Calculation and regularization of 3N interactions up to N3LO: status update and recent developments

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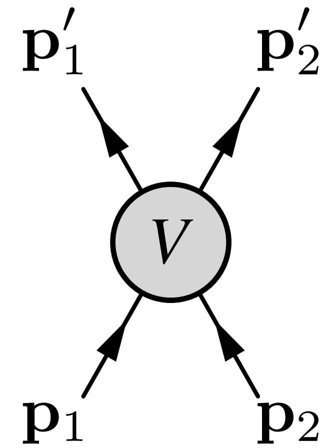
Regularization schemes for NN interactions

Separation of long- and short-range physics



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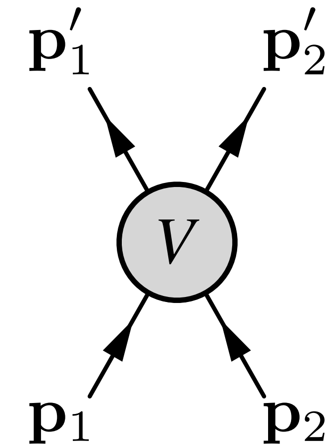

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nonlocal $$V_{\mathrm{NN}}(\mathbf{p},\mathbf{p}') \rightarrow \exp\left[-\left((p^2+p'^2)/\Lambda^2\right)^n\right] V_{\mathrm{NN}}(\mathbf{p},\mathbf{p}')$$

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

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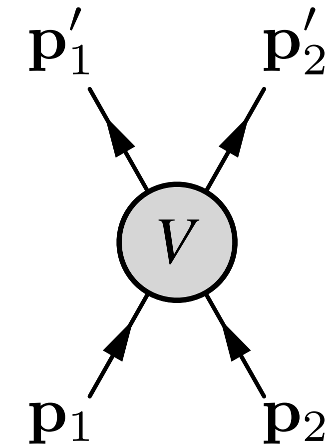

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(momentum space)

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

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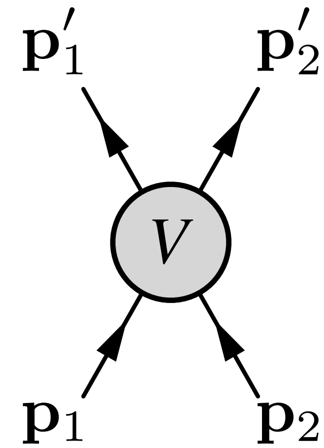

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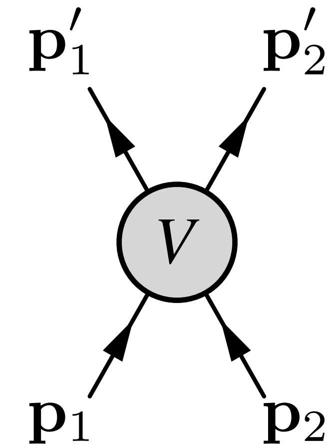
local (coordinate space)

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

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

Regularization schemes for NN interactions

Separation of long- and short-range physics



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

semi-local

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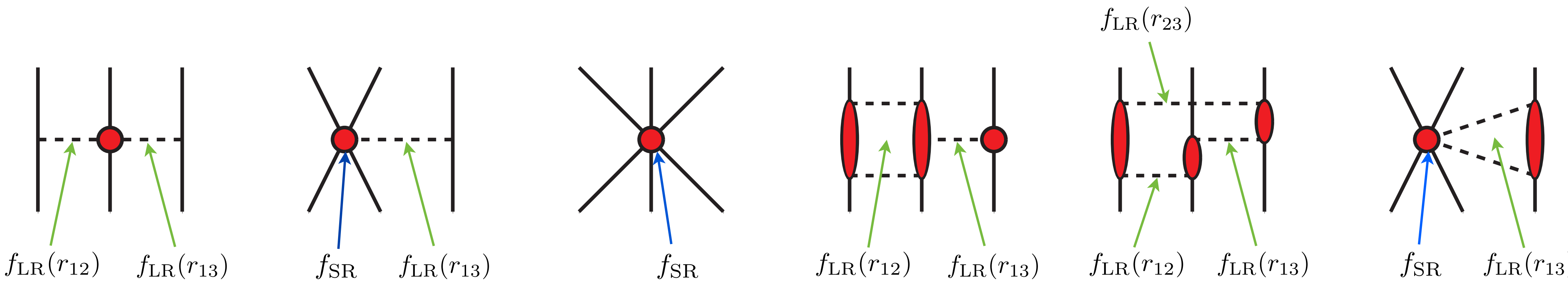
$$\delta(\mathbf{r}) \to C \to \exp\left[-\left((p^2 + p'^2)/\Lambda^2\right)^n\right] C$$

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

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



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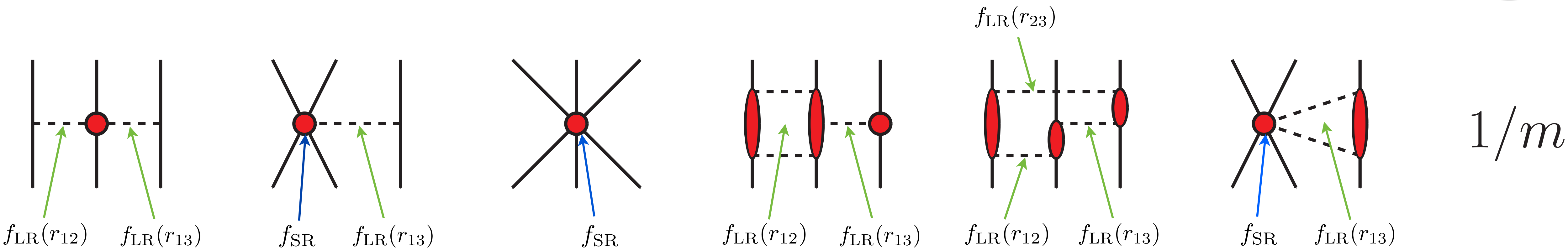


Computational strategy:

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

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:

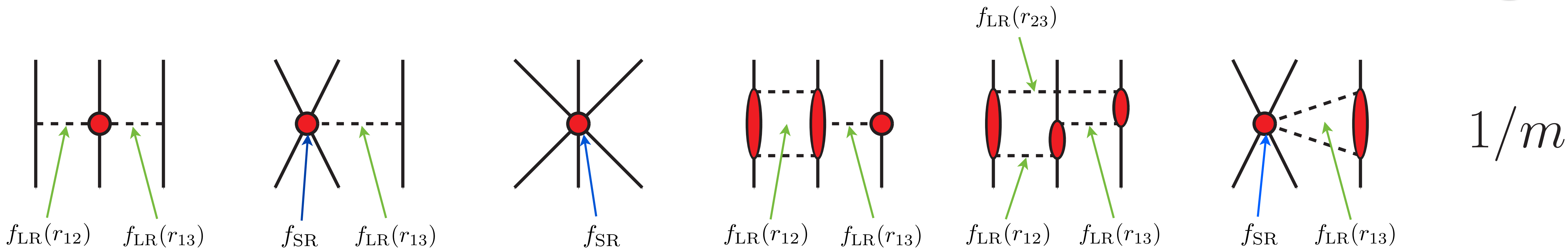
- use that all interaction contributions (except rel. corr.) are local:

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

$\longrightarrow$ 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

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



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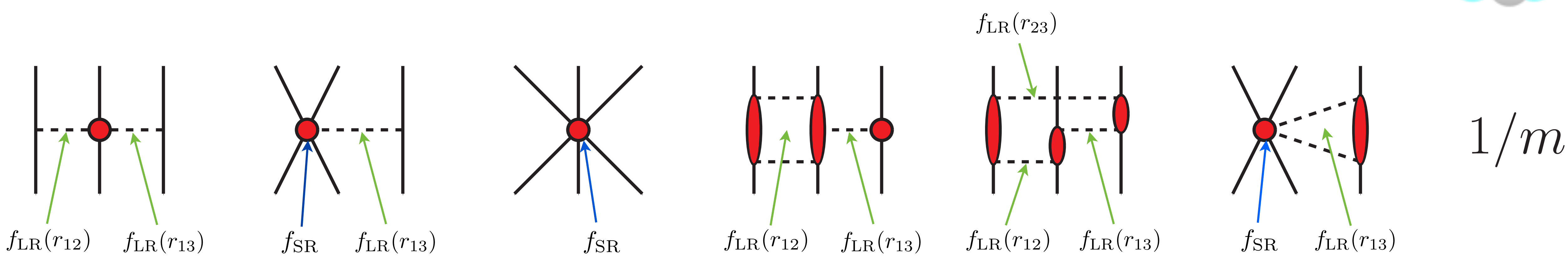

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(3) decompose regulator f_{LR} in partial wave momentum basis

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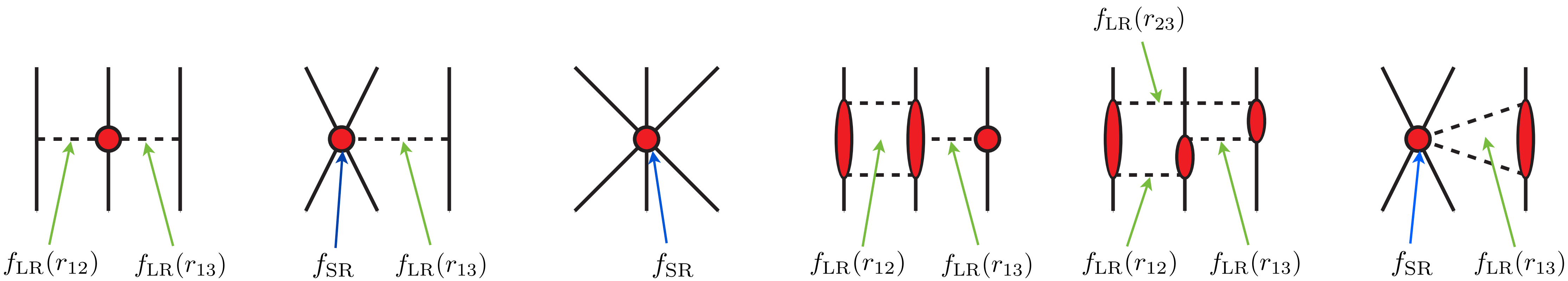

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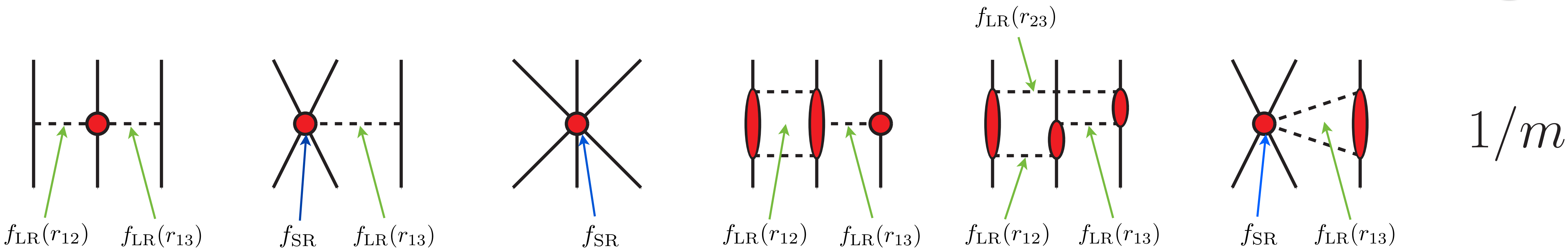
(4) perform convolution integrals:

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

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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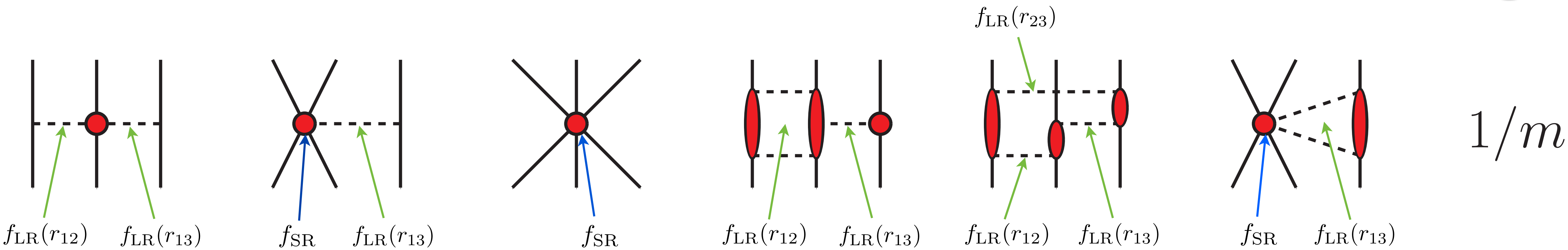

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(5) regularize short-range parts in interactions with non-local regulator

(6) antisymmetrize interactions (optional)

Calculation of convolution integrals: option one

$$V_{reg}(\mathbf{r}_{12}, \mathbf{r}_{13}, \mathbf{r}_{23}) = V(\mathbf{r}_{12}, \mathbf{r}_{13}, \mathbf{r}_{23}) F(r_{12}) F(r_{13}) F(r_{23})$$

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with $F(r_{ij}) = (1 - \exp(-r_{ij}^2/R^2))^{n_{exp}}$

Calculation of convolution integrals:
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Problem:
for practical calculation of the convolution integrals we need to explicitly separate the delta function part

$$\langle \mathbf{pq}|V_{reg}|\mathbf{p}'\mathbf{q}'\rangle = \int d\tilde{\mathbf{p}}d\tilde{\mathbf{q}}\,\langle \mathbf{pq}|V|\tilde{\mathbf{p}}\tilde{\mathbf{q}}\rangle\,\langle \tilde{\mathbf{p}}\tilde{\mathbf{q}}|R|\mathbf{p}'\mathbf{q}'\rangle$$

$$= \boxed{\int d\tilde{\mathbf{p}}d\tilde{\mathbf{q}}\,\langle \mathbf{pq}|V|\tilde{\mathbf{p}}\tilde{\mathbf{q}}\rangle\,\langle \tilde{\mathbf{p}}\tilde{\mathbf{q}}|R-1|\mathbf{p}'\mathbf{q}'\rangle} + \boxed{\langle \mathbf{pq}|V|\mathbf{p}'\mathbf{q}'\rangle}$$

delicate cancellation!

