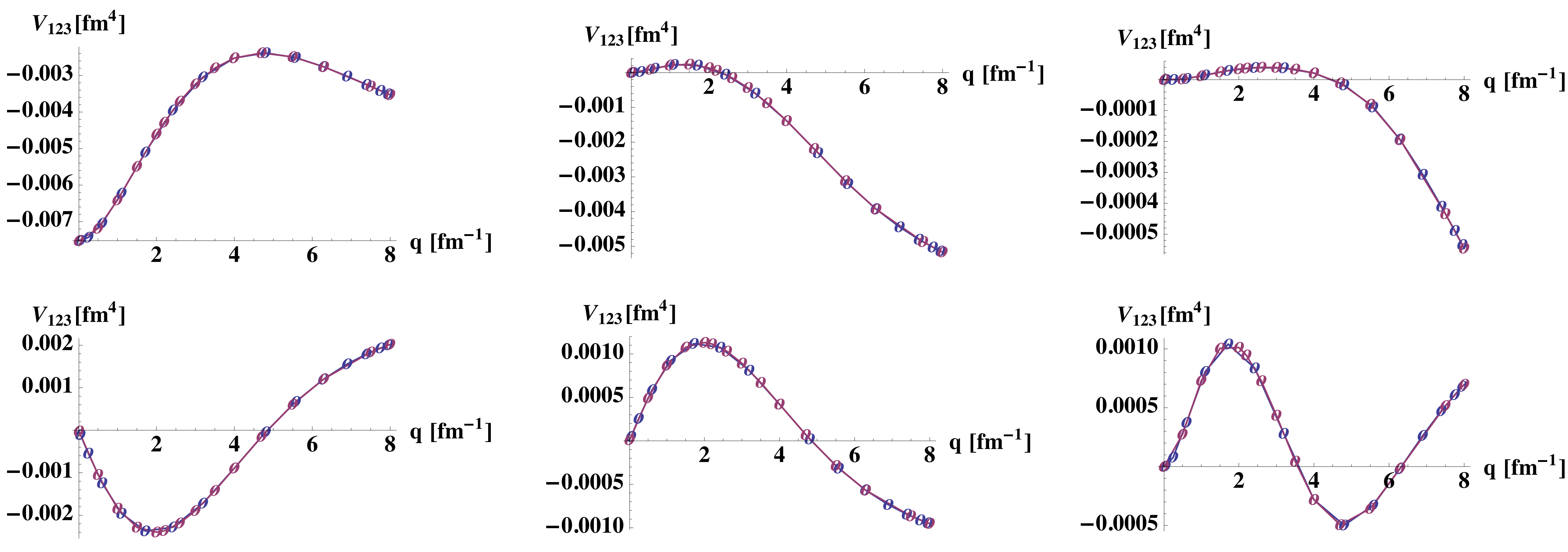
In-medium SRG



Required inputs:

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

Tests of the new framework

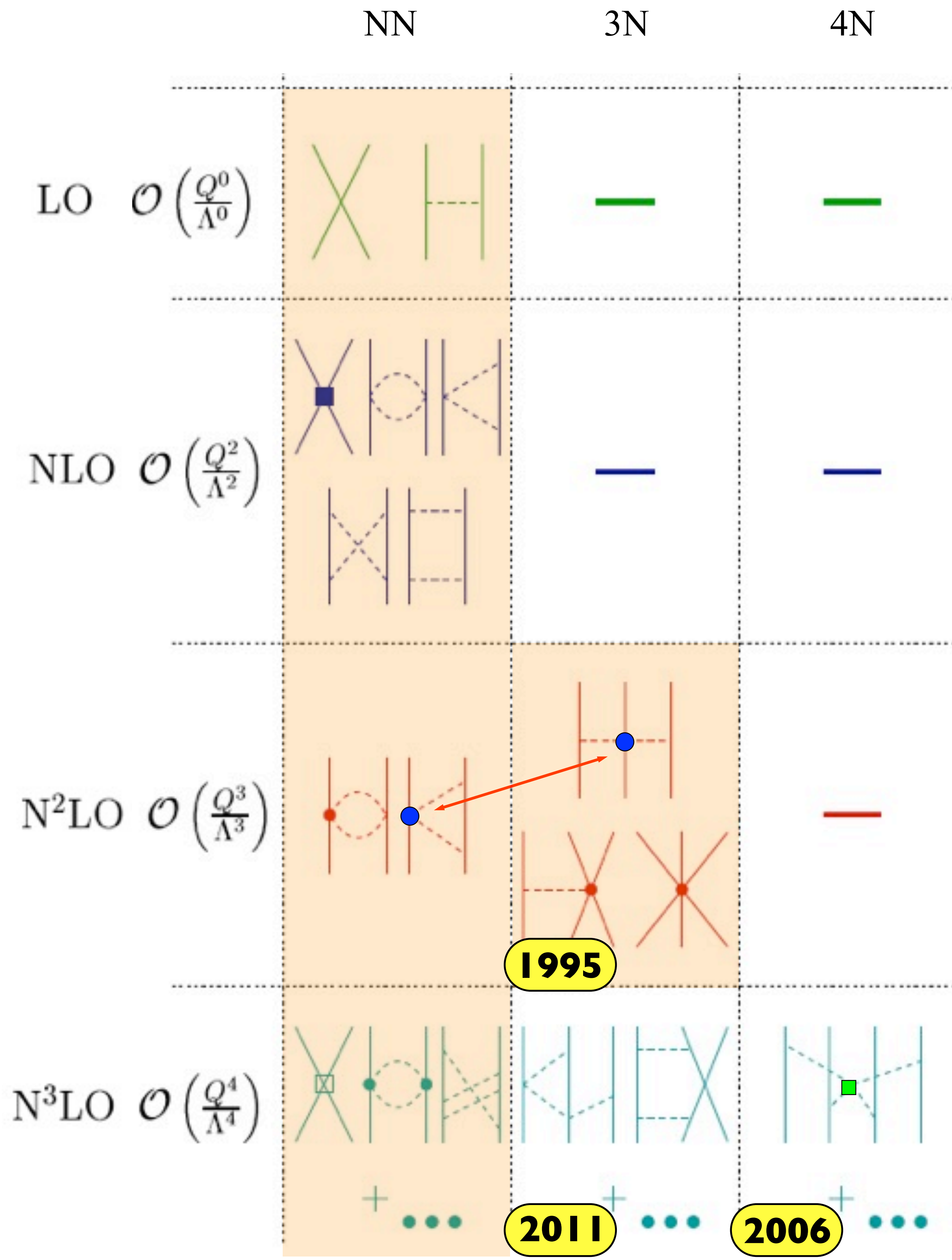


- **perfect agreement** with results based on traditional approach
- **speedup** factors of >1000
- **very general**, can also be applied to
  - pion-full EFT
  - N^{4}LO terms
  - currents?
- **efficient:** allows to study systematically alternative regulators

