Implementation and applications of 3N interactions and nuclear currents

Kai Hebeler

Trento, June 6, 2018

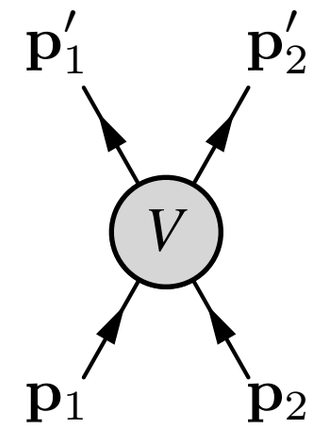
ECT* workshop
“New Ideas in Constraining Nuclear Forces”

SFB 1245

TECHNISCHE UNIVERSITÄT DARMSTADT

Regularization schemes for nuclear interactions (here: NN)

Separation of long- and short-range physics



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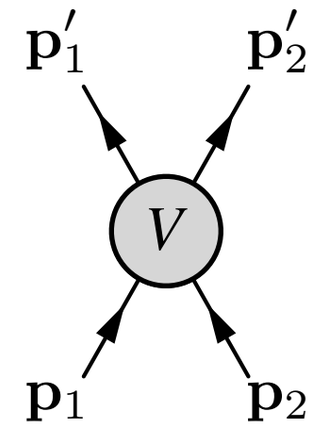

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$$V_{\mathrm{NN}}(\mathbf{p}, \mathbf{p}') \to \exp\left[-\left((p^2 + p'^2)/\Lambda^2\right)^n\right] V_{\mathrm{NN}}(\mathbf{p}, \mathbf{p}')$$

Epelbaum, Glöckle, Meissner, NPA 747, 362 (2005)
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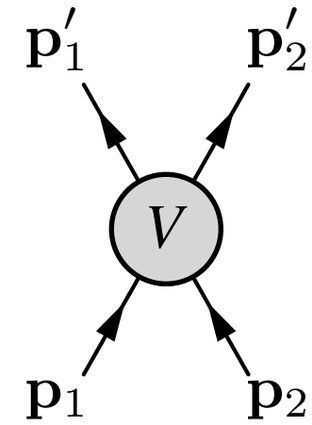

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cf. Navratil, Few-body Systems 41, 117 (2007)

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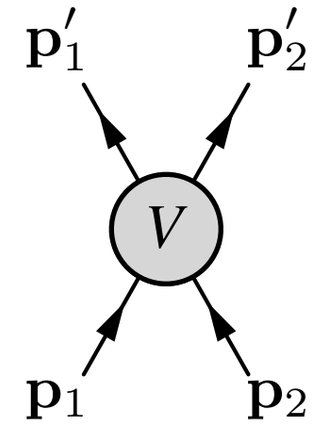

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Gezerlis et. al, PRL, 111, 032501 (2013)

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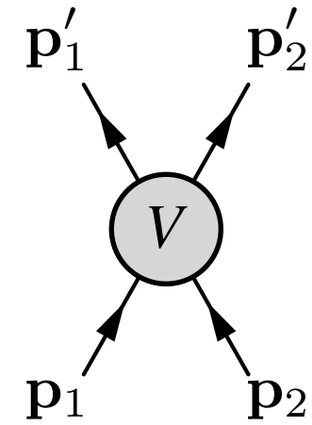

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semi-local

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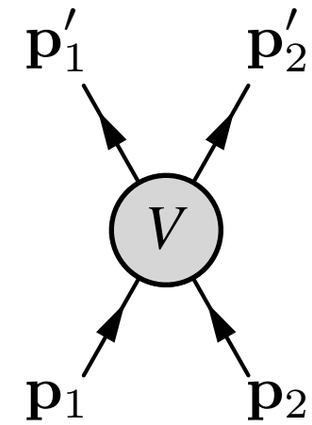

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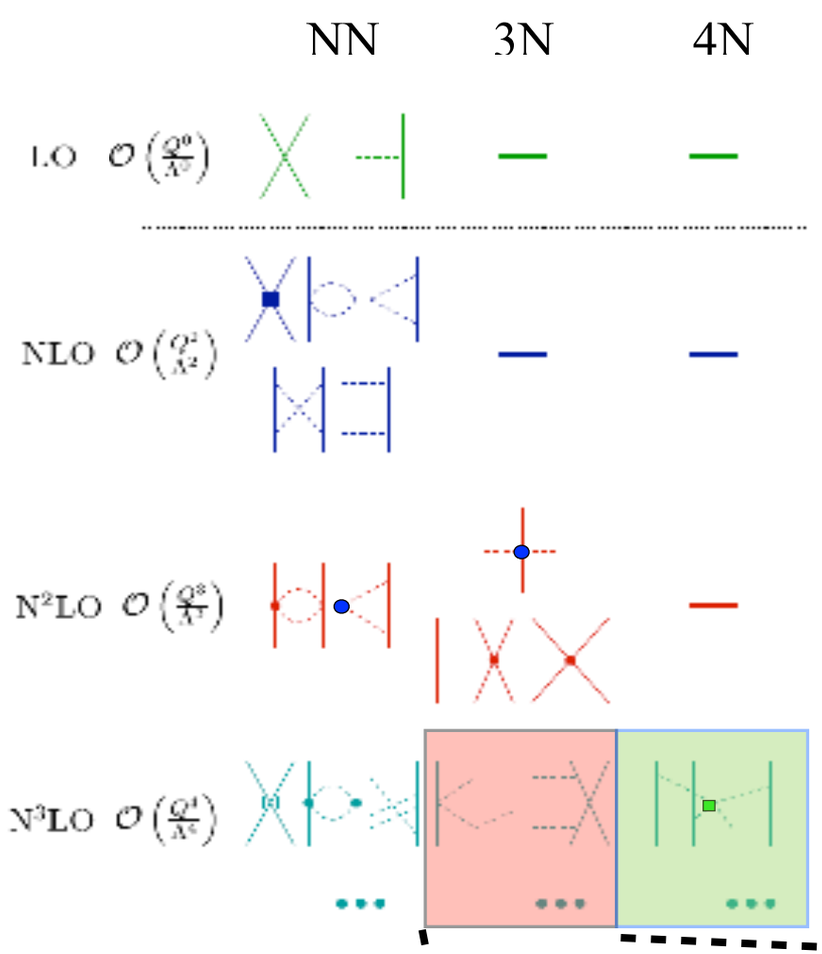
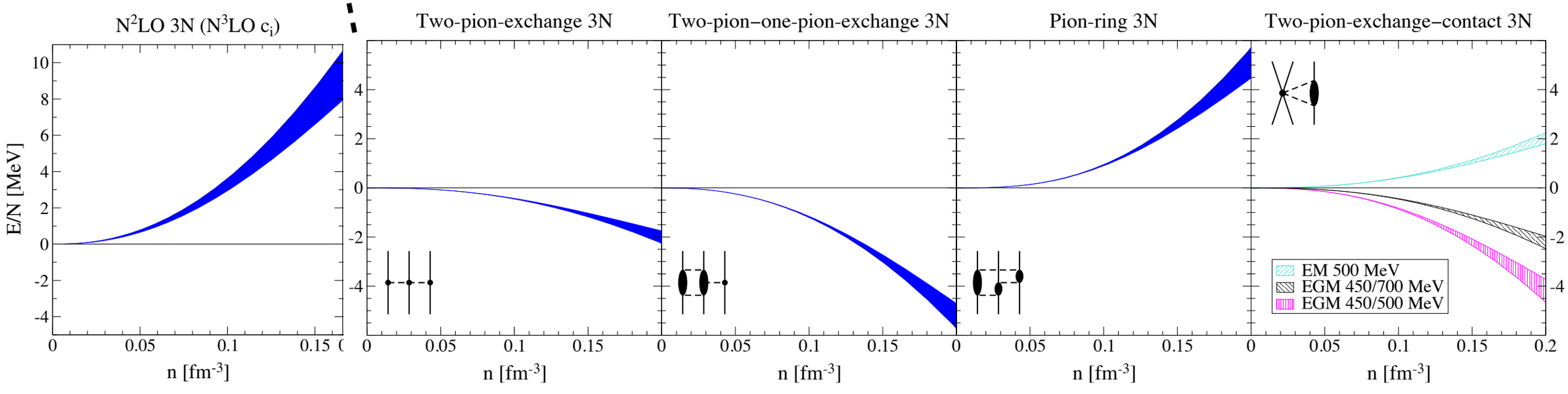
Power counting in chiral 3N sector (nonlocal): Contributions of many-body forces at N³LO in neutron matter