Calculation of convolution integrals: option one

in practice the cancellation needs to happen between even more than two terms

Calculation of convolution integrals: option one

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The regulator can be Fourier transformed analytically by expanding all binomials and decompose them in partial waves separately:

$$\tilde{R}_1 = \int d^3\mathbf{r}_{12} d^3\mathbf{r}_{23} e^{-i\mathbf{q}_1\cdot\mathbf{r}_{12}} e^{-i\mathbf{q}_3\cdot\mathbf{r}_{23}} e^{-\alpha_{12} r_{12}^2/R_0^2} = (2\pi)^3 \delta(\mathbf{q}_3) \left(\frac{\pi R_0^2}{\alpha_{12}}\right)^{3/2} e^{-R_0^2 q_1^2/(4\alpha_{12})}$$

$$\tilde{R}_2 = \int d^3\mathbf{r}_{12} d^3\mathbf{r}_{23} e^{-i\mathbf{q}_1\cdot\mathbf{r}_{12}} e^{-i\mathbf{q}_3\cdot\mathbf{r}_{23}} e^{-\alpha_{13} r_{13}^2/R_0^2} = (2\pi)^3 \delta(\mathbf{q}_2) \left(\frac{\pi R_0^2}{\alpha_{13}}\right)^{3/2} e^{-R_0^2 q_1^2/(4\alpha_{13})}$$

$$\tilde{R}_3 = \int d^3\mathbf{r}_{12} d^3\mathbf{r}_{23} e^{-i\mathbf{q}_1\cdot\mathbf{r}_{12}} e^{-i\mathbf{q}_3\cdot\mathbf{r}_{23}} e^{-\alpha_{23} r_{23}^2/R_0^2} = (2\pi)^3 \delta(\mathbf{q}_1) \left(\frac{\pi R_0^2}{\alpha_{23}}\right)^{3/2} e^{-R_0^2 q_3^2/(4\alpha_{23})}$$

$$\tilde{R}_4 = \int d^3\mathbf{r}_{12} d^3\mathbf{r}_{23} e^{-i\mathbf{q}_1\cdot\mathbf{r}_{12}} e^{-i\mathbf{q}_3\cdot\mathbf{r}_{23}} e^{-(\alpha_{12} r_{12}^2 + \alpha_{13} r_{13}^2)/R_0^2} = \left(\frac{\pi R_0^2}{\alpha_{12}}\right)^{3/2} \left(\frac{\pi R_0^2}{\alpha_{13}}\right)^{3/2} e^{-R_0^2 q_2^2/(4\alpha_{12})} e^{-R_0^2 q_3^2/(4\alpha_{13})}$$

$$\tilde{R}_5 = \int d^3\mathbf{r}_{12} d^3\mathbf{r}_{23} e^{-i\mathbf{q}_1\cdot\mathbf{r}_{12}} e^{-i\mathbf{q}_3\cdot\mathbf{r}_{23}} e^{-(\alpha_{12} r_{12}^2 + \alpha_{23} r_{23}^2)/R_0^2} = \left(\frac{\pi R_0^2}{\alpha_{12}}\right)^{3/2} \left(\frac{\pi R_0^2}{\alpha_{23}}\right)^{3/2} e^{-R_0^2 q_1^2/(4\alpha_{12})} e^{-R_0^2 q_3^2/(4\alpha_{23})}$$

$$\tilde{R}_6 = \int d^3\mathbf{r}_{12} d^3\mathbf{r}_{23} e^{-i\mathbf{q}_1\cdot\mathbf{r}_{12}} e^{-i\mathbf{q}_3\cdot\mathbf{r}_{23}} e^{-(\alpha_{13} r_{13}^2 + \alpha_{23} r_{23}^2)/R_0^2} = \left(\frac{\pi R_0^2}{\alpha_{13}}\right)^{3/2} \left(\frac{\pi R_0^2}{\alpha_{23}}\right)^{3/2} e^{-R_0^2 q_1^2/(4\alpha_{13})} e^{-R_0^2 q_2^2/(4\alpha_{23})}$$

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Calculation of convolution integrals: option one

in practice the cancellation needs to happen between even more than two terms

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$$\tilde{R}_7 = \int d^3\mathbf{r}_{12} d^3\mathbf{r}_{23} e^{-i\mathbf{q}_1} \ldots \overline{\ldots 3 + \alpha_{13}\alpha_{23}}\Bigg)^{3/2} \exp[\ldots]$$

hard to decompose in partial waves for

$$\mathbf{q}_2 = \mathbf{p} - \mathbf{p}' - \frac{\mathbf{q} - \mathbf{q}'}{2}, \mathbf{q}_3 = -\mathbf{p} + \mathbf{p}' - \frac{\mathbf{q} - \mathbf{q}'}{2}$$

use instead:

$$\tilde{R}_1 = P_{123} \tilde{R}_3 P_{123}^{-1}$$

Calculation of convolution integrals:
option one

that means for the ring topology we obtain:

$$V_{reg}(\mathbf{r}_{12},\mathbf{r}_{13},\mathbf{r}_{23}) = V(\mathbf{r}_{12},\mathbf{r}_{13},\mathbf{r}_{23})F(r_{12})F(r_{13})F(r_{23})$$

$$R(r_{12},r_{13},r_{23}) = (1-e^{-r_{12}^2/R_0^2})^n(1-e^{-r_{13}^2/R_0^2})^n(1-e^{-r_{23}^2/R_0^2})^n$$

$$\boxed{V_{reg} = V + \tilde{R}_{123}V + \tilde{R}_3 V + P_{123}\tilde{R}_3 P_{123}^{-1}V + P_{123}^{-1}\tilde{R}_3 P_{123}V}$$

numerical problems, especially at large momenta:

- for large Jacobi momenta $V_{reg} \to 0$, but V does not!
- very delicate cancellation necessary

Calculation of convolution integrals:

option two: use preregularization

consider a N2LO long-range topology:

$$V(\mathbf{r}_{13}, \mathbf{r}_{23}) = \int \frac{d\mathbf{q}_1}{(2\pi)^3} \int \frac{d\mathbf{q}_2}{(2\pi)^3} e^{i\mathbf{q}_2 \cdot \mathbf{r}_{13}} e^{i\mathbf{q}_3 \cdot \mathbf{r}_{23}} V(\mathbf{q}_2, \mathbf{q}_3)$$

Calculation of convolution integrals:
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for the calculation of the regularized interaction we insert an identity

$$V_{\rm reg}(\mathbf{r}_{13},\mathbf{r}_{23}) = V(\mathbf{r}_{13},\mathbf{r}_{23}) \frac{Q(r_{13}^2)}{Q(r_{13}^2)} \frac{Q(r_{23}^2)}{Q(r_{23}^2)} \left(1 - e^{-r_{13}^2/R^2}\right)^6 \left(1 - e^{-r_{23}^2/R^2}\right)^6$$

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and define a *preregularized* interaction:

$$V_{\rm prereg}(\mathbf{q}_2, \mathbf{q}_3) = \int d\mathbf{r}_{13} \int d\mathbf{r}_{23} e^{-i\mathbf{q}_2 \cdot \mathbf{r}_{13}} e^{-i\mathbf{q}_3 \cdot \mathbf{r}_{23}} Q(r_{13}^2) Q(r_{23}^2) V(\mathbf{r}_{13}, \mathbf{r}_{23}) = Q(-\Delta_{q_2}) Q(-\Delta_{q_3}) V(\mathbf{q}_2, \mathbf{q}_3)$$

Calculation of convolution integrals:

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$$V_{\mathrm{reg}}(\mathbf{r}_{13}, \mathbf{r}_{23}) = V(\mathbf{r}_{13}, \mathbf{r}_{23}) \frac{Q(r_{13}^2)}{Q(r_{13}^2)} \frac{Q(r_{23}^2)}{Q(r_{23}^2)} \left(1 - e^{-r_{13}^2/R^2}\right)^6 \left(1 - e^{-r_{23}^2/R^2}\right)^6$$

and define a *preregularized* interaction:

$$V_{\mathrm{prereg}}(\mathbf{q}_2, \mathbf{q}_3) = \int d\mathbf{r}_{13} \int d\mathbf{r}_{23} e^{-i\mathbf{q}_2\cdot\mathbf{r}_{13}} e^{-i\mathbf{q}_3\cdot\mathbf{r}_{23}} Q(r_{13}^2) Q(r_{23}^2) V(\mathbf{r}_{13}, \mathbf{r}_{23}) = Q(-\Delta_{q_2}) Q(-\Delta_{q_3}) V(\mathbf{q}_2, \mathbf{q}_3)$$

the *preregularized* regulator reads accordingly:

$$R_{\mathrm{prereg}}(\mathbf{q}_2, \mathbf{q}_3) = \int \frac{d\mathbf{r}_{13}}{(2\pi)^3} \int \frac{d\mathbf{r}_{23}}{(2\pi)^3} e^{-i\mathbf{q}_2\cdot\mathbf{r}_{13}} e^{-i\mathbf{q}_3\cdot\mathbf{r}_{23}} \frac{\left(1 - e^{-r_{13}^2/R^2}\right)^6 \left(1 - e^{-r_{23}^2/R^2}\right)^6}{Q(r_{13}^2) Q(r_{23}^2)}$$

Calculation of convolution integrals:

option two: use preregularization

consider a N2LO long-range topology:

$$V(\mathbf{r}_{13},\mathbf{r}_{23}) = \int \frac{d\mathbf{q}_1}{(2\pi)^3} \int \frac{d\mathbf{q}_2}{(2\pi)^3} e^{i\mathbf{q}_2\cdot\mathbf{r}_{13}} e^{i\mathbf{q}_3\cdot\mathbf{r}_{23}} V(\mathbf{q}_2,\mathbf{q}_3)$$

for the calculation of the regularized interaction we insert an identity

$$V_{\rm reg}(\mathbf{r}_{13},\mathbf{r}_{23}) = V(\mathbf{r}_{13},\mathbf{r}_{23}) \frac{Q(r_{13}^2)}{Q(r_{13}^2)} \frac{Q(r_{23}^2)}{Q(r_{23}^2)} \left(1-e^{-r_{13}^2/R^2}\right)^6 \left(1-e^{-r_{23}^2/R^2}\right)^6$$

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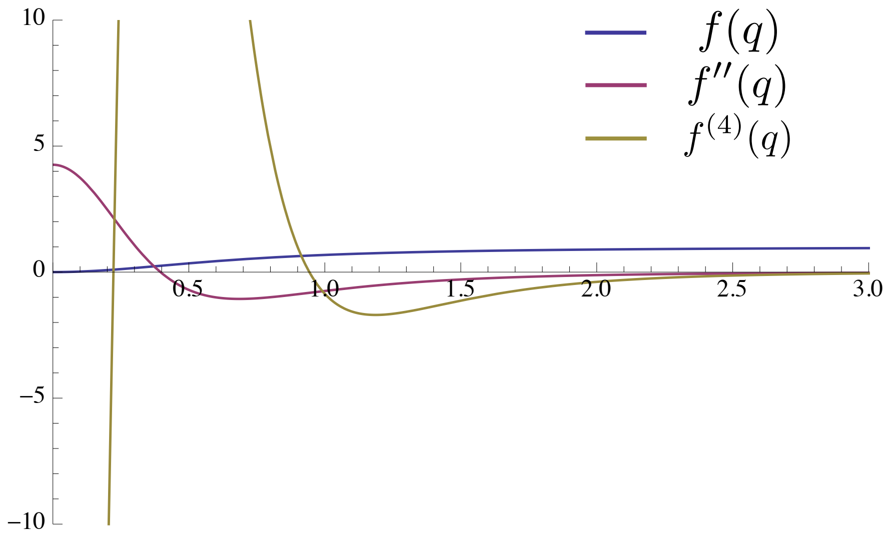
For $Q(r^2) = r^2, r^4$ all integrals are finite and can be calculated without subtraction!