Chiral effective field theory for nuclear forces

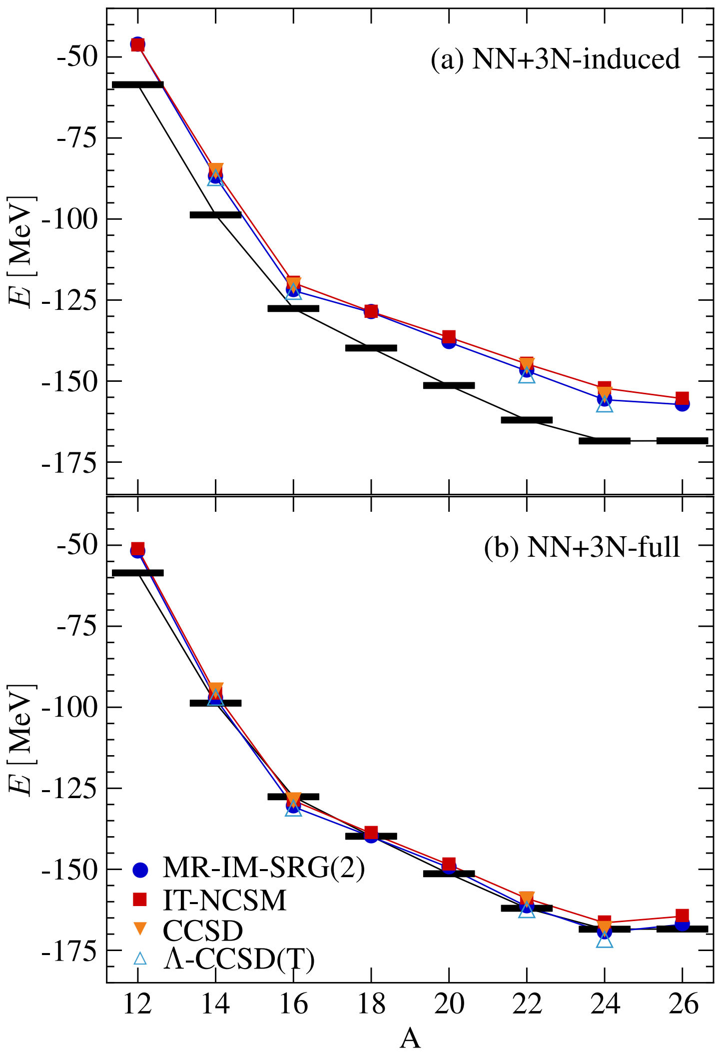
- choose relevant degrees of freedom: here nucleons and pions
- operators constrained by symmetries of QCD
- short-range physics captured in few short-range couplings
- separation of scales: Q << Λ_b, breakdown scale Λ_b~500 MeV
- power-counting: expand in powers Q/Λ_b
- systematic: work to desired accuracy,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