- first calculations of N³LO 3NF and 4NF contributions to EOS of neutron matter
- found large contributions in Hartree Fock appr., comparable to size of N²LO contributions

Krüger, Tews, KH, Schwenk, PRC 88, 025802 (2013)

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



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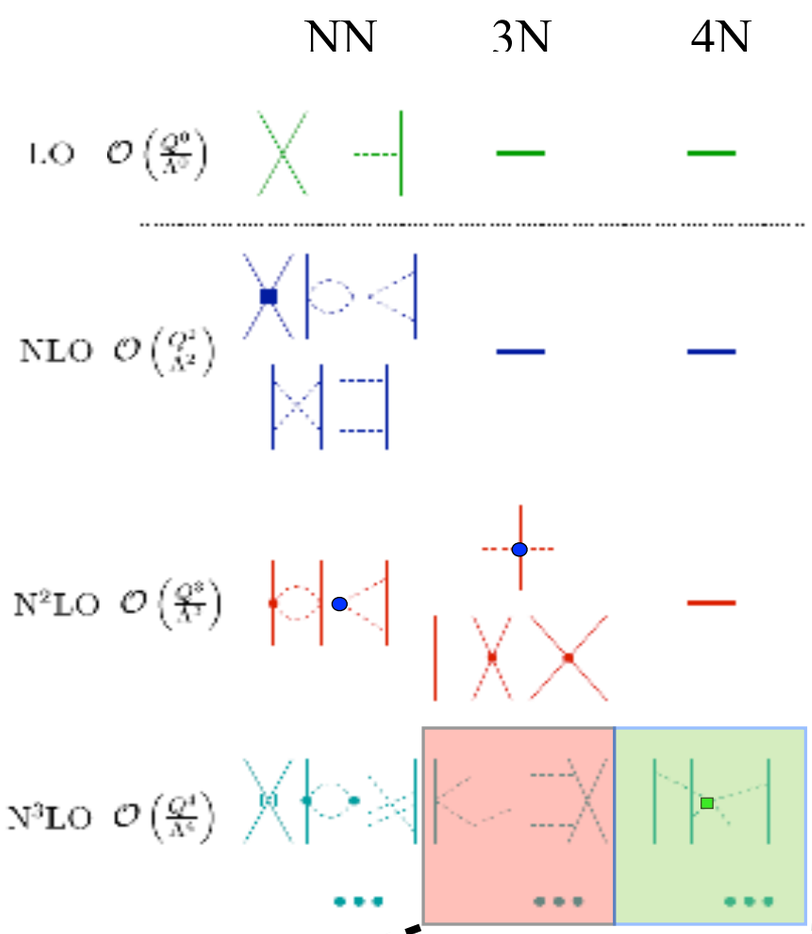

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- 4NF contributions small

Krüger, Tews, KH, Schwenk, PRC 88, 025802 (2013)