Calculation of convolution integrals:
option two: use preregularization

comments and status:

- each application of Laplacians leads to more pronounced peak structures for interactions, try to minimize number of derivatives



$$f(q) = \frac{q^2}{q^2 + m_\pi^2}$$

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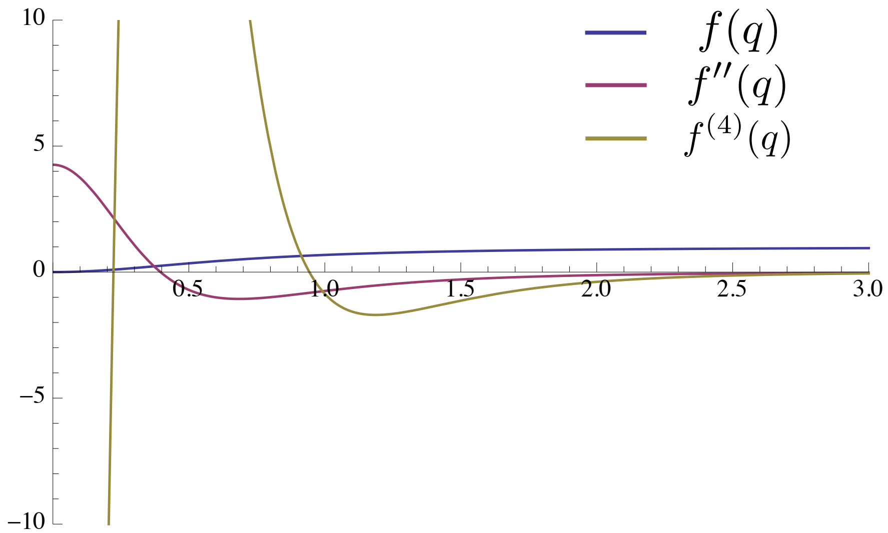

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• finished calculations of all N2LO matrix elements and also N3LO 2pi-contact matrix elements (using $Q(r^2) = r^2$) up to J=7/2

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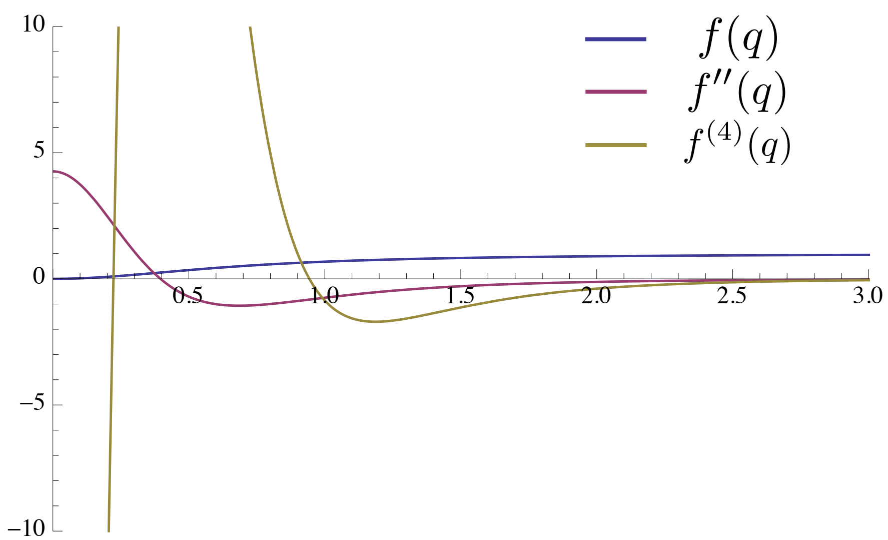

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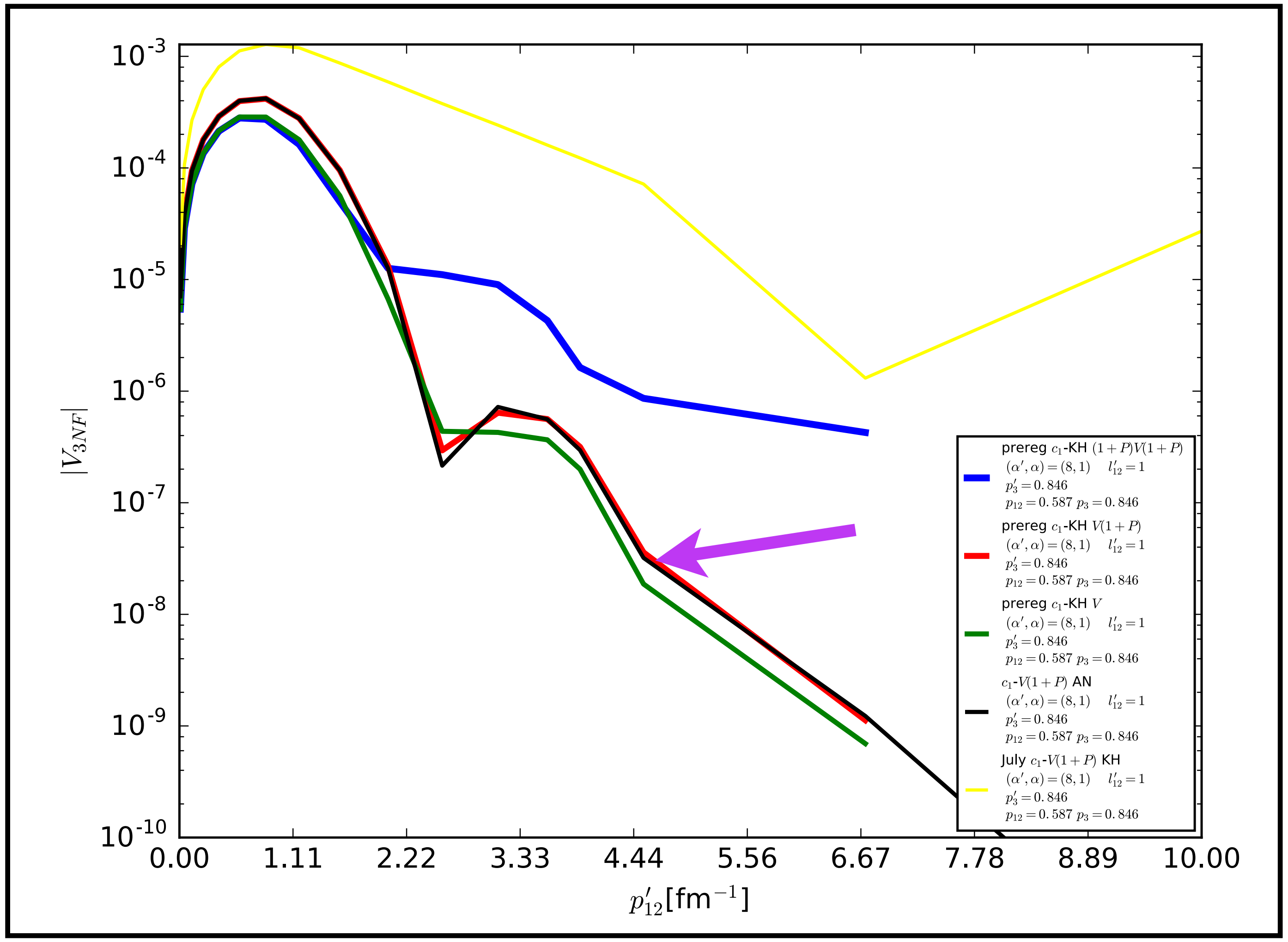
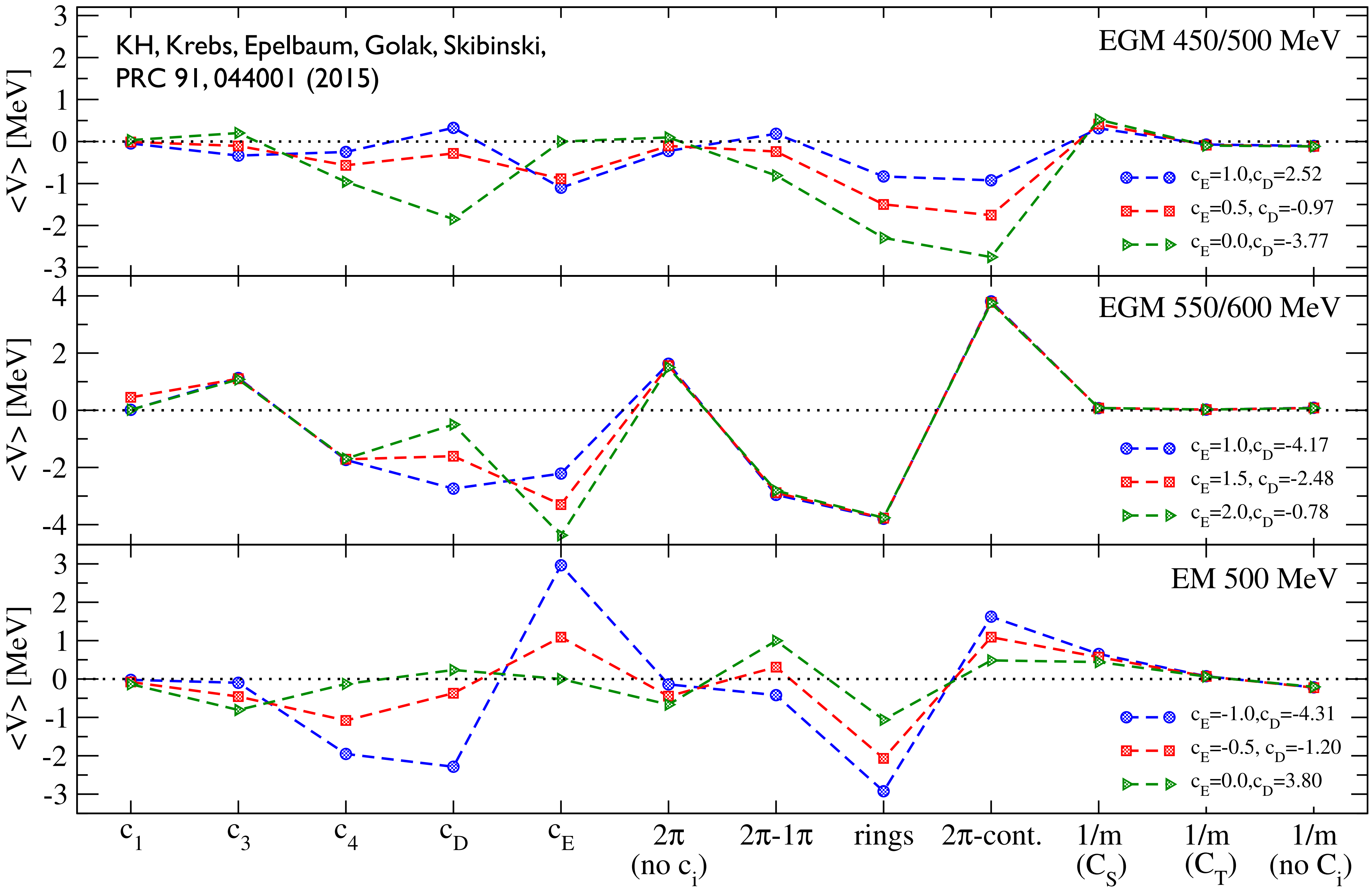