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



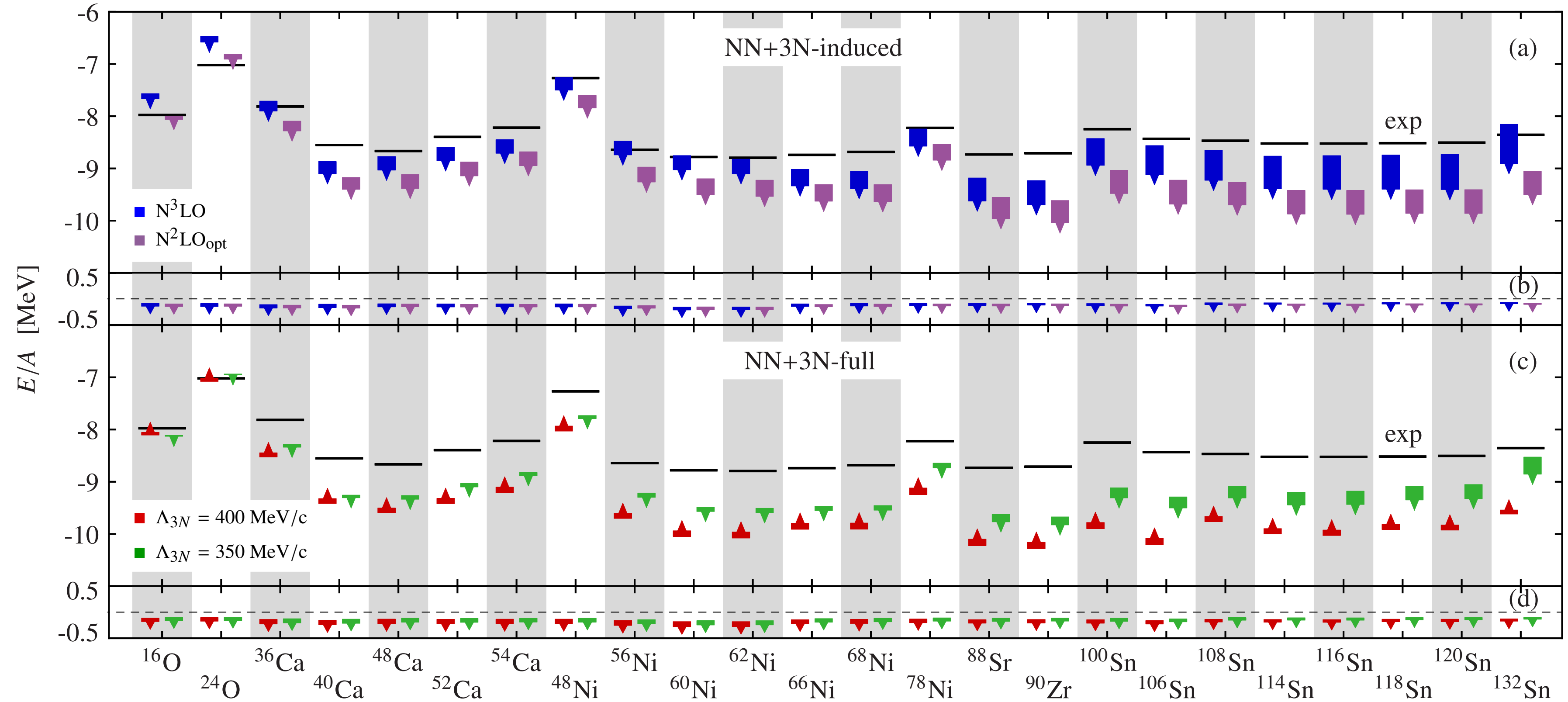
Open issues in nuclear interactions

oxygen chain



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

heavy nuclei

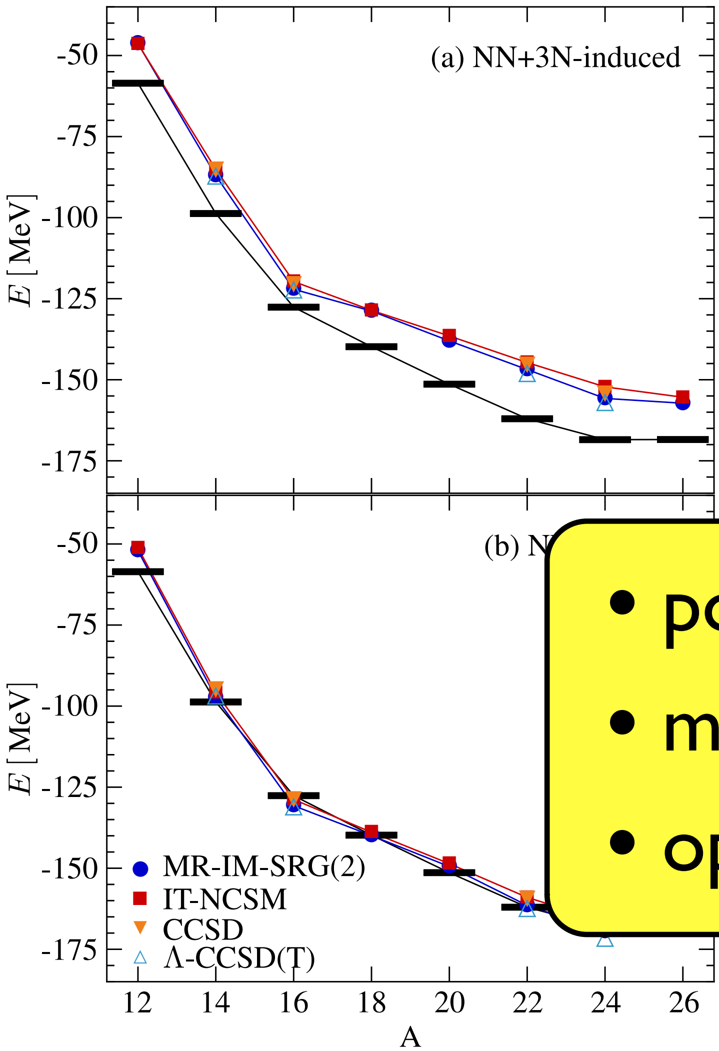


Binder et al., Phys. Lett B 736, 119 (2014)