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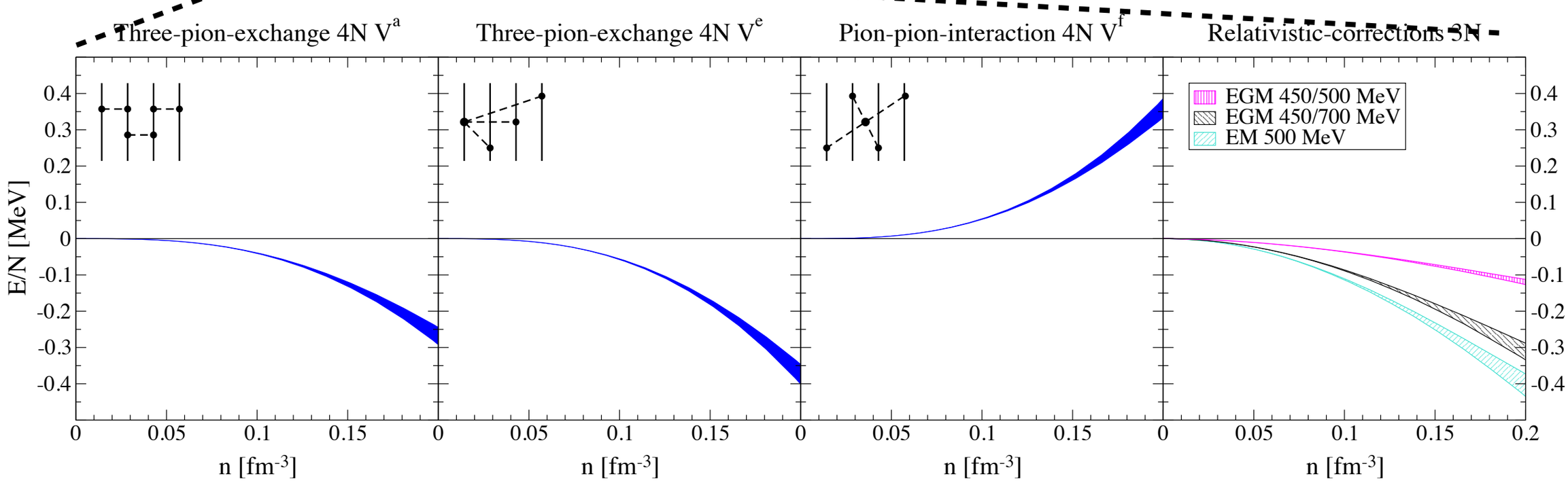
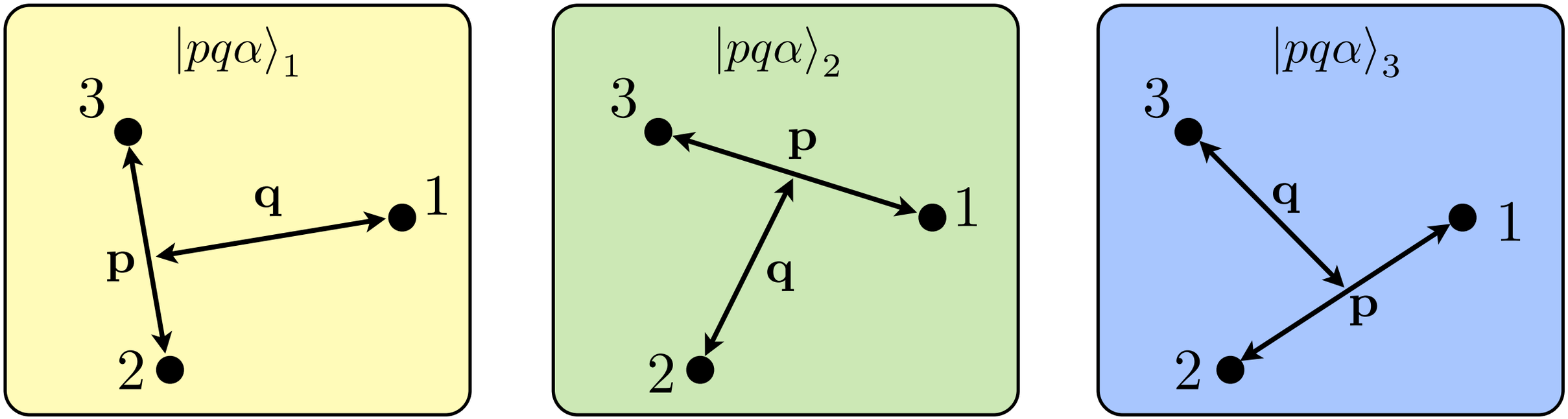


Representation of 3N interactions in momentum space

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



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

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

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

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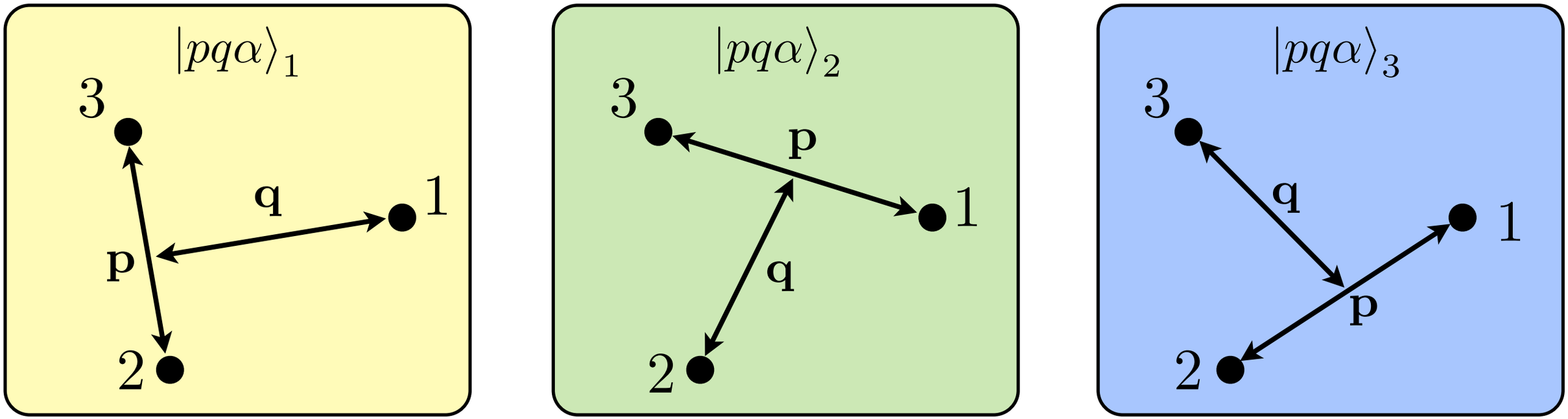

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A 'new' algorithm allows efficient calculation.

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

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:

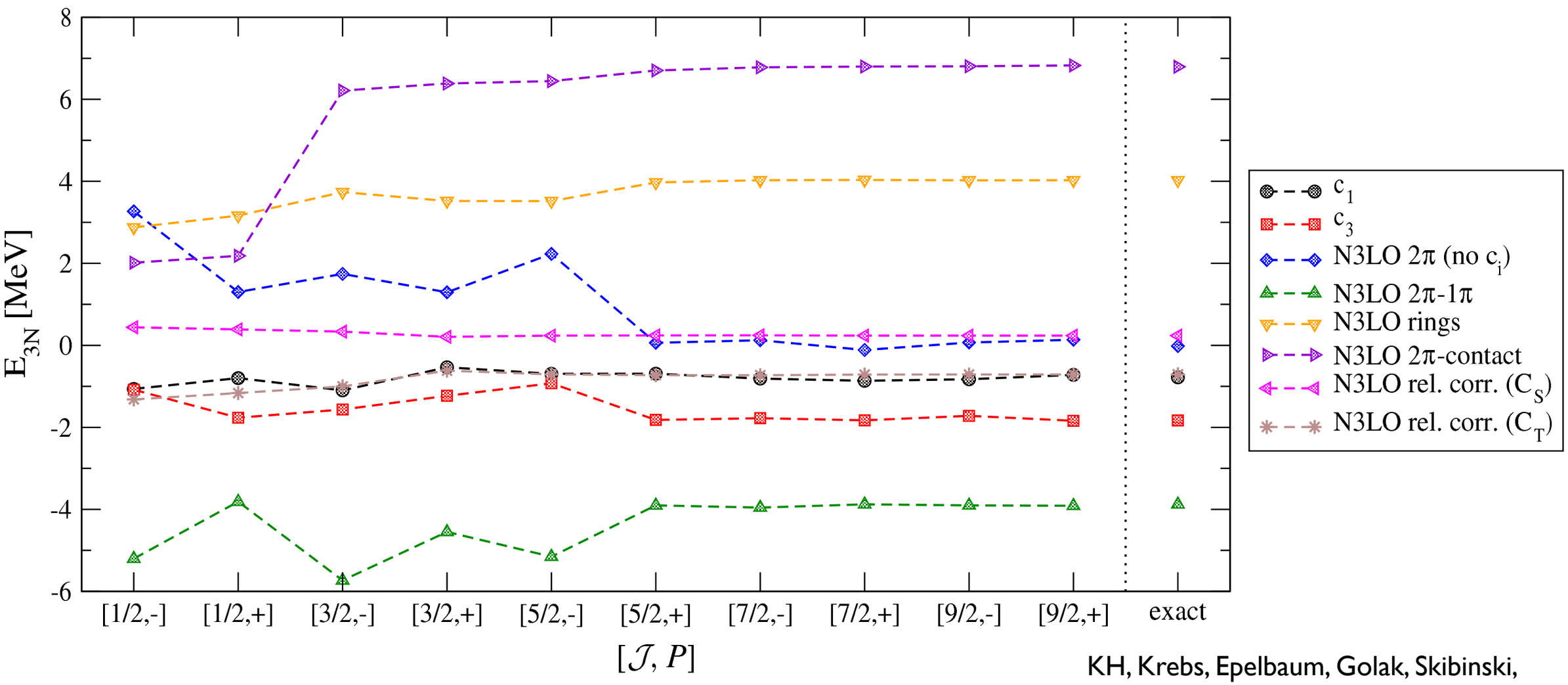
$$\begin{aligned}\langle \mathbf{pq}|V_{123}|\mathbf{p}'\mathbf{q}'\rangle &= V_{123}(\mathbf{p}-\mathbf{p}', \mathbf{q}-\mathbf{q}') \\ &= V_{123}(p-p', q-q', \cos\theta)\end{aligned}$$

$\longrightarrow$ 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

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

neutron matter:

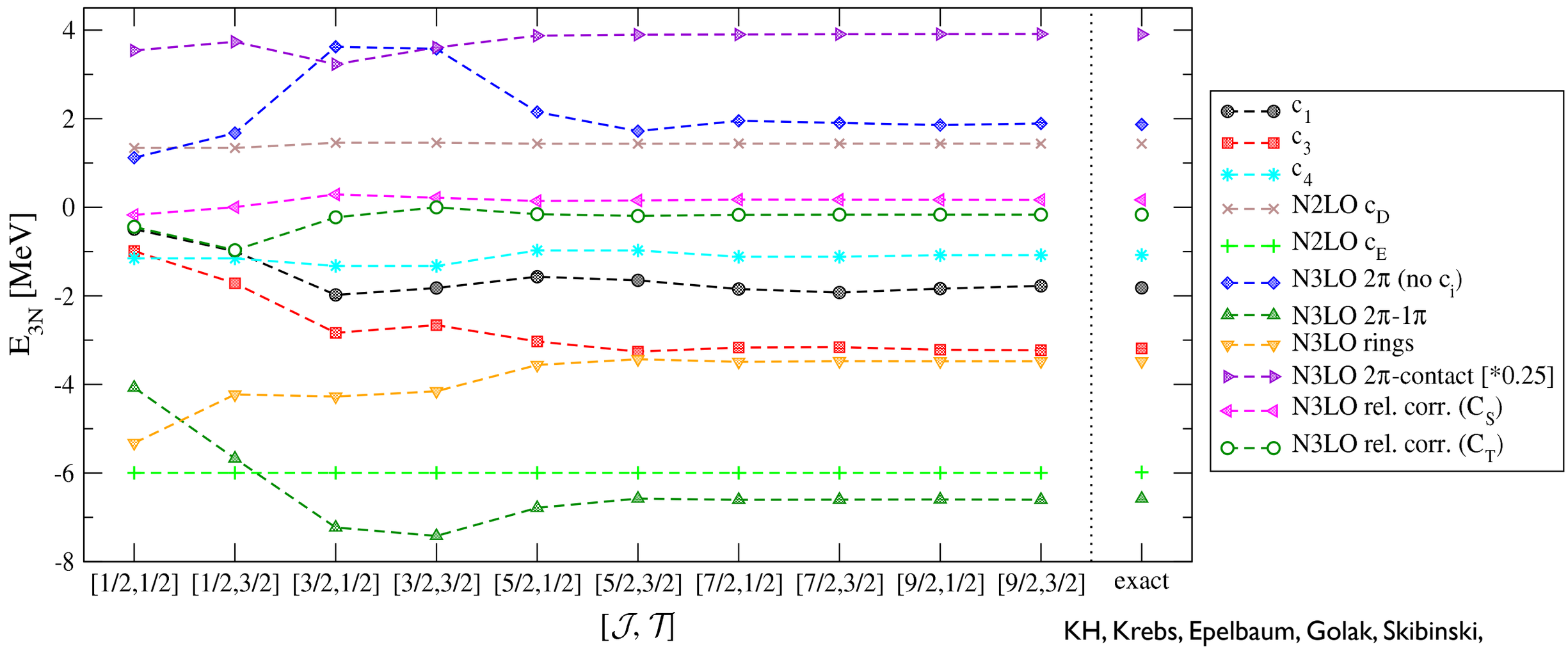


KH, Krebs, Epelbaum, Golak, Skibinski, PRC 91, 044001 (2015)

- 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:



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

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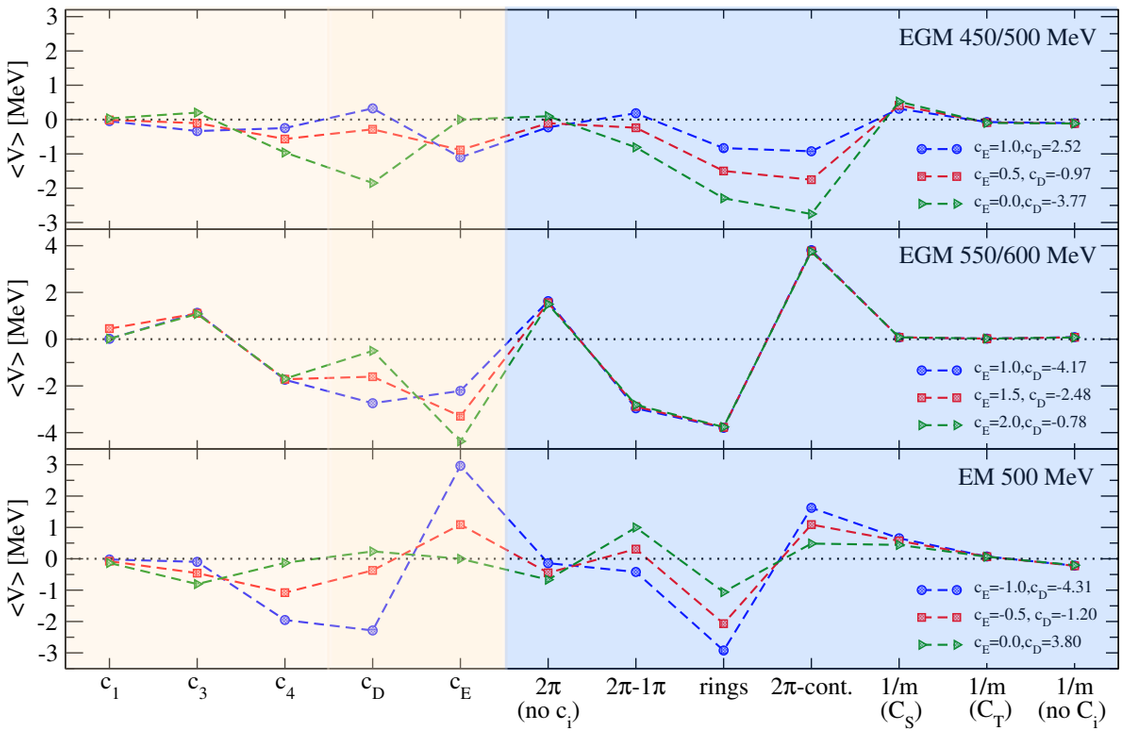
3NF power counting in 3H for different regulators

nonlocal

N2LO N3LO



KH et al.,
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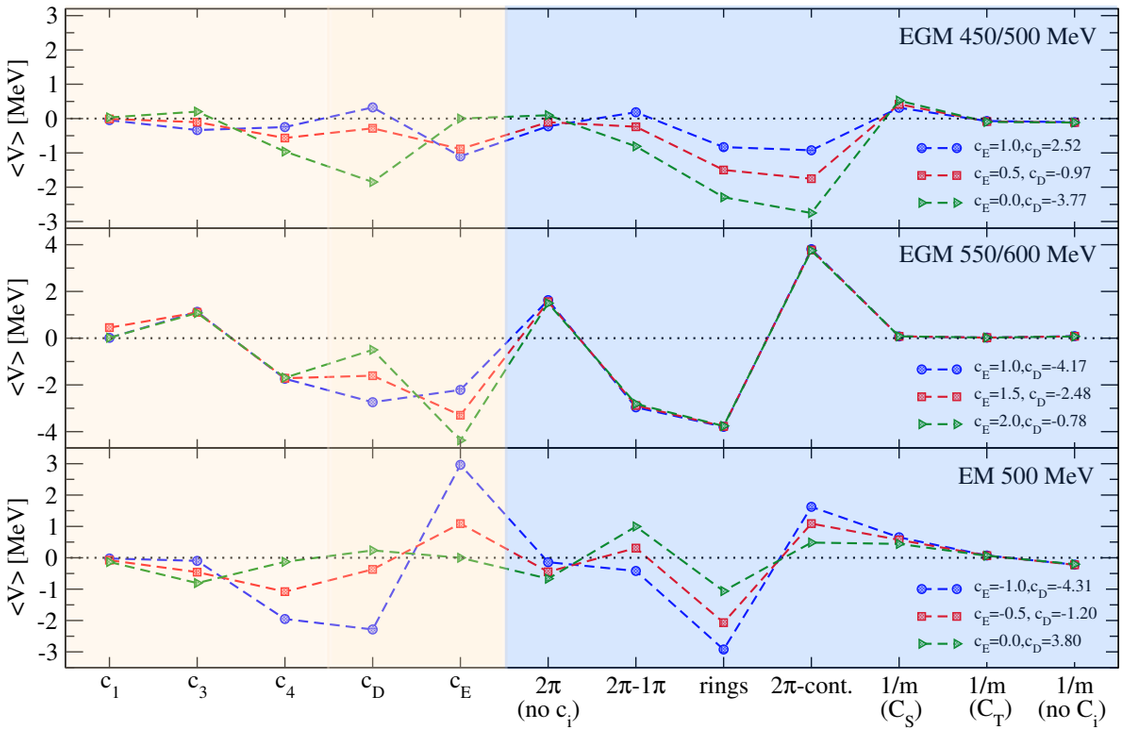