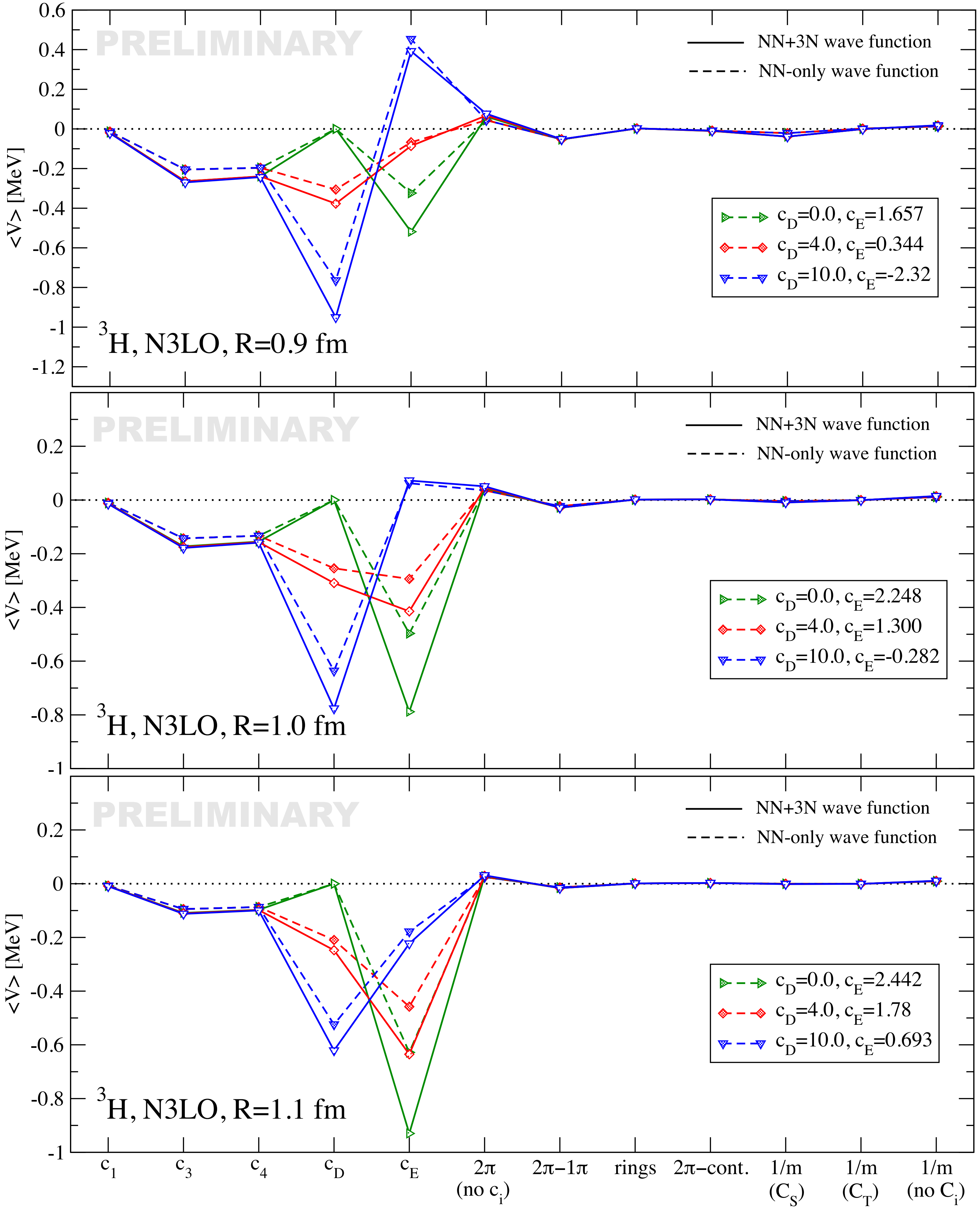
- finished calculations of all N2LO matrix elements and also N3LO 2pi-contact matrix elements (using $Q(r^2) = r^2$) up to J=7/2
- good agreement with previously calculated 3H expectation values
- excellent agreement with Andreas' results on matrix element level
- no numerical problems in first scattering benchmark calculations (Evgeny)

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



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

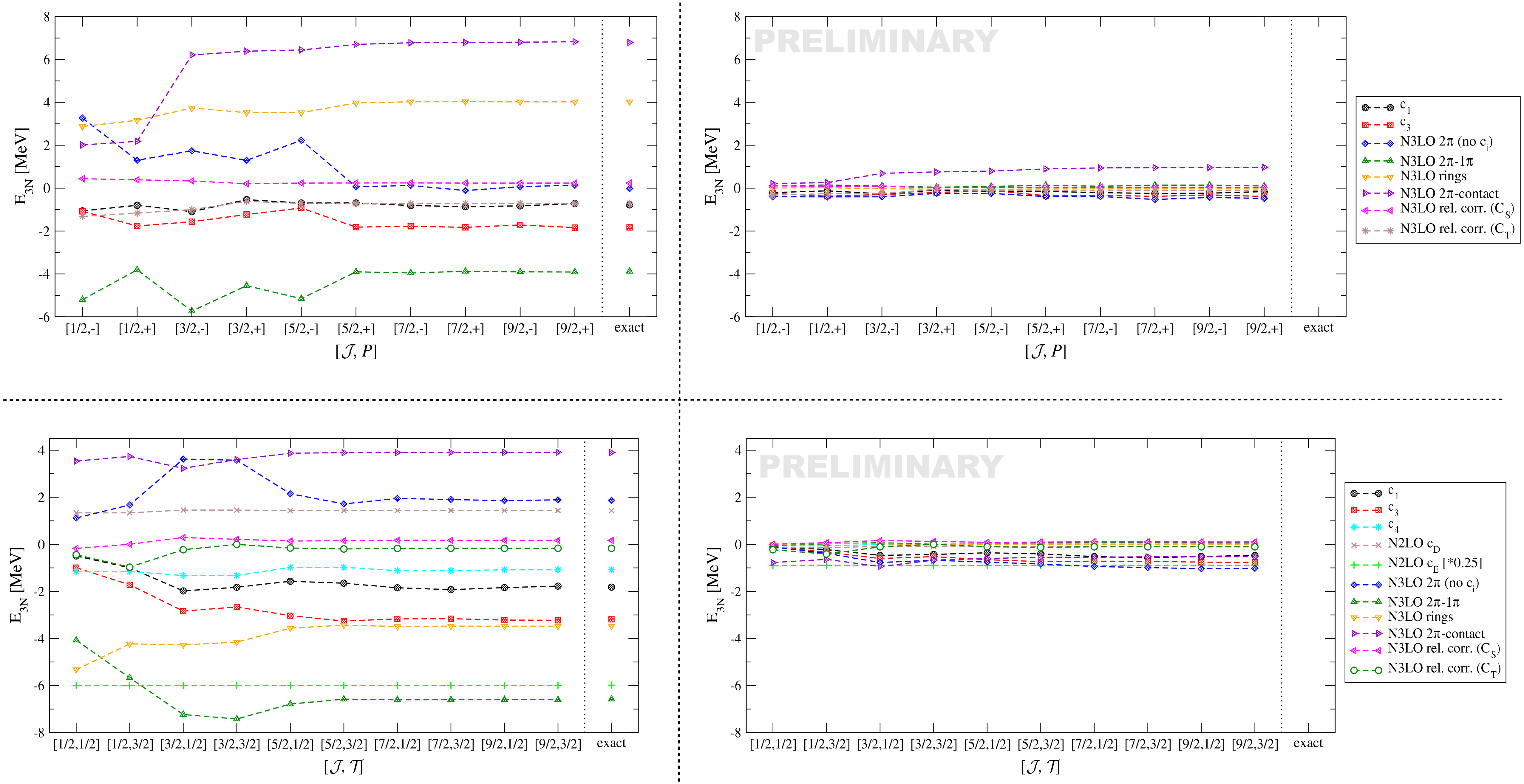
Hartree-Fock energy of infinite matter (based on old mat. elems.)

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 (based on old mat. elems.)

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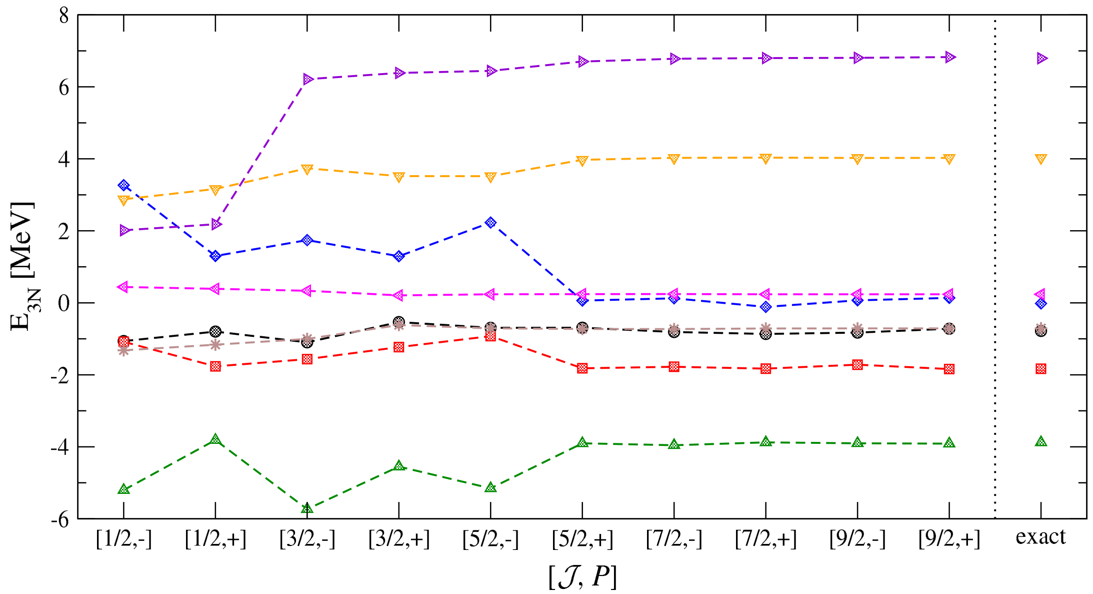

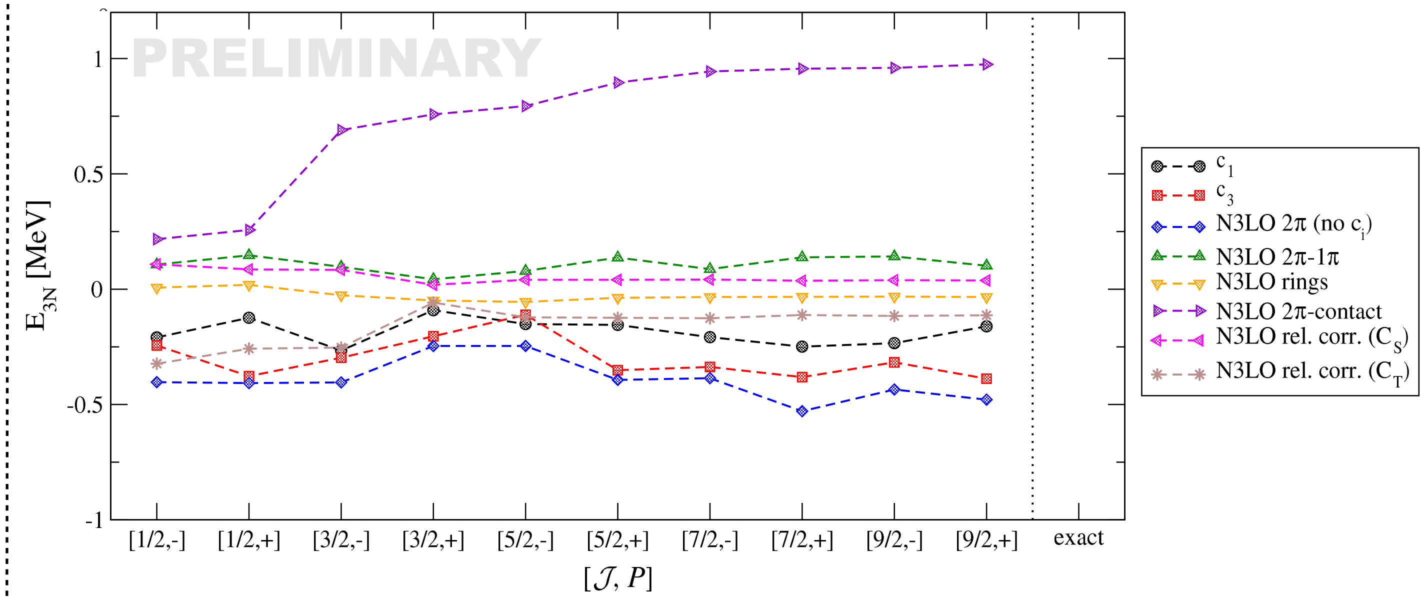

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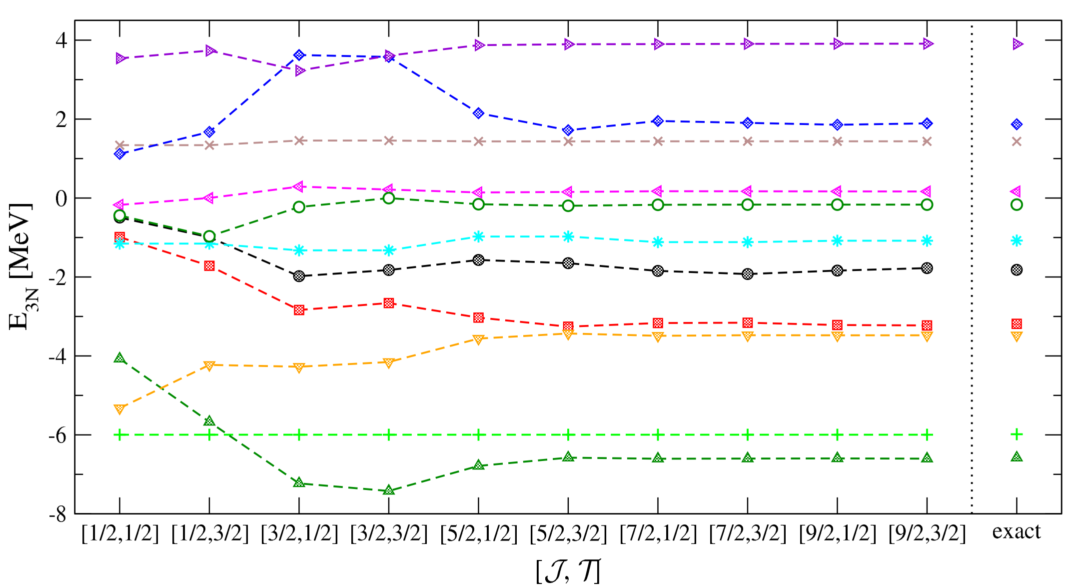