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

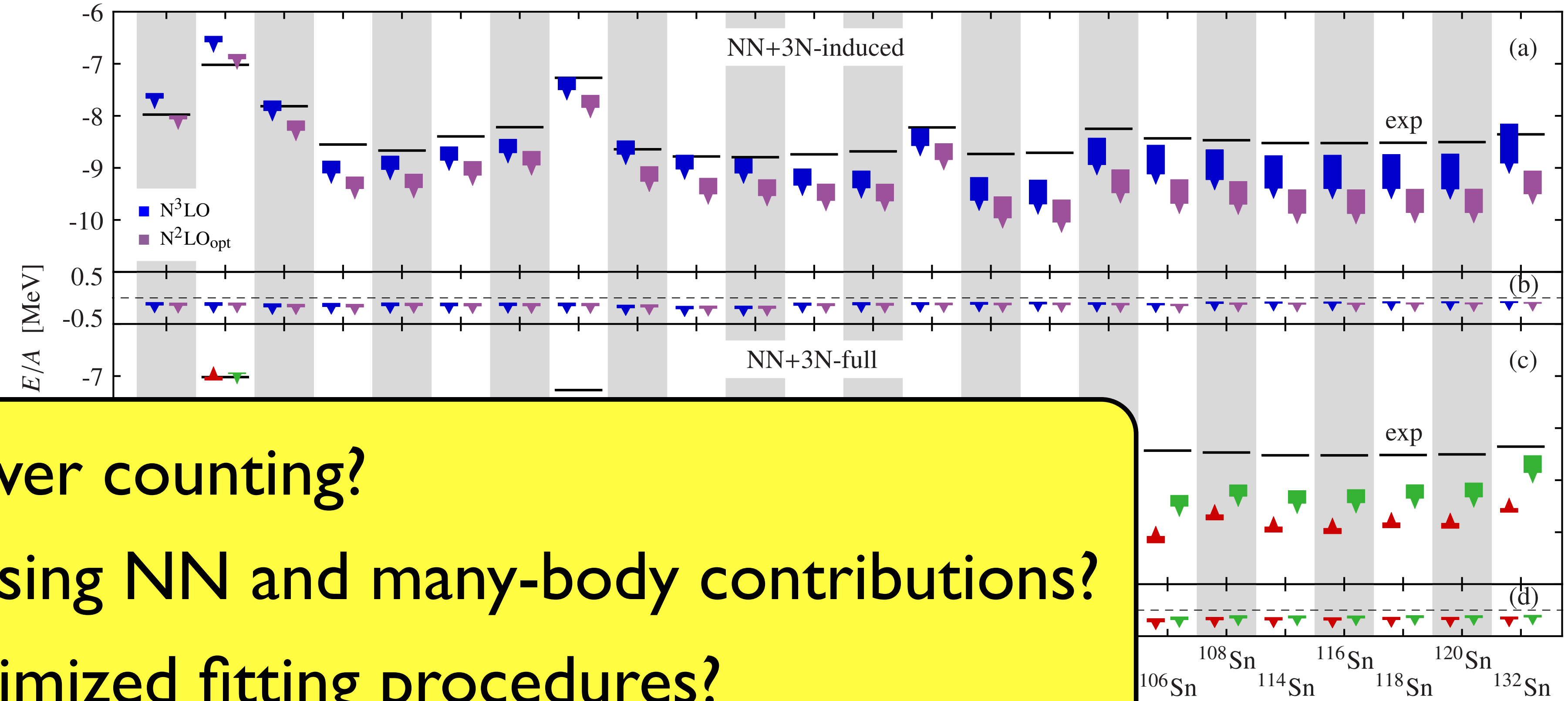
Open issues in nuclear interactions

oxygen chain



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

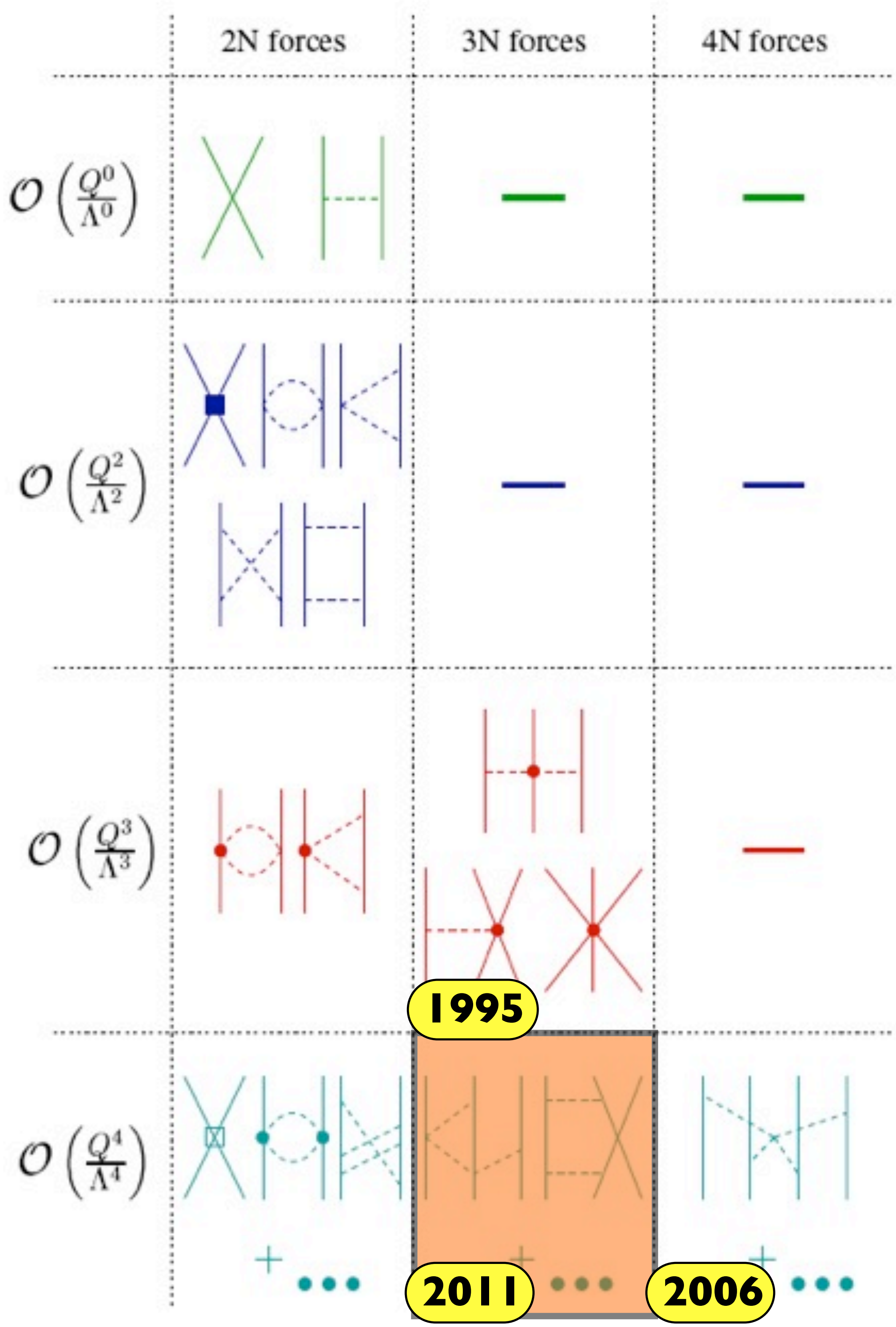
heavy nuclei

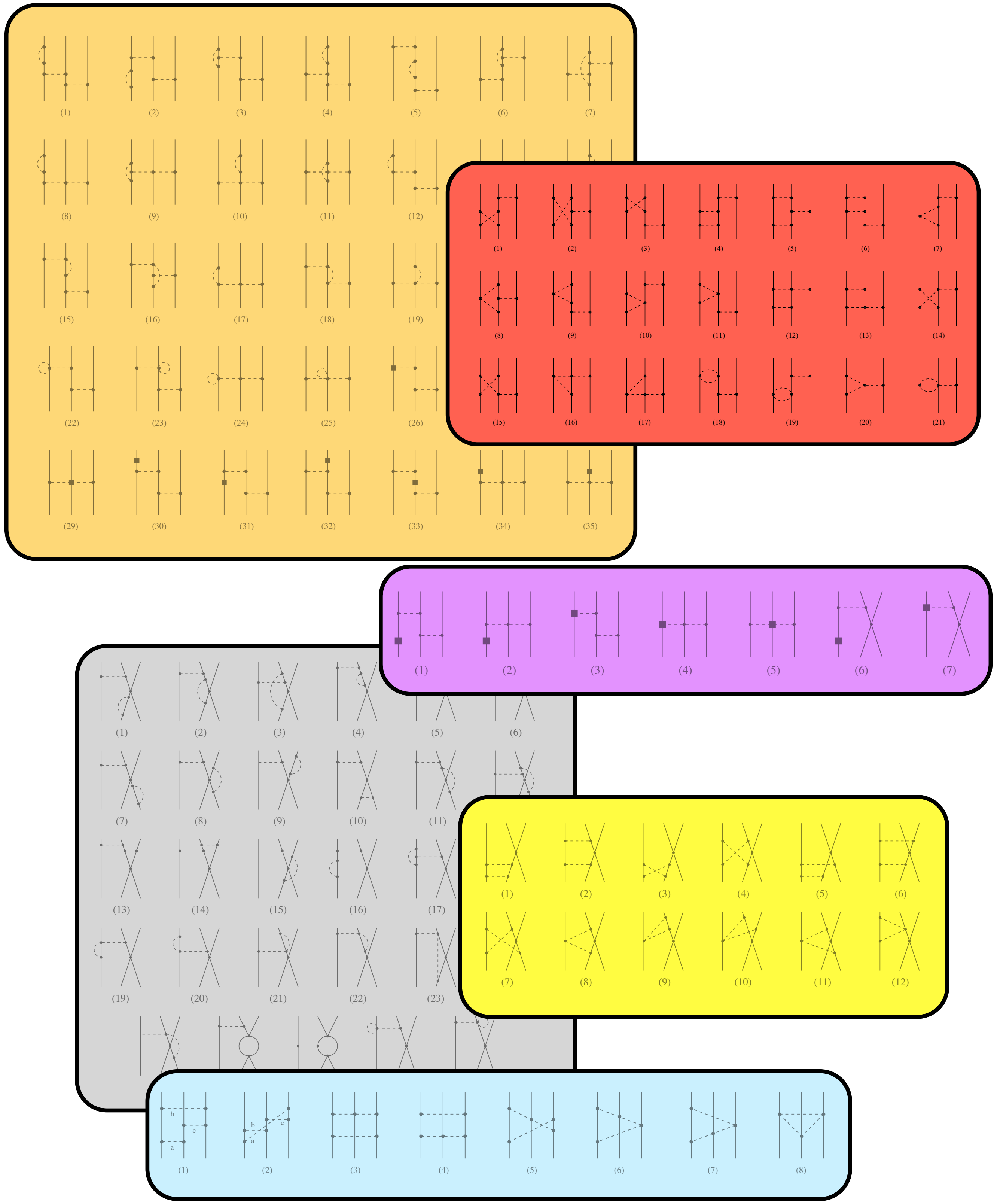


- power counting?
- missing NN and many-body contributions?
- optimized fitting procedures?