KH et al.,
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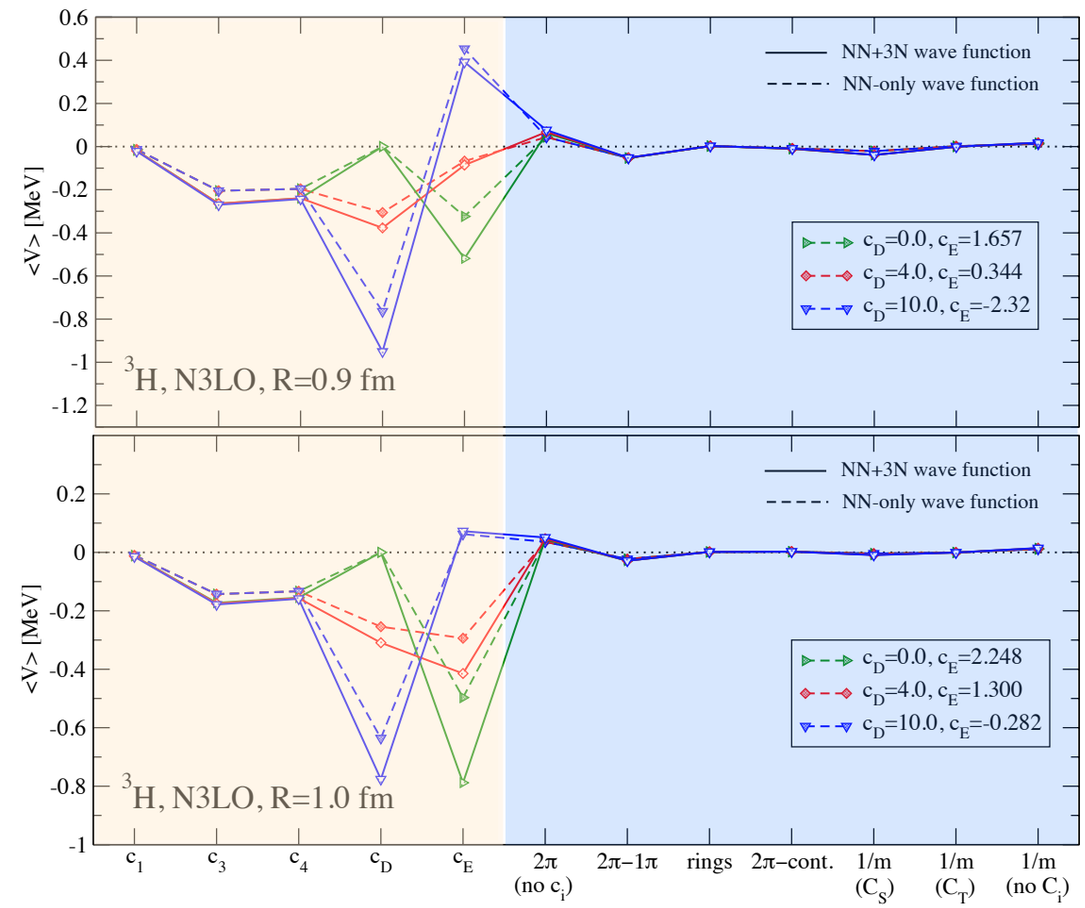
semilocal (coordinate space)

N2LO N3LO



- size of N3LO contribution not suppressed for shown nonlocal interactions
- N3LO contributions suppressed for semilocal interactions
- technical challenges for semilocal interactions:
  - ⋆ forces non-perturbative, large basis spaces/RG evolution needed
  - ⋆ implementation of 3N forces hard, stability problems for scattering calculations
  - ⋆ derivation and implementation of nuclear currents hard

3NF power counting for different regulators

nonlocal

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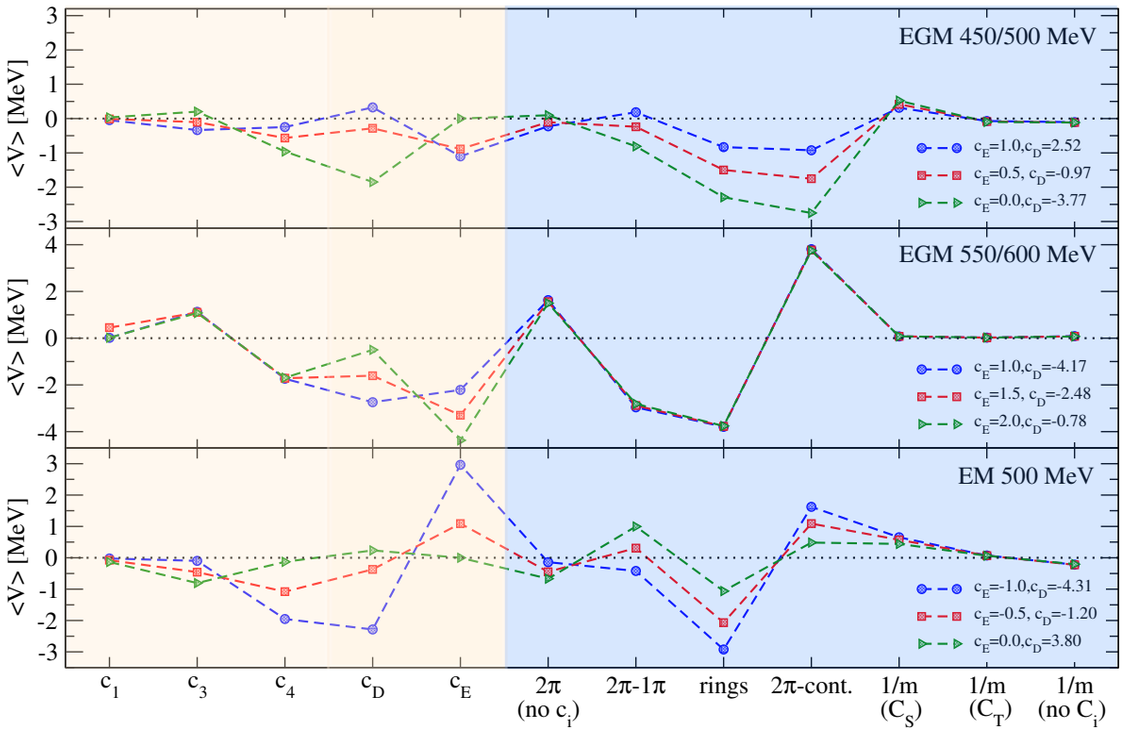