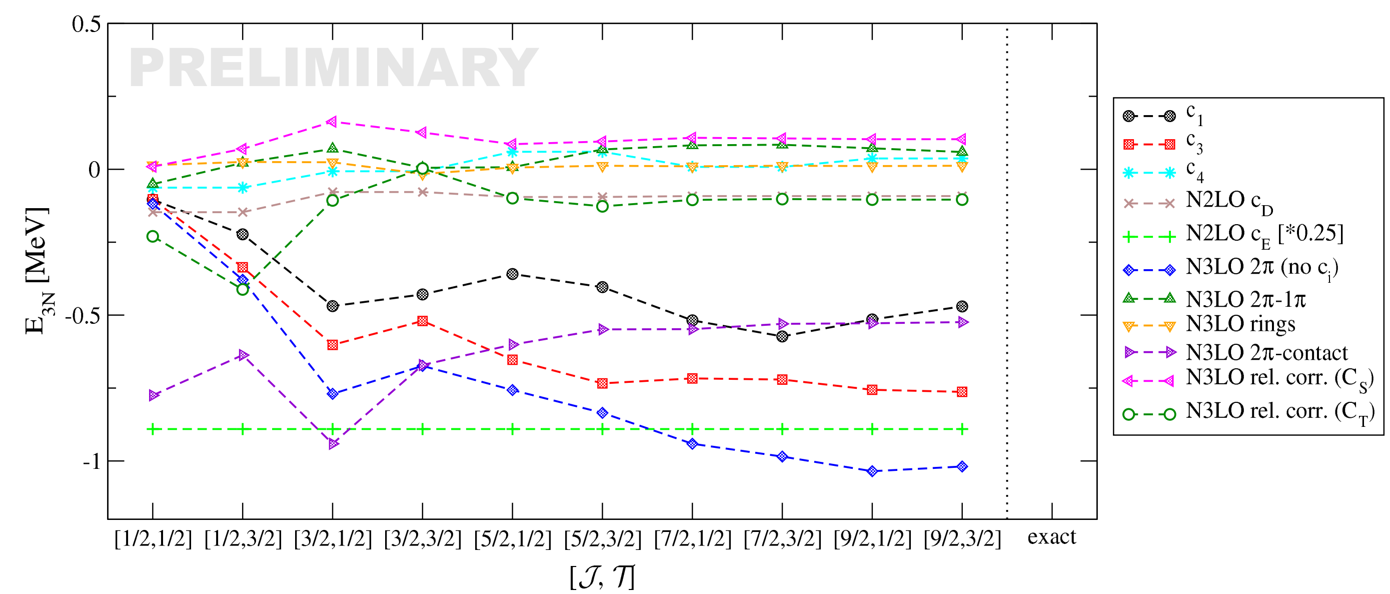

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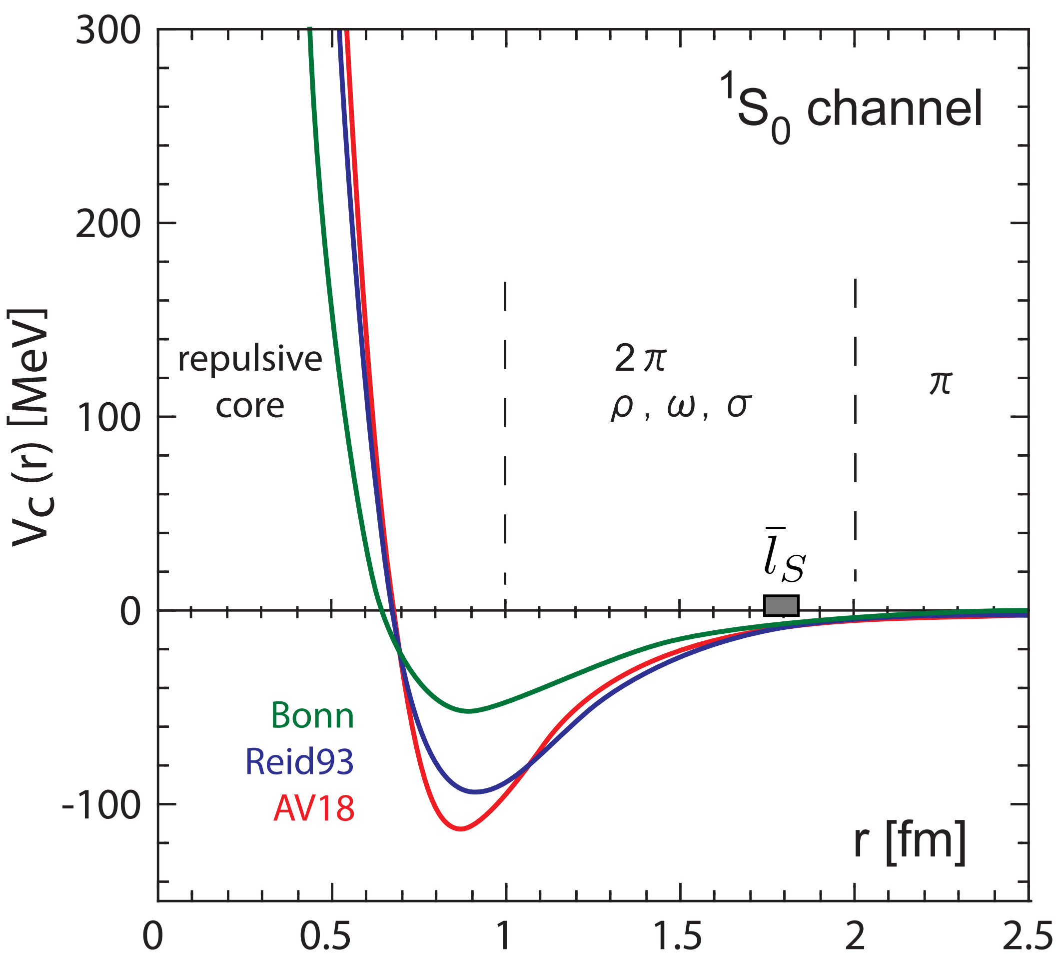
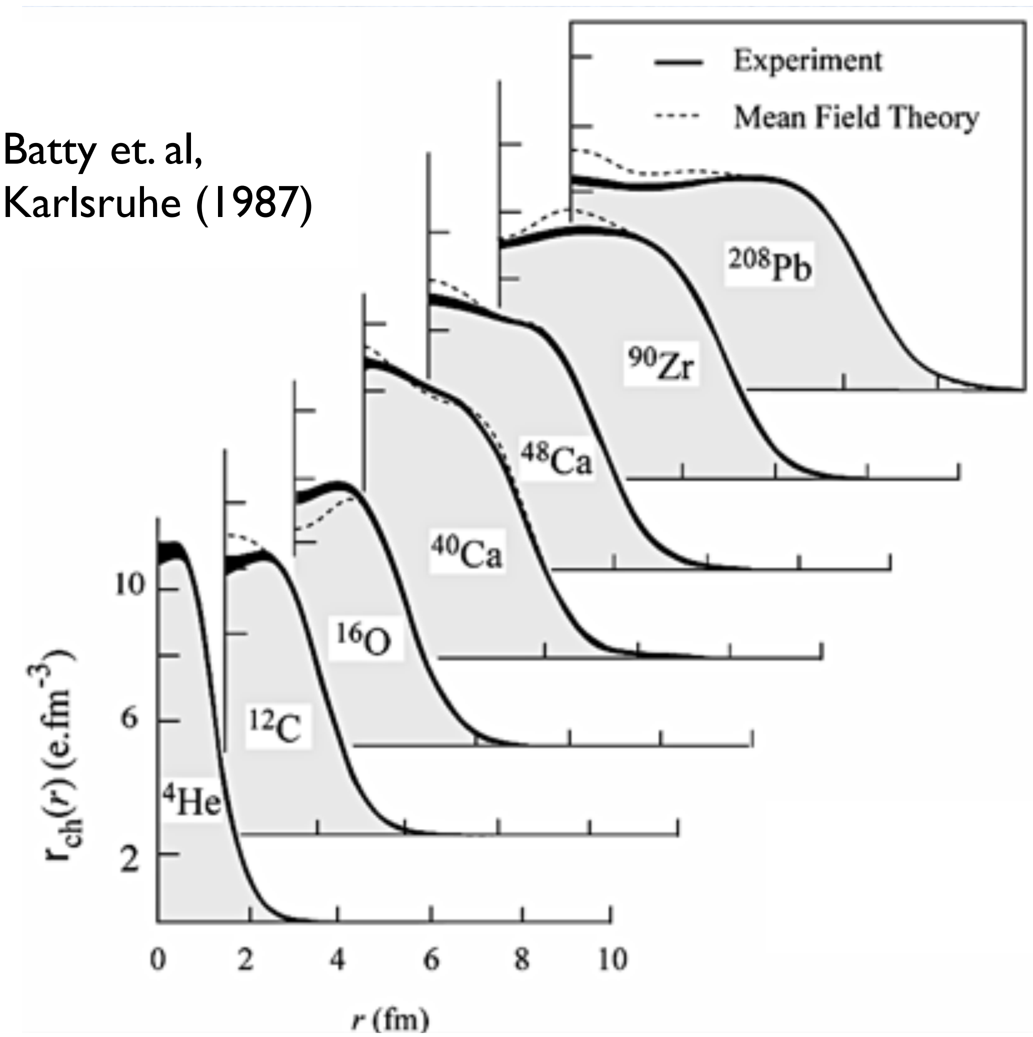
Equation of state of symmetric nuclear matter: nuclear saturation





Batty et. al, Karlsruhe (1987)

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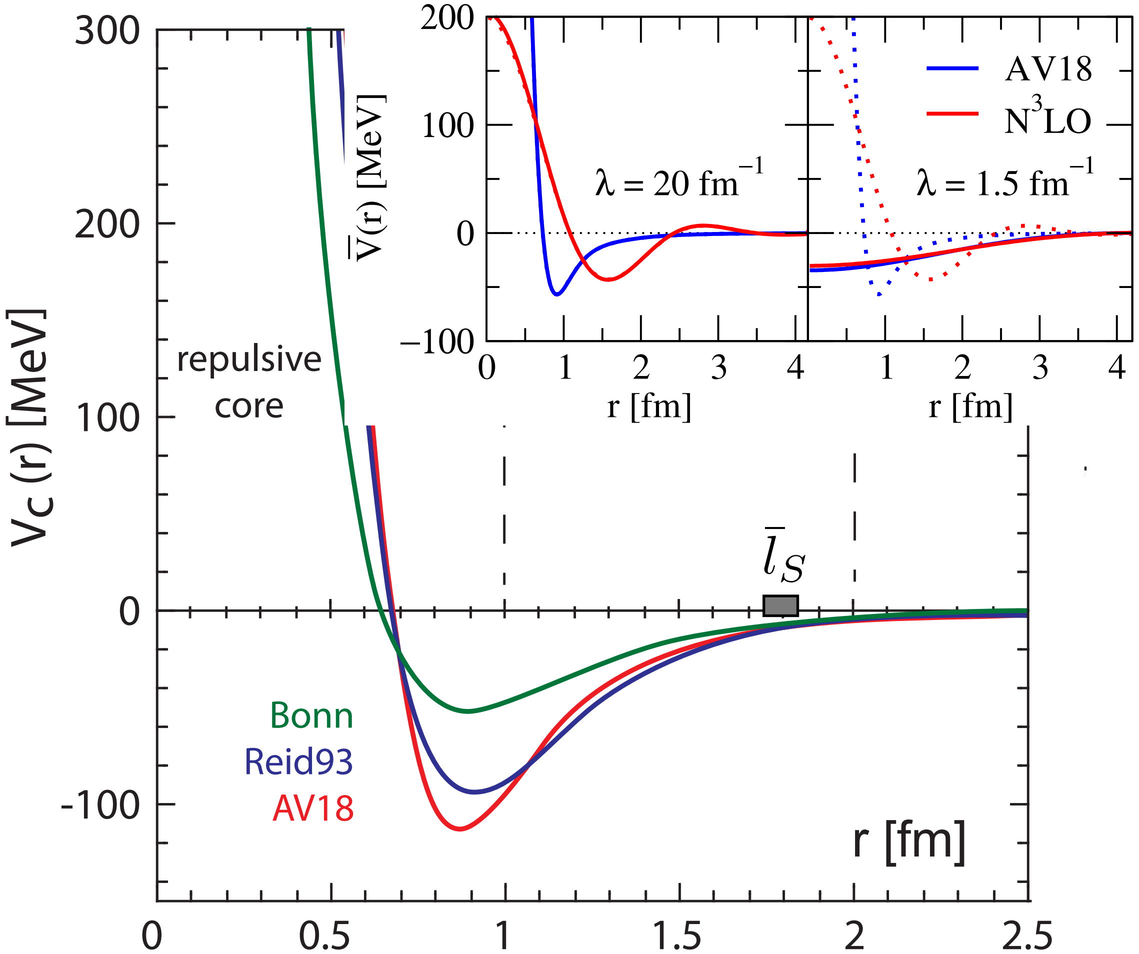