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

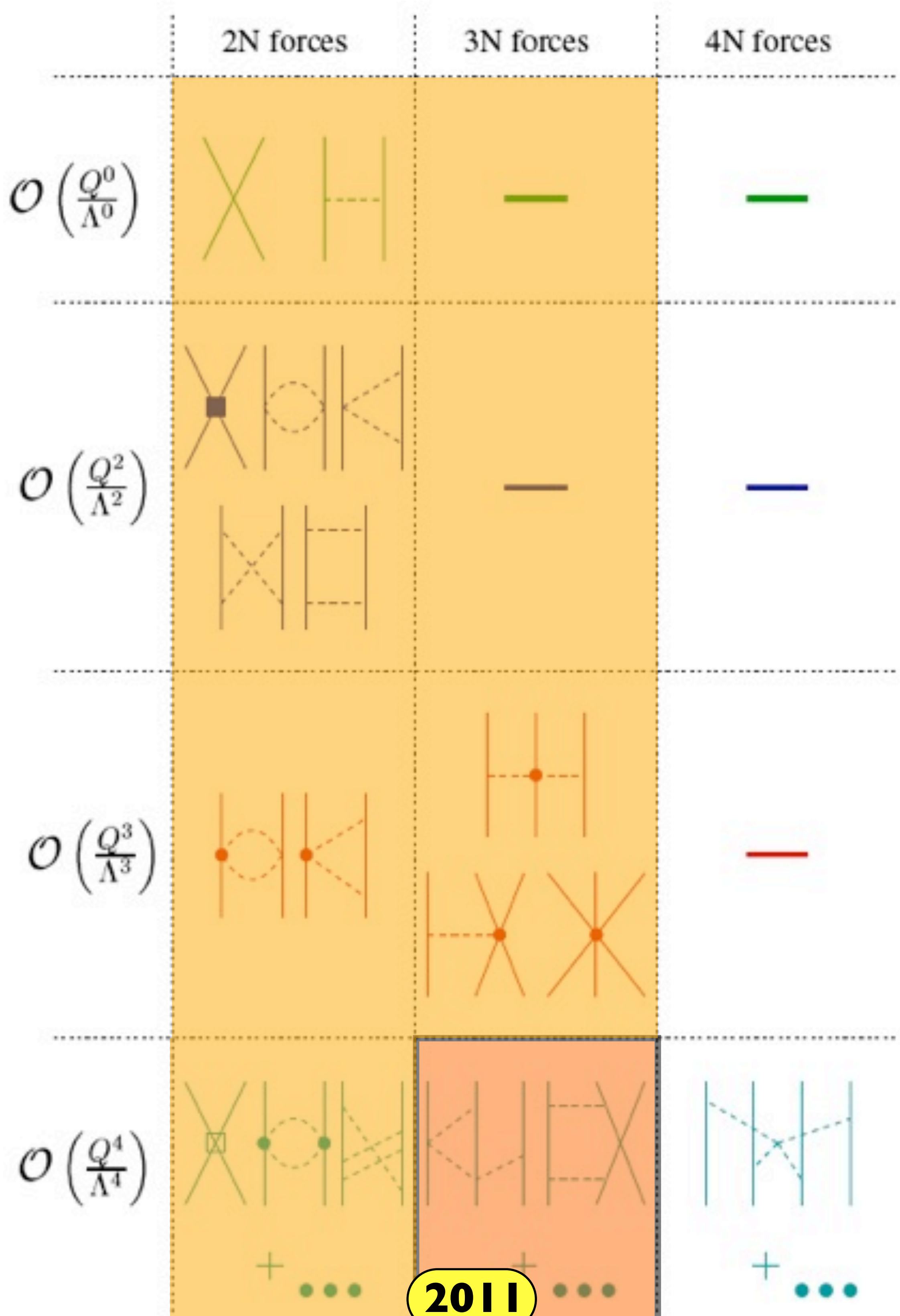
Chiral 3N forces at subleading order (N^{3}LO)

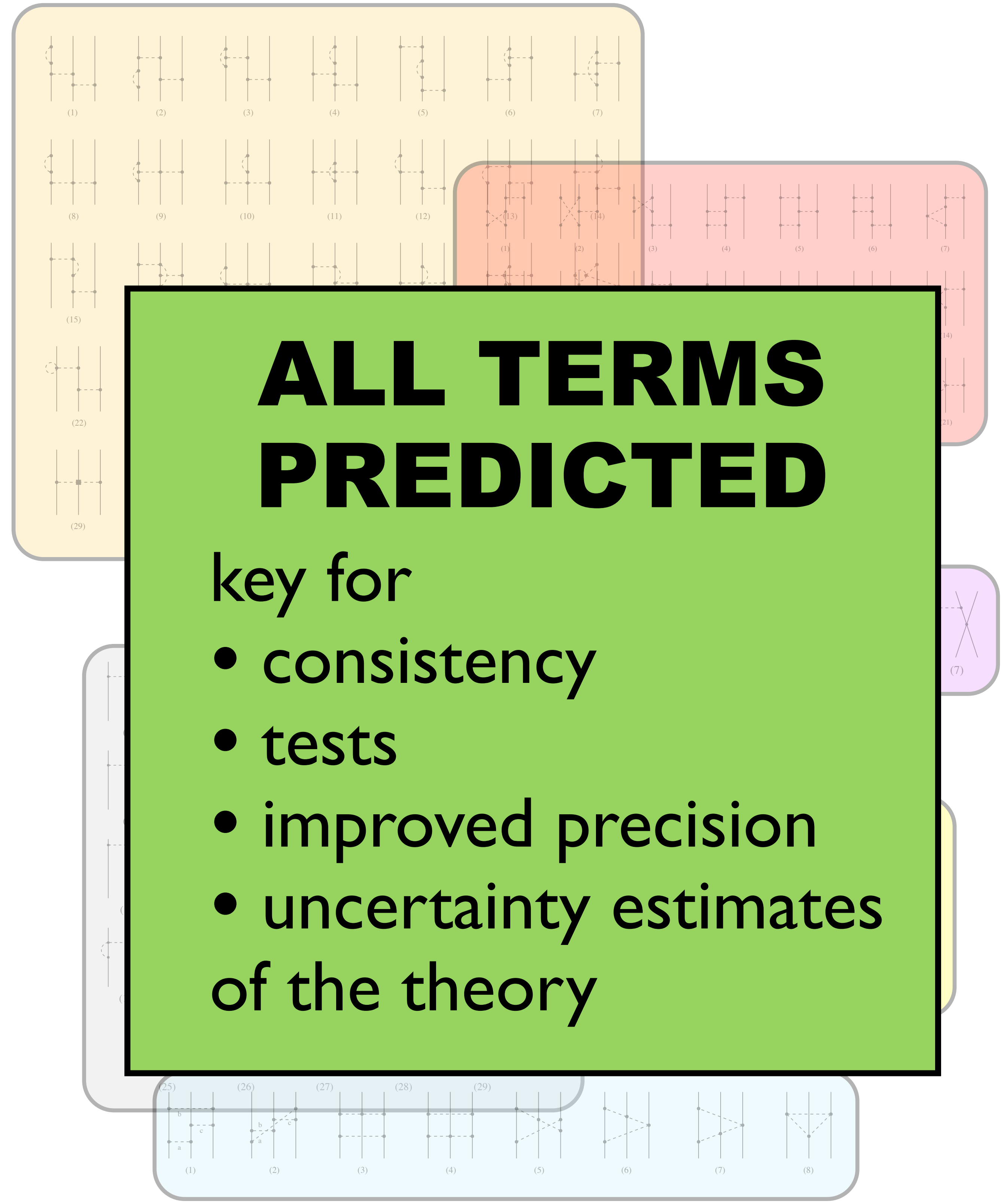




Bernard et al., PRC 77, 064004 (2008)
Bernard et al., PRC 84, 054001 (2011)
Krebs et al., PRC 85, 054006 (2012)
Krebs et al., PRC 87, 054007 (2013)