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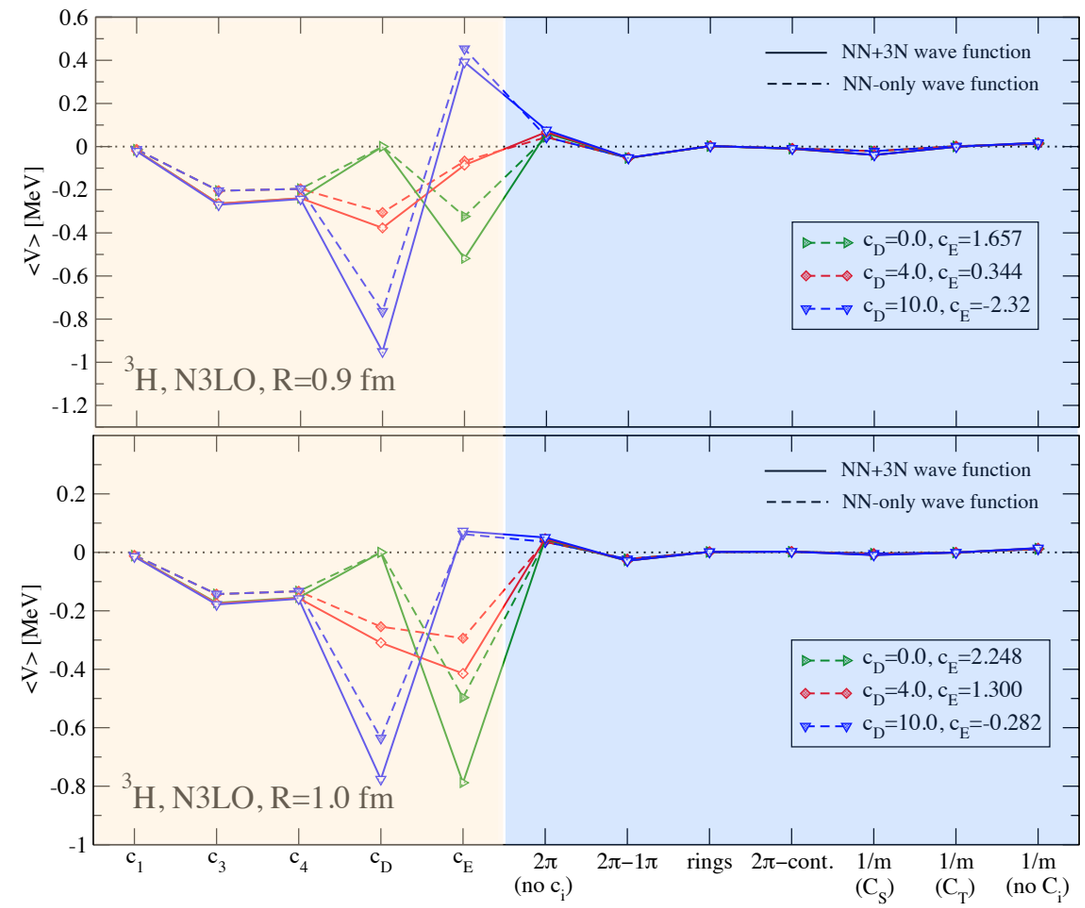


Development of improved novel semilocal NN+3N interactions regularised in momentum space.

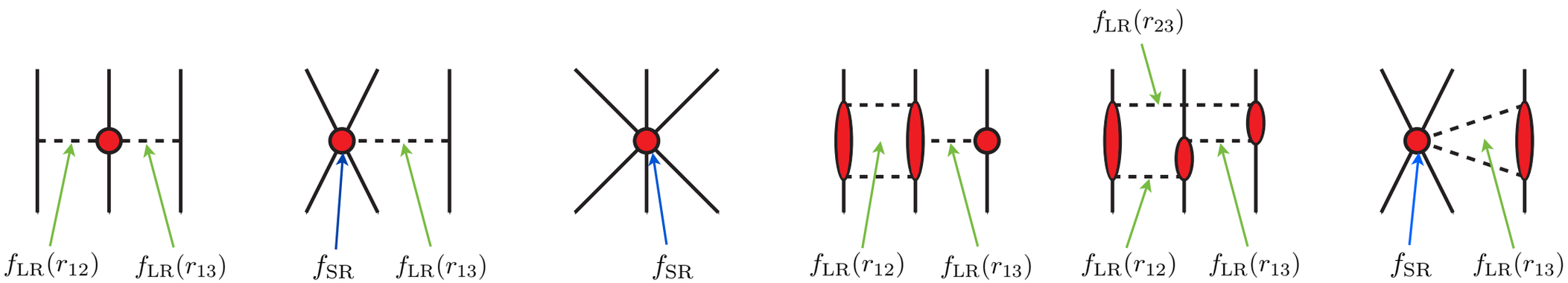
$$V_\pi(\mathbf{p},\mathbf{p}') \to V_\pi(\mathbf{p},\mathbf{p}')e^{-(\mathbf{q}^2+m_\pi^2)/\Lambda^2}$$

Reinert et al.,
arXiv:1711.08821

→ *Hermann's /Evgeny's talk*

Calculation of N2LO 3NFs completed.
N3LO contributions progress!

Semi-local regularization of 3NF (coordinate space)



$1/m$

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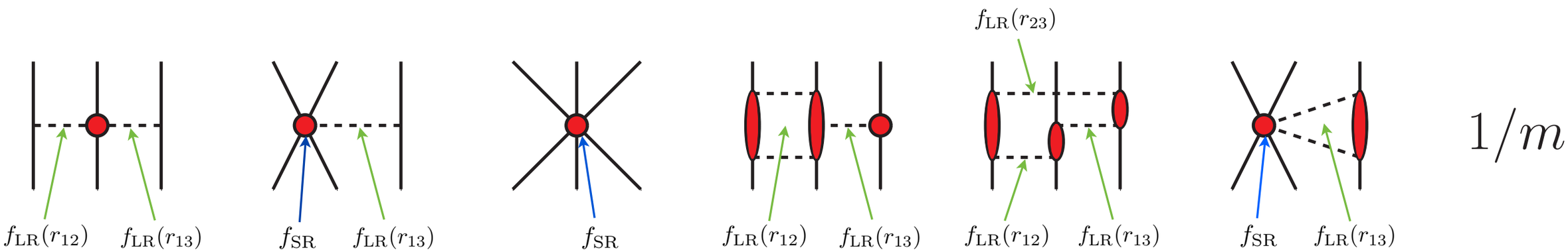

Computational strategy:

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

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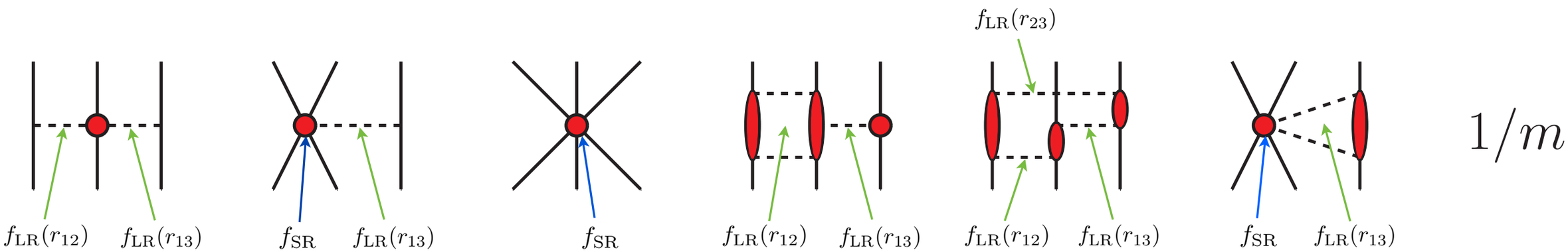