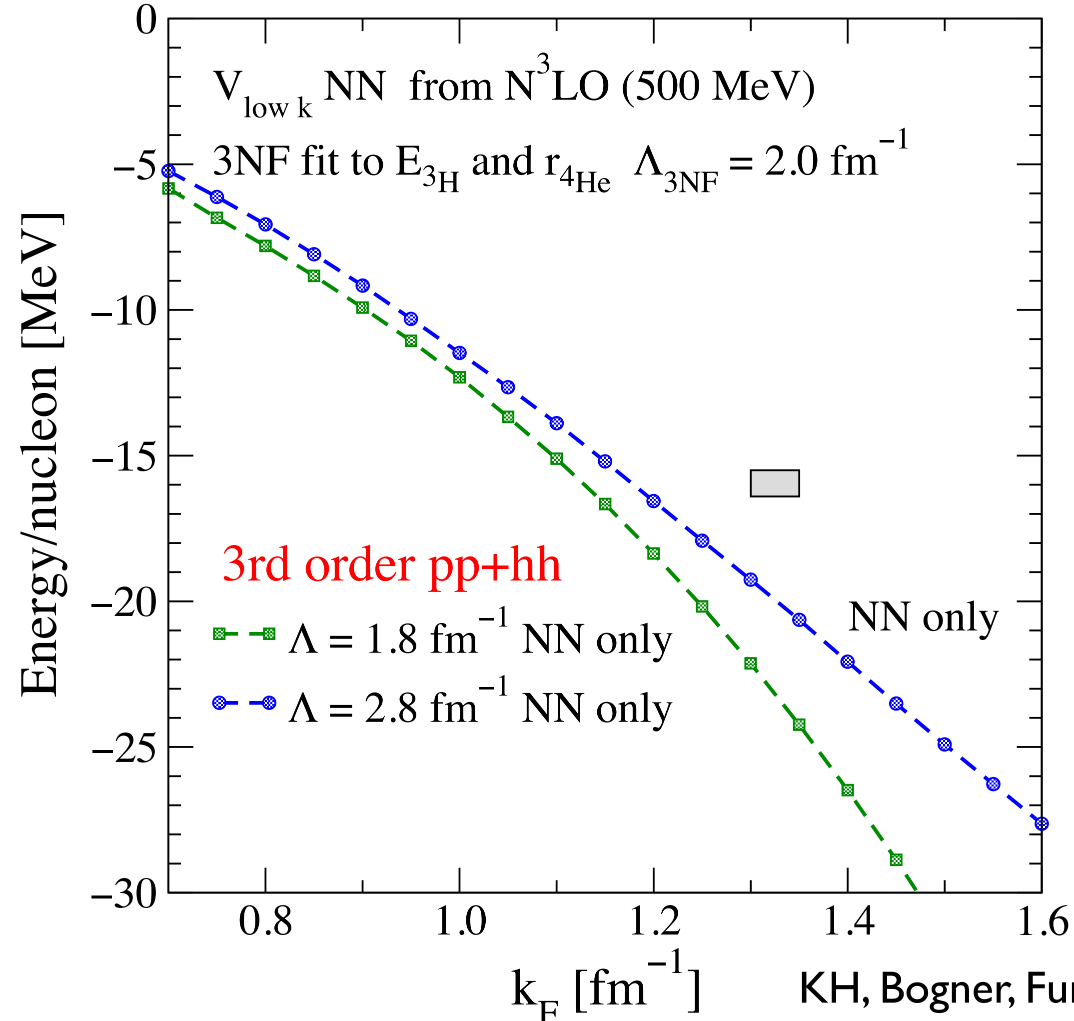

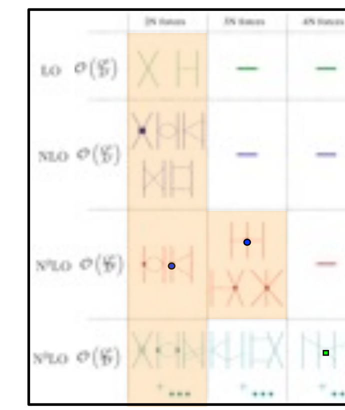

KH, Bogner, Furnstahl, Nogga, PRC(R) 83, 031301 (2011)

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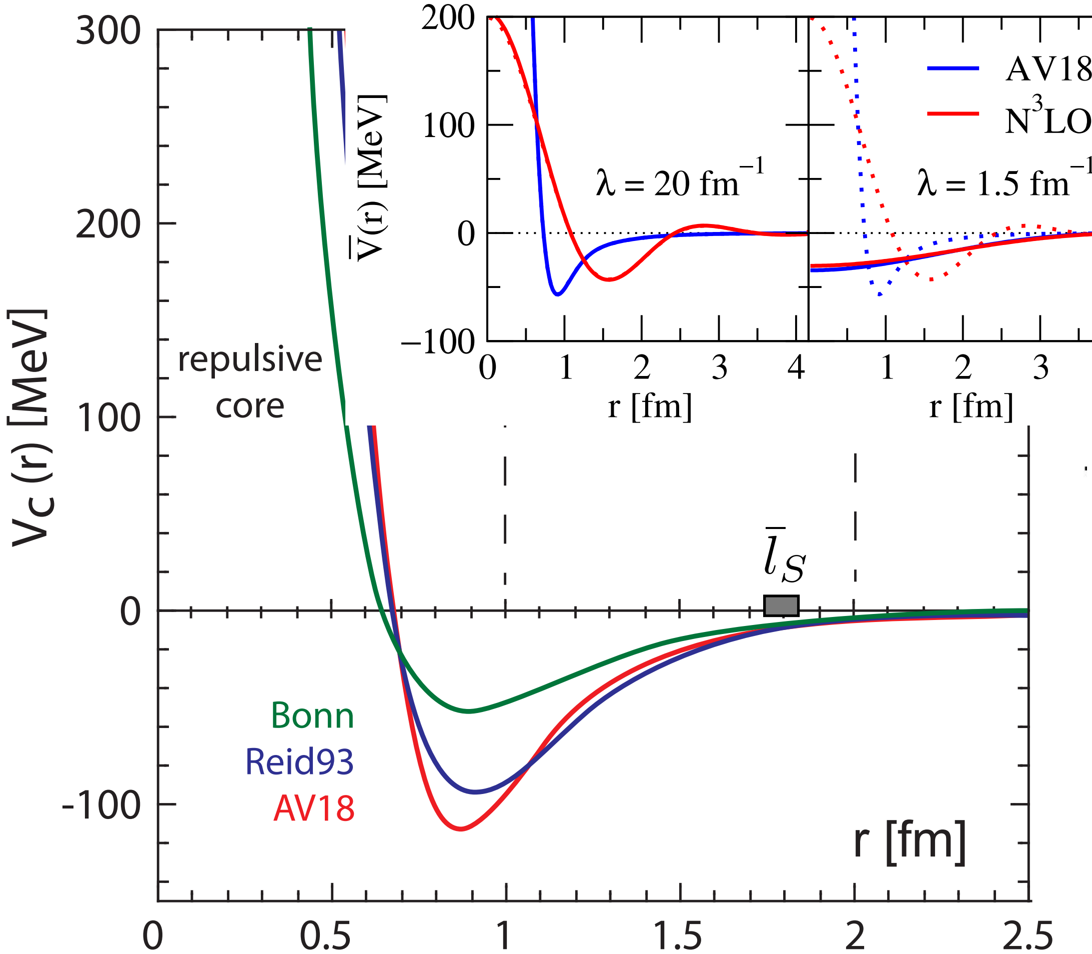

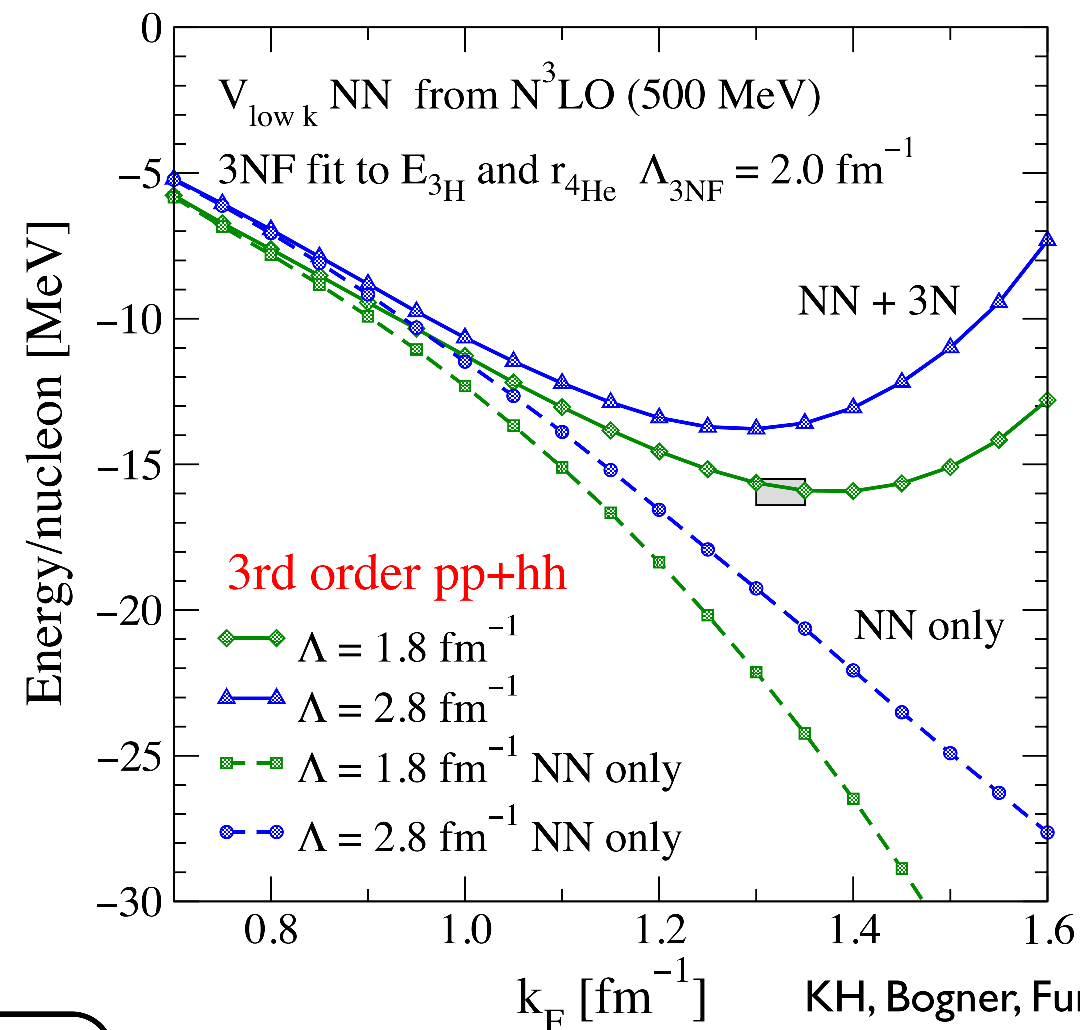

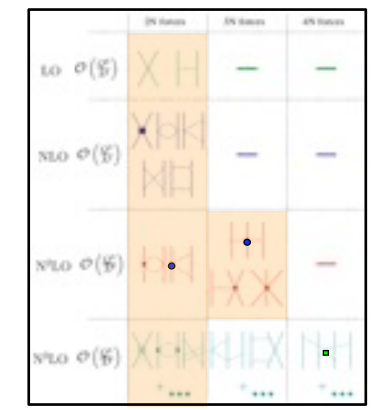

KH, Bogner, Furnstahl, Nogga, PRC(R) 83, 031301 (2011)