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





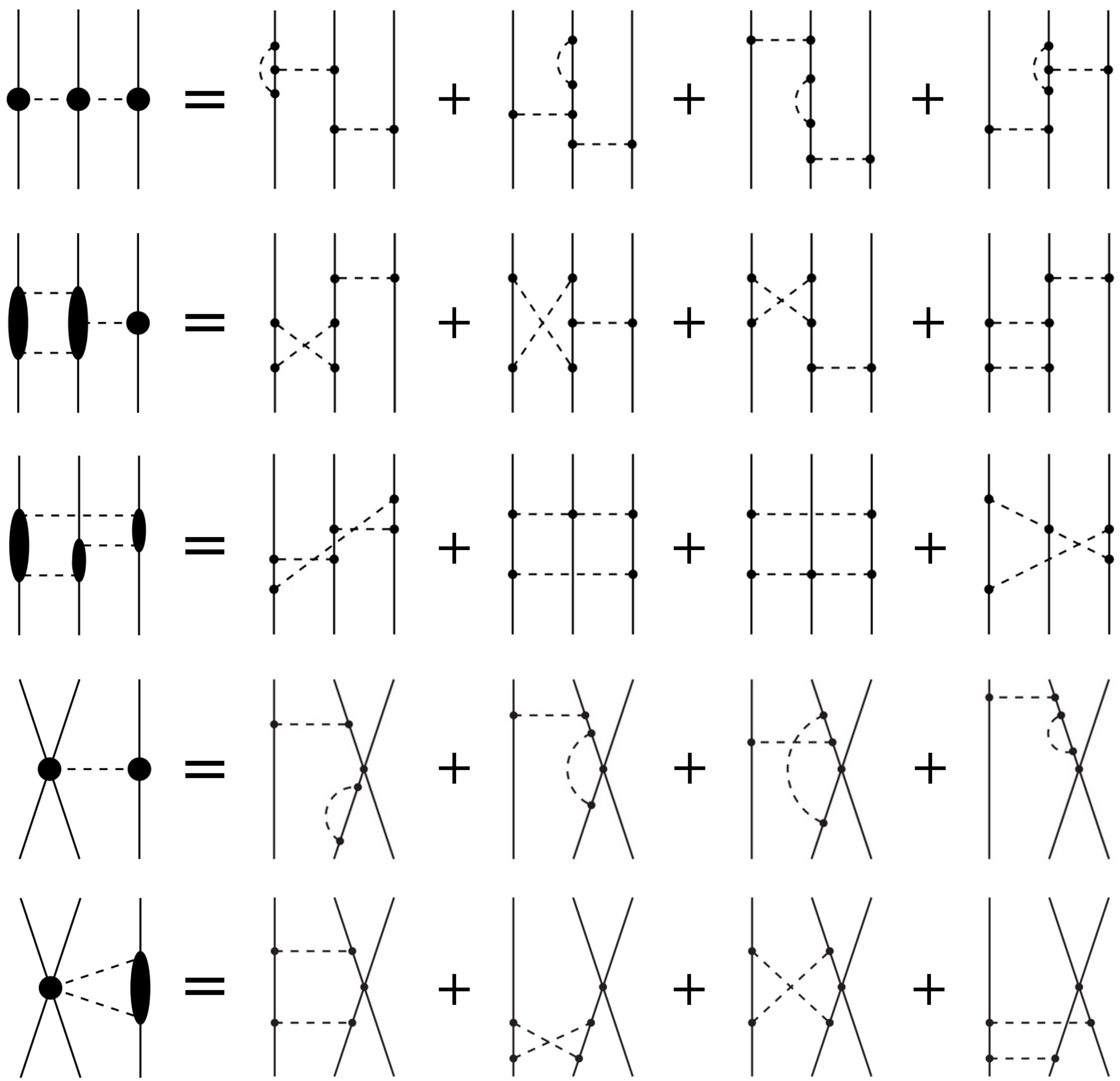
ALL TERMS PREDICTED

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

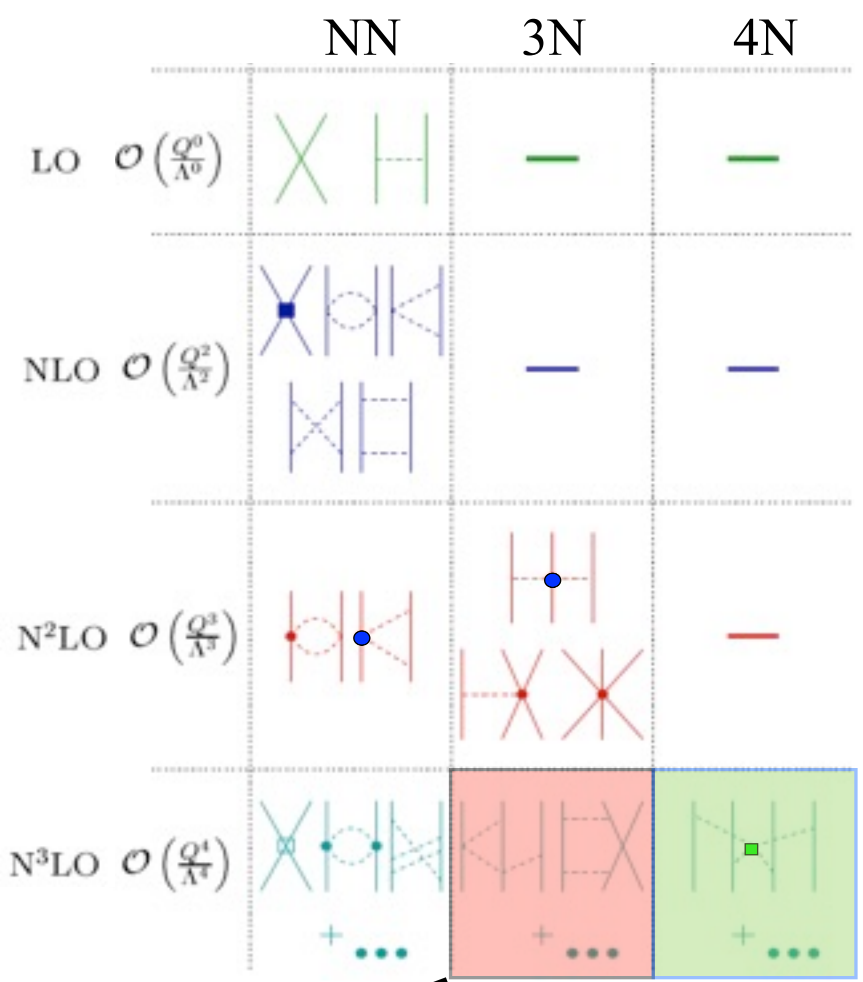
pion rings

1pi-contact

2pi-contact

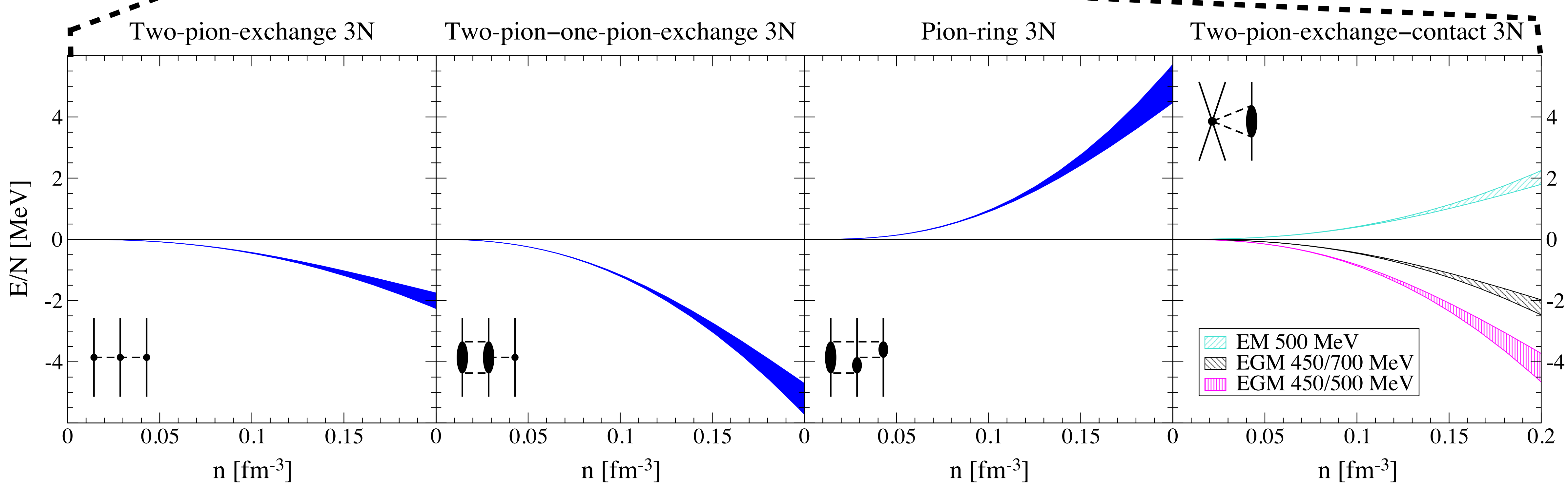