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

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

c_1, c_3, c_4 terms $\quad c_D$ term $\quad c_E$ term

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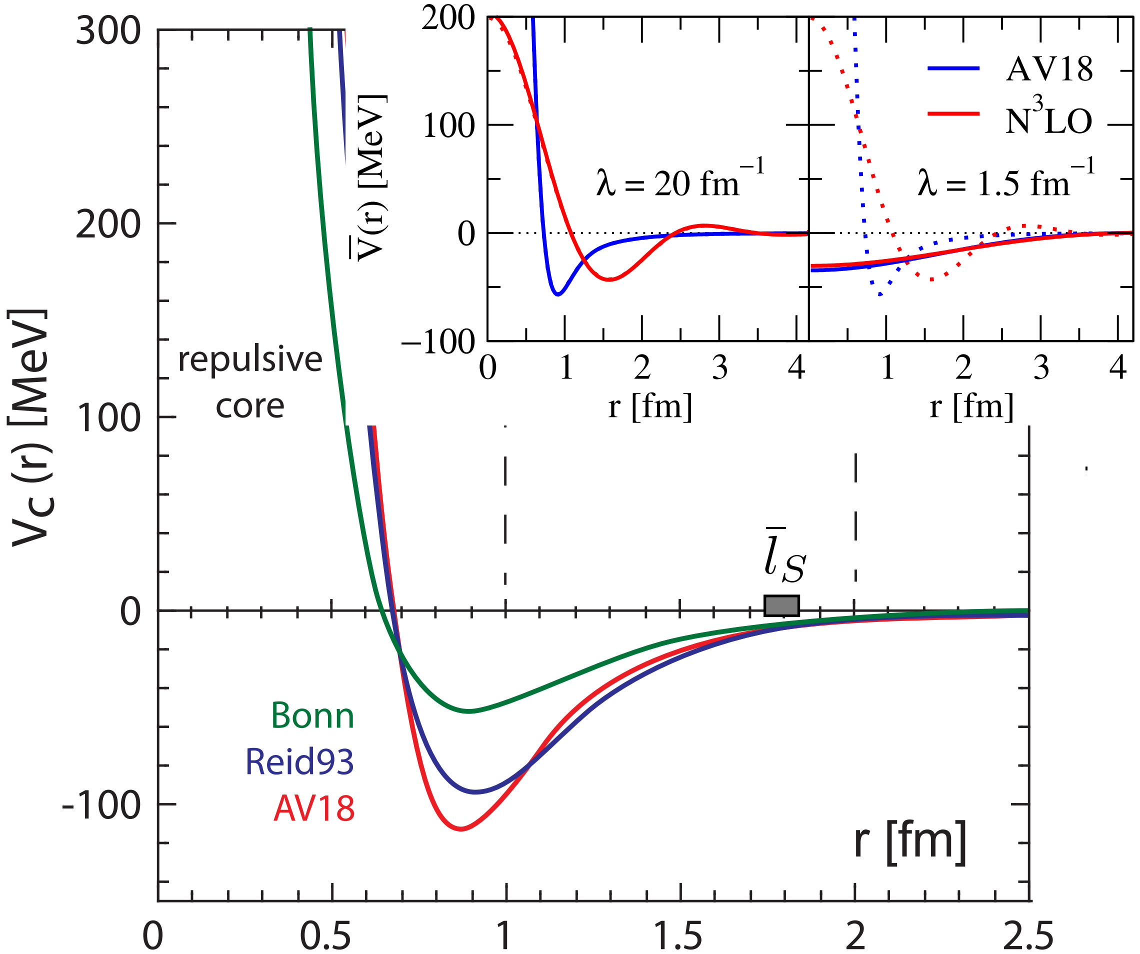

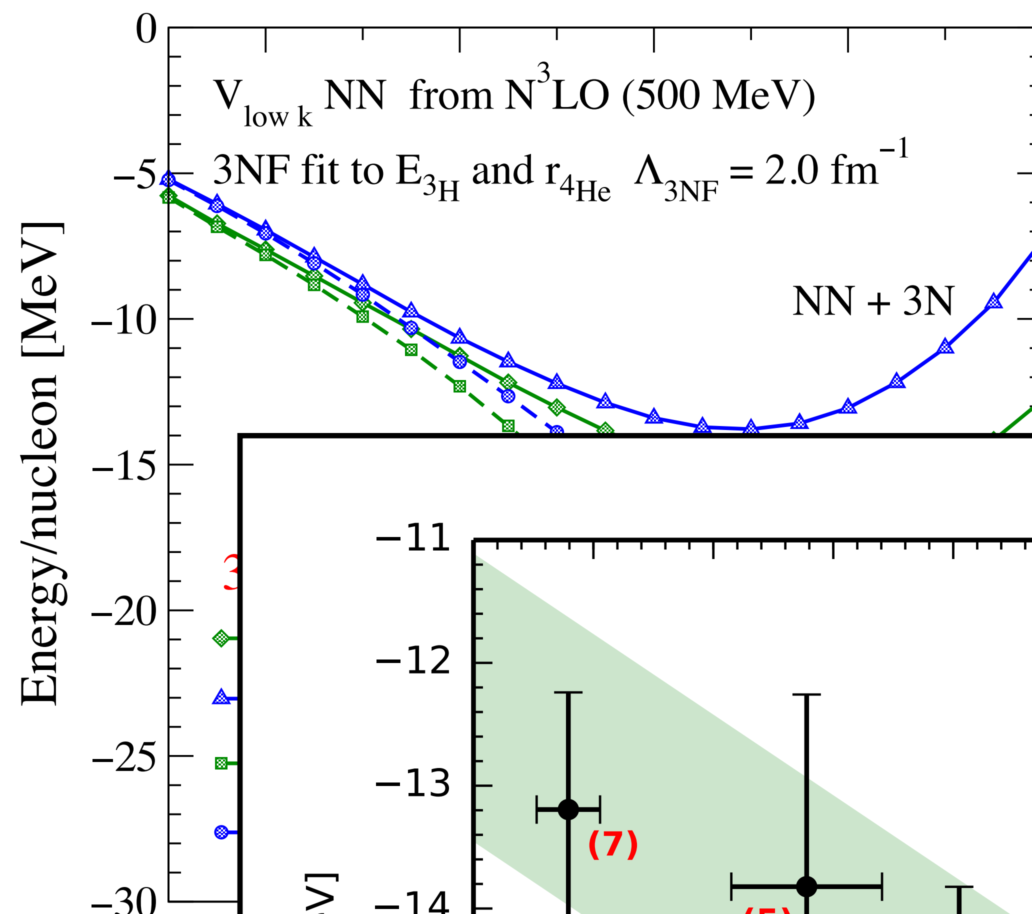

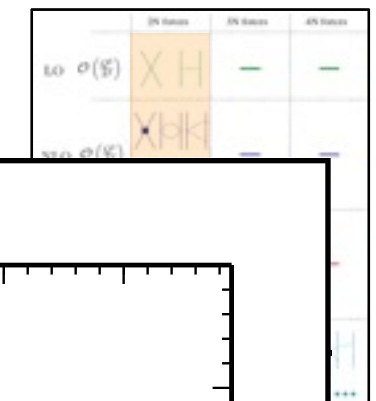

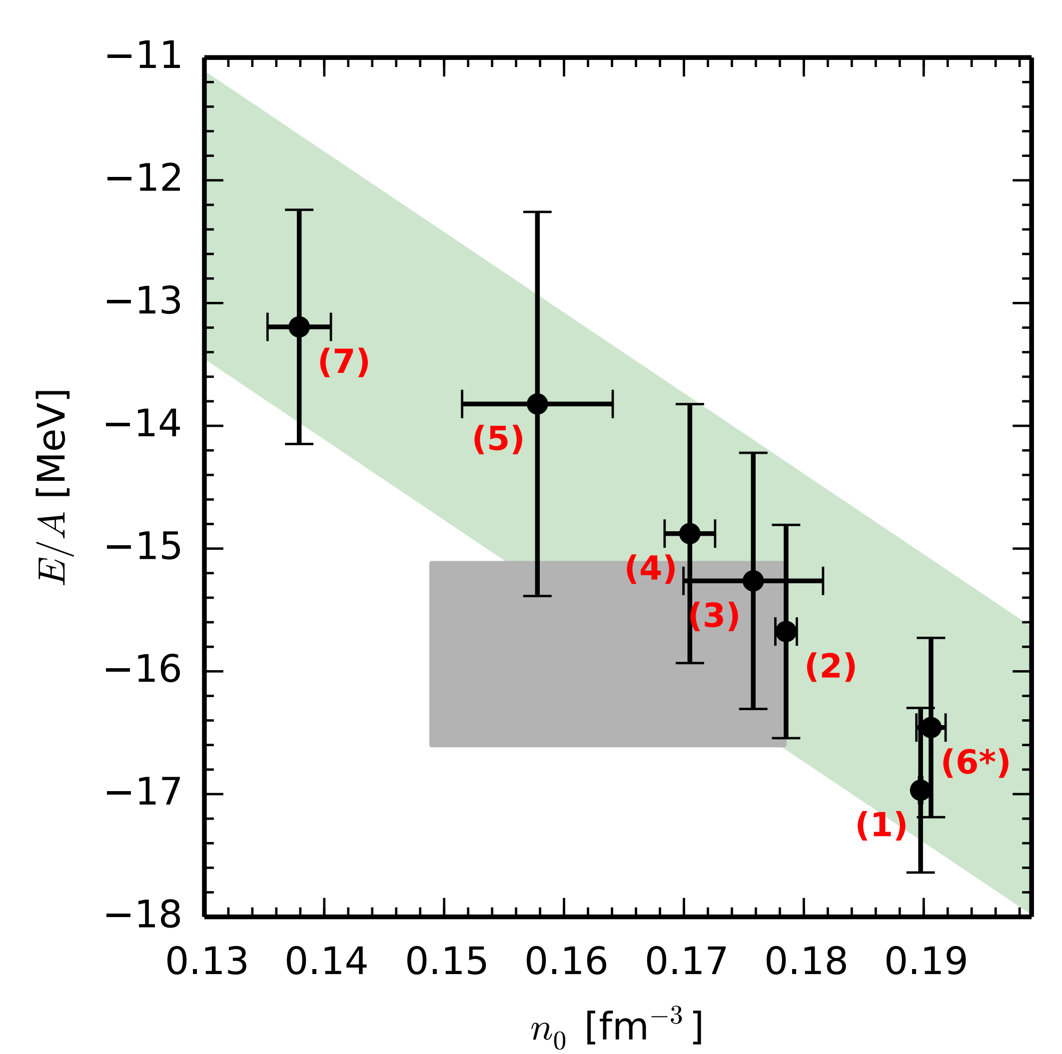

Drischler, KH, Schwenk, PRC93, 054314 (2016)

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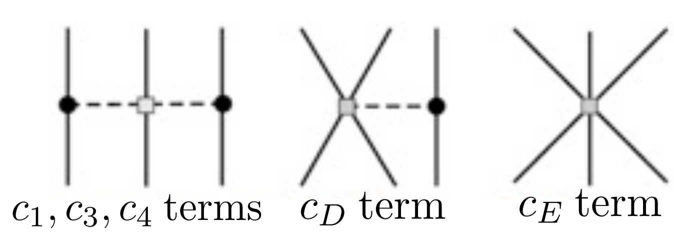
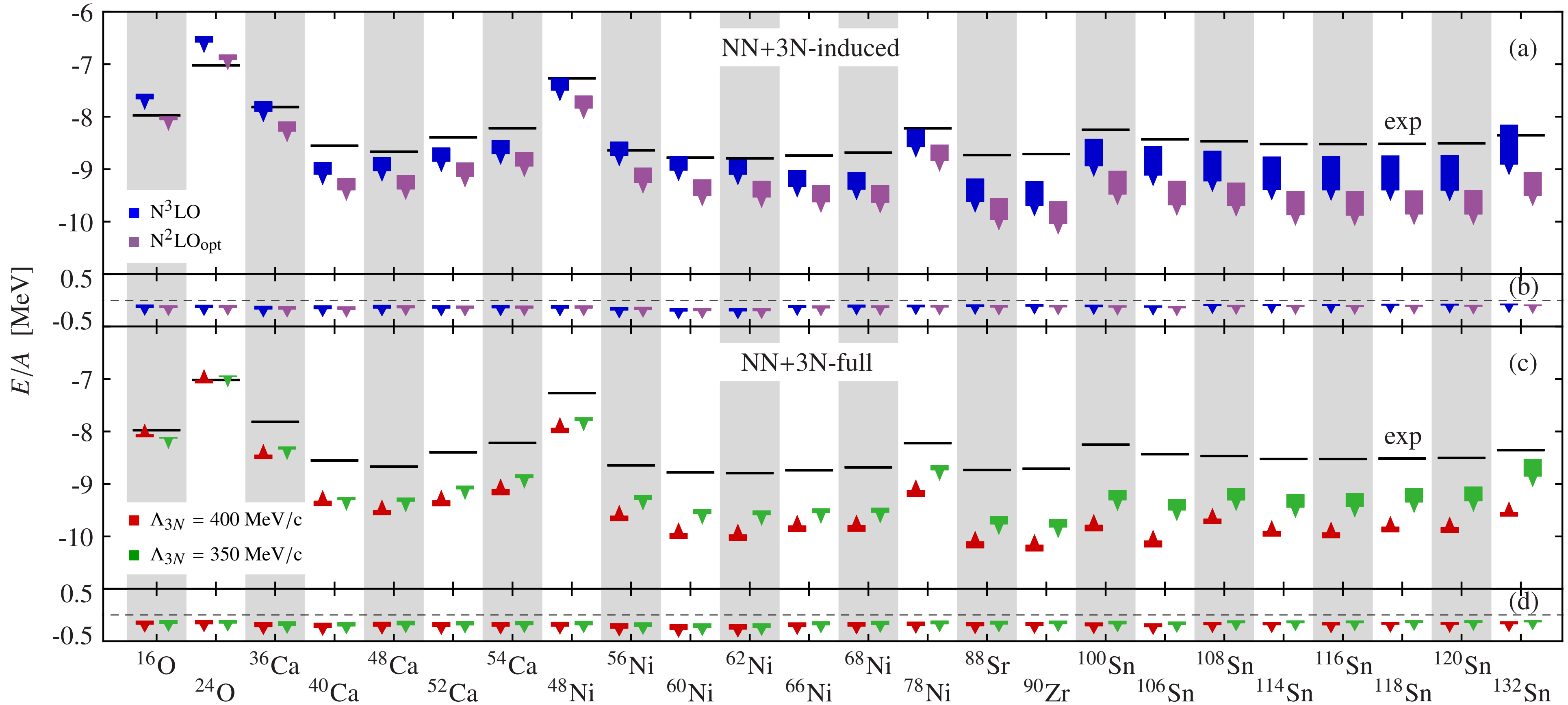
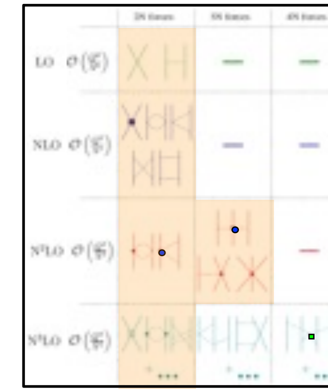