rel. corrections

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

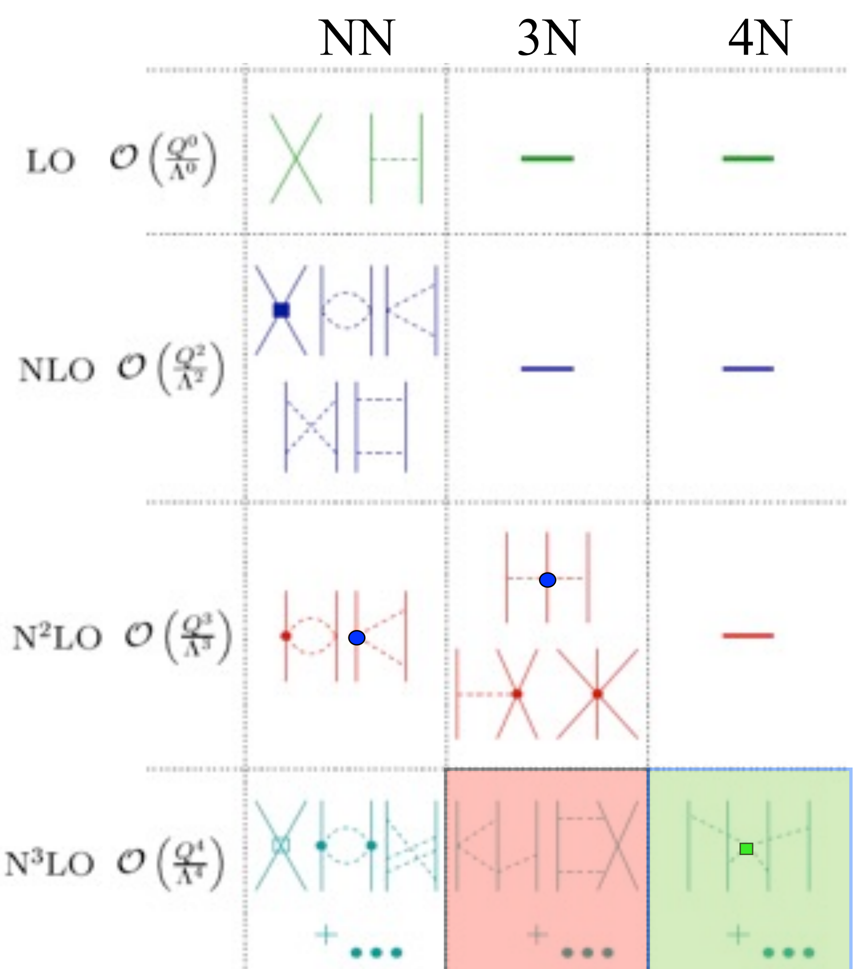


- first calculations of N^3LO 3NF and 4NF contributions to EOS of neutron matter
- found large contributions in Hartree Fock appr., comparable to size of N^2LO contributions