Ab initio calculations of heavier nuclei

coupled cluster (CC) framework



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



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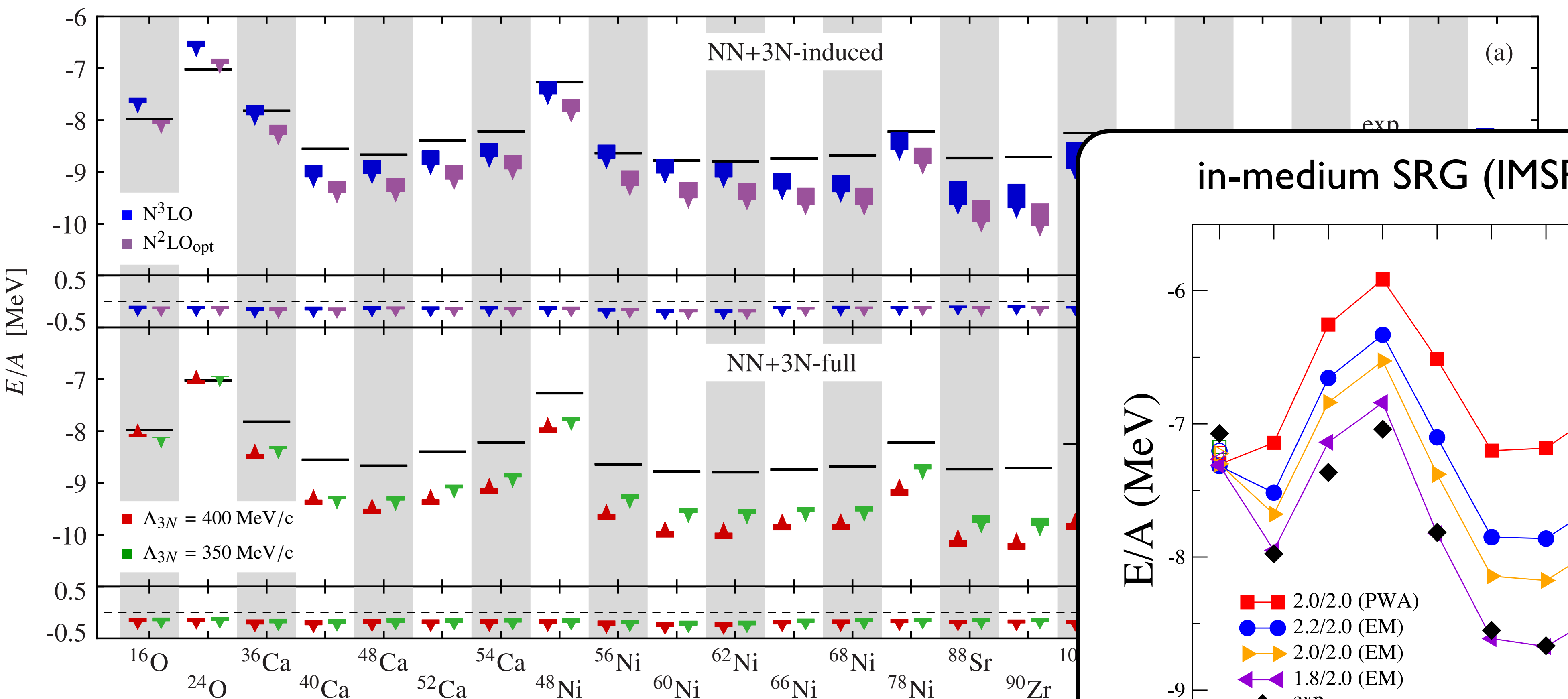
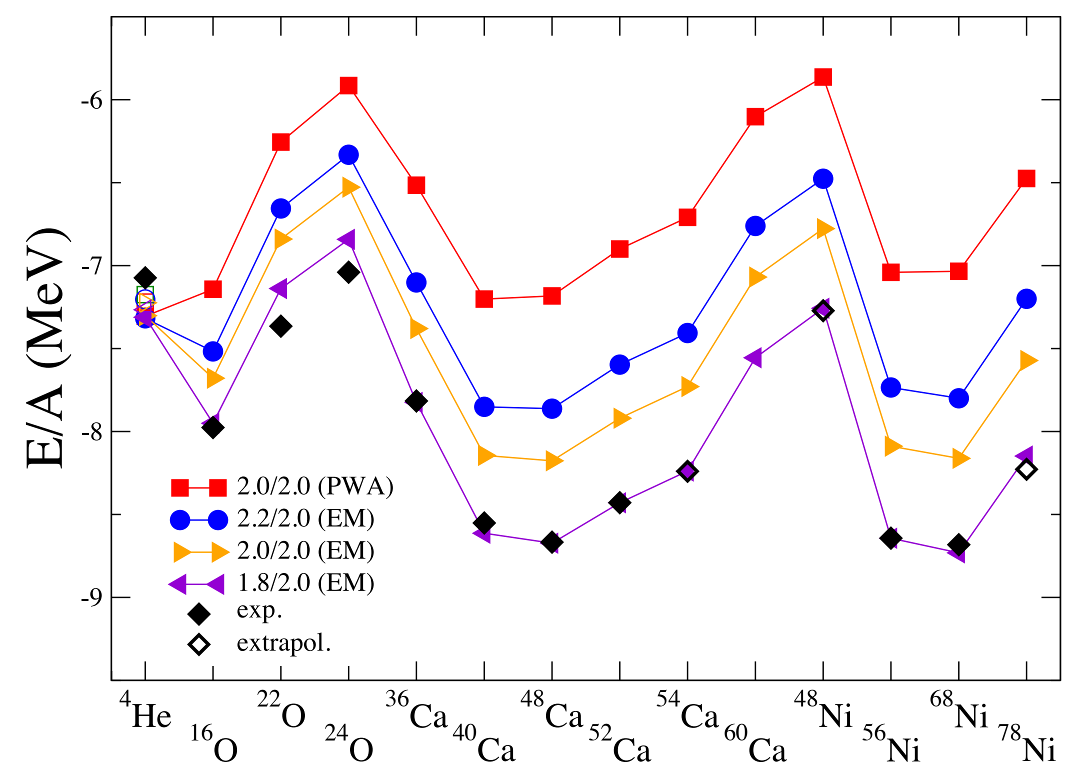


Binder et al., Phys. Lett B 736, 119 (2014)

in-medium SRG (IMSRG) framework



Simonis, Stroberg et al., in preparation

- significant discrepancies to experimental data for heavy nuclei for (most of) presently used nuclear interactions
- significance of realistic nuclear matter properties for heavier nuclei?
- need to quantify theoretical uncertainties

Efficient many-body framework for nuclear matter

Developer:

Christian Drischler

Goal:

Develop efficient framework that allows to calculate dense matter (runtime ~few minutes). Suitable for incorporating information of nuclear matter in fitting frameworks for nuclear forces.

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Calculate MBPT diagrams NN-complete up to 4th order by sampling phase space integrals in vector basis using Monte-Carlo techniques.

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Status:

Implementation of NN plus 3N forces up to N3LO complete.

Implementation of non-local NN and 3N interactions.

Ongoing benchmarks regarding required number of sampling points.

Efficient many-body framework for nuclear matter

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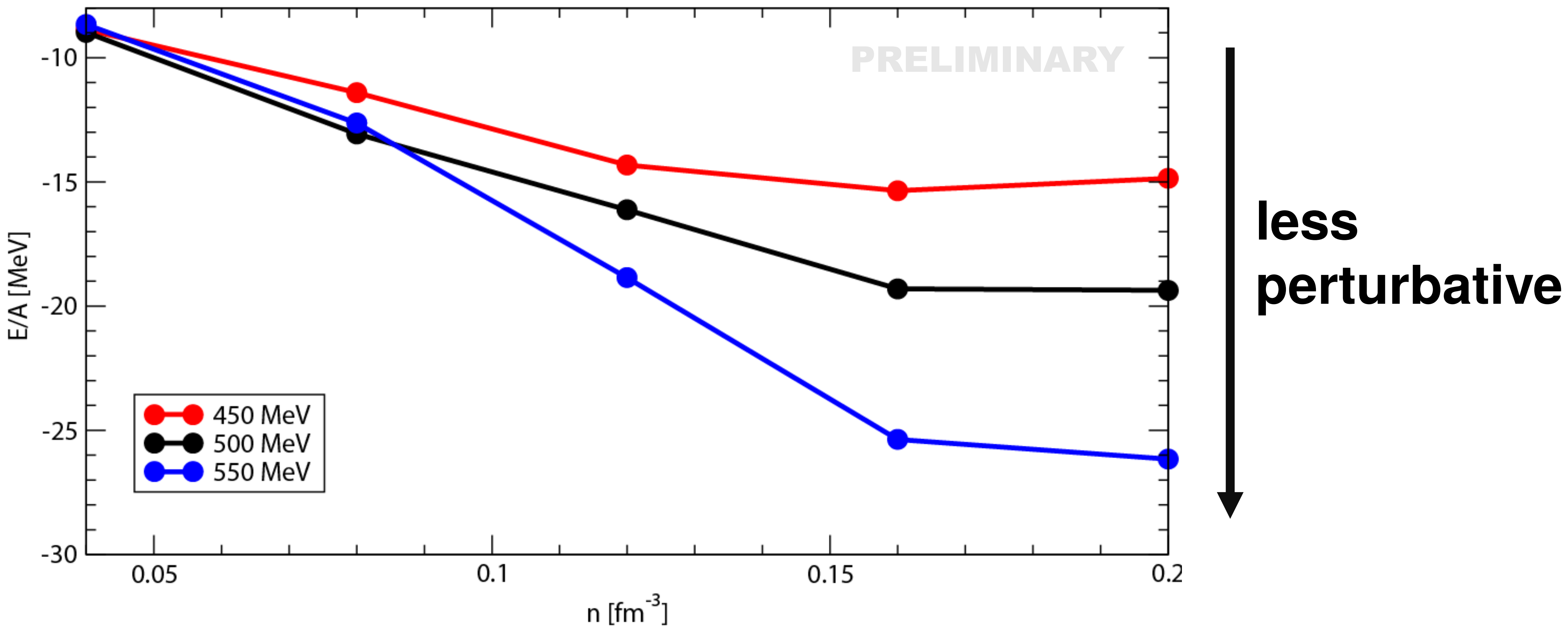
first results for some N2LO sim potentials



N^{2}LOsim	$E_{NN}^{(3)}(n_0)$ [MeV]	$E_{NN}^{(4)}(n_0)$ [MeV]	$E_{tot}^{(IV)}(n_0)$ [MeV]
450 MeV	**+1.1**	**+0.3**	**–15.4**
500 MeV	+1.6	–1.5	–19.3
550 MeV	+3.3	–4.1	–25.4

Status and achievements

significant increase in scope of ab initio many-body frameworks

remarkable agreement between different ab intio many-body methods

discrepancies to experiment dominated by deficiencies of present nuclear interactions

Current developments and open questions

presently active efforts to develop improved nuclear interactions (fits of LECs, power counting, regularization, incorporation of NM info?,...)

Key goals

unified study of nuclei, nuclear matter and reactions based on novel interactions

systematic estimates of theoretical uncertainties