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

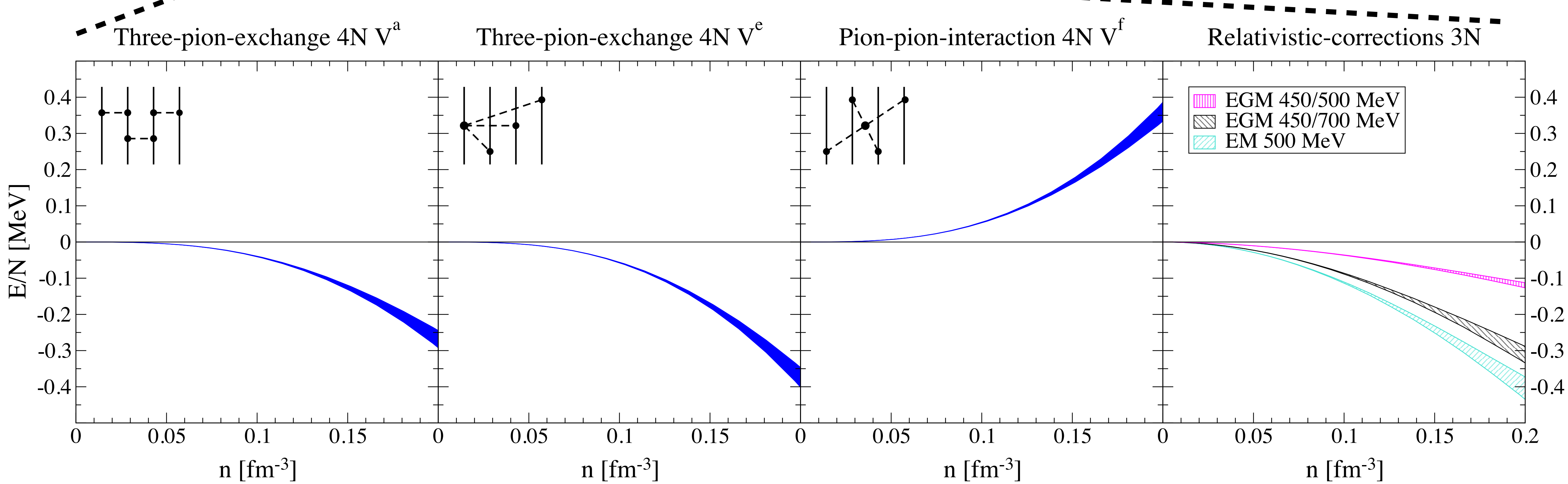


Contributions of many-body forces at N^{3}LO in neutron matter

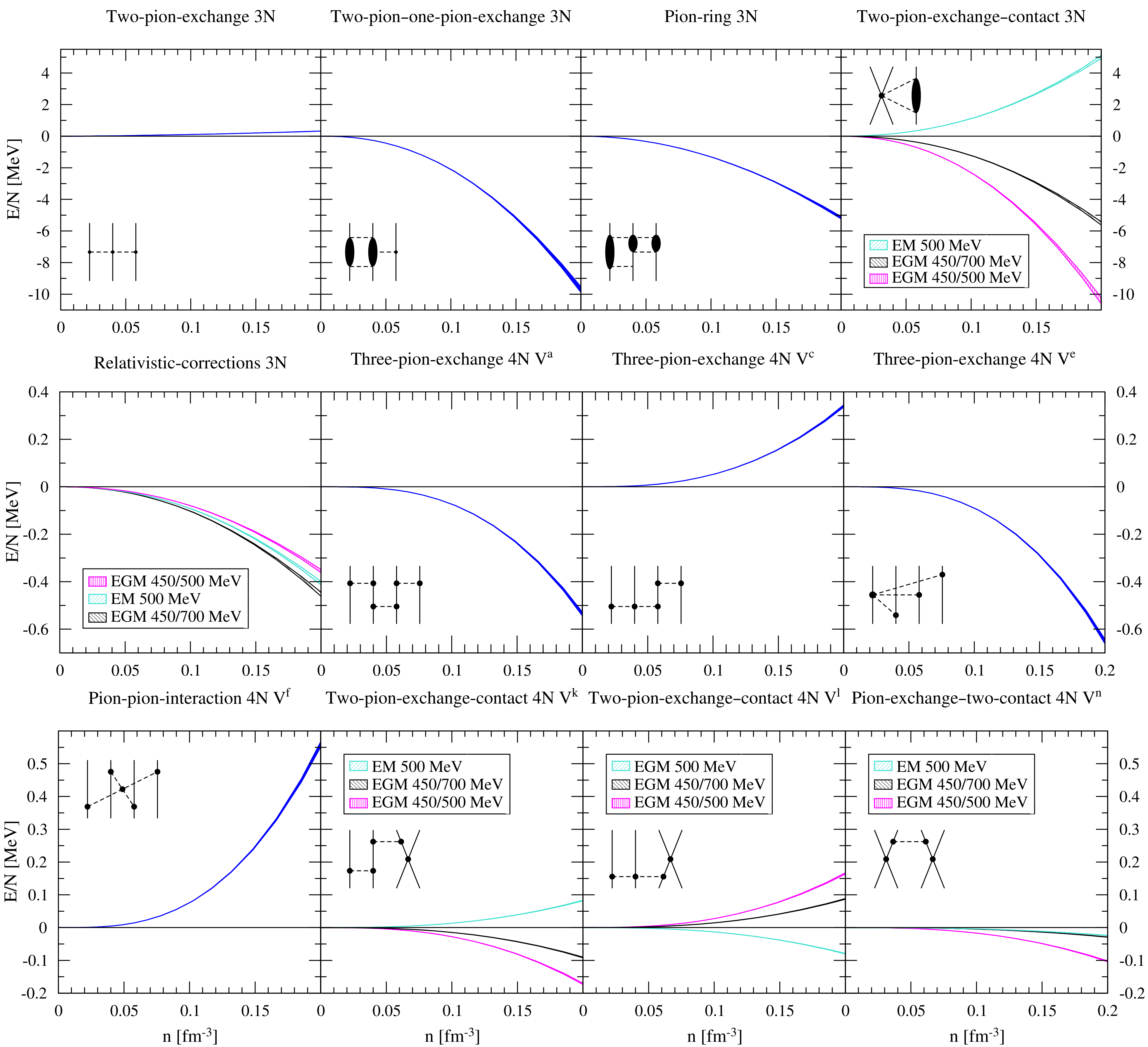


- first calculations of N^{3}LO 3NF and 4NF contributions to EOS of neutron matter
- found large contributions in Hartree Fock appr., comparable to size of N^{2}LO contributions
- 4NF contributions small

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

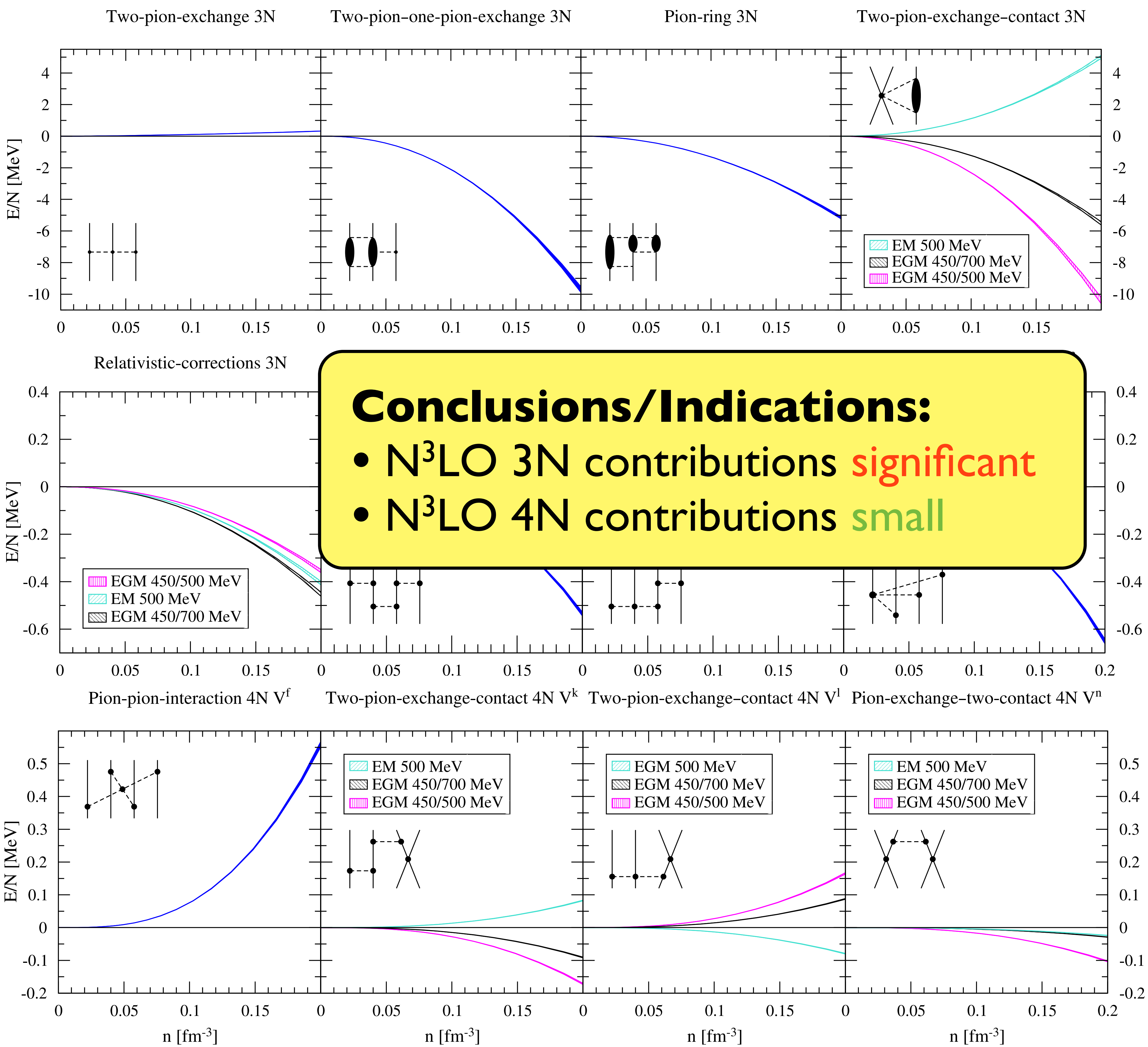


N^3LO contributions in nuclear matter (Hartree Fock)



Krüger, 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

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