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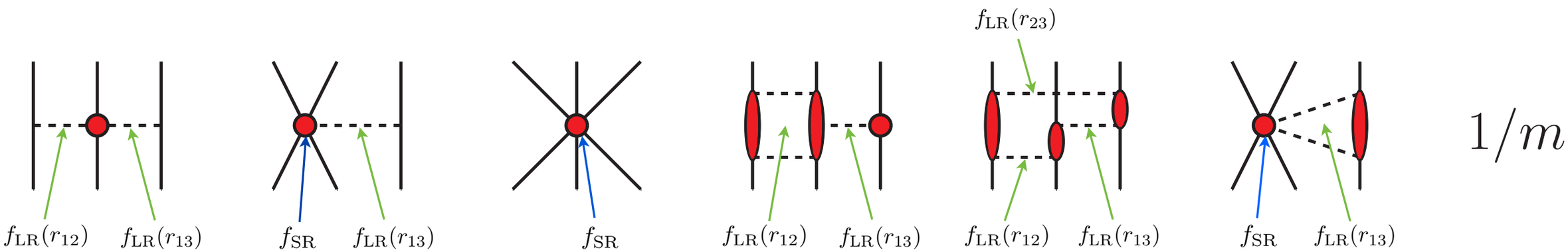

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(4) perform convolution integrals:

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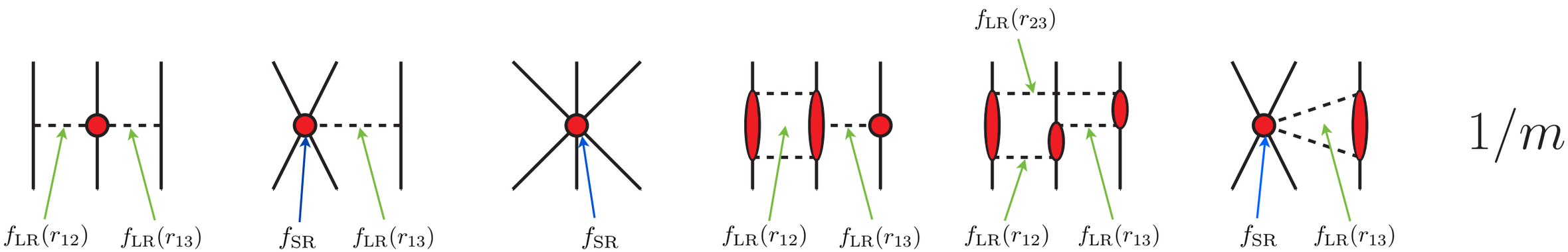

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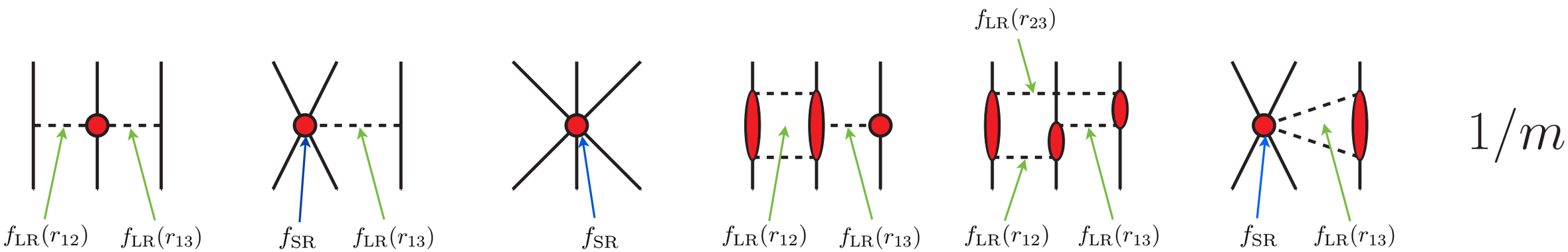

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(5) regularize short-range parts in interactions with non-local regulator

(6) antisymmetrize interactions (optional)

Naive calculation of convolution integrals: Problem!

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

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

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

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

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

delicate cancellation!

More clever way to calculate convolution integrals: Preregularization!

with Hermann Krebs

consider a N2LO long-range topology:

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

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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:

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

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the *preregularized* regulator reads accordingly:

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

More clever way to calculate convolution integrals: Preregularization!

with Hermann Krebs

consider a N2LO long-range topology:

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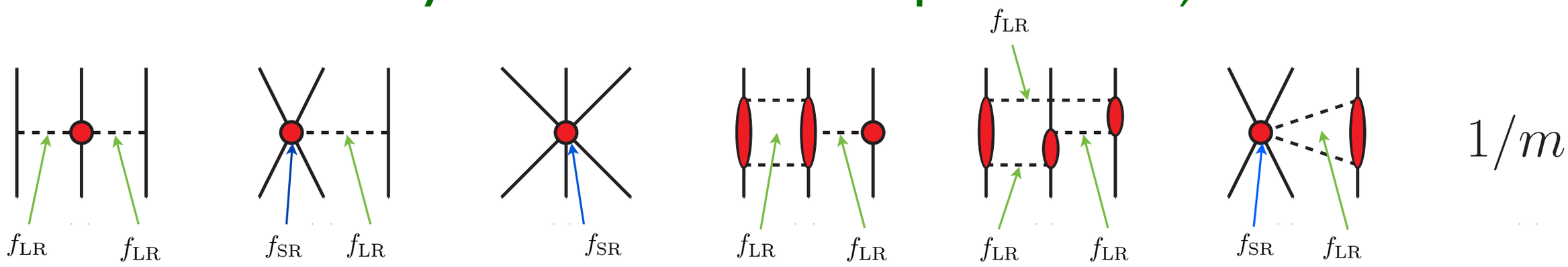
For $Q(r^2) = r^2$ all integrals are finite and can be calculated without subtraction!

Momentum space regularized semi-local 3NF

Easy and efficient to implement! :-)



$$f_{\rm LR} = f_{\rm LR}(\mathbf{q}) = \exp\left[-(\mathbf{q}^2 + m_\pi^2)/\Lambda^2\right]$$ → *Hermann's talk*

$$V_{123} = V_{123}(p-p', q-q', \cos\theta) = V_{123}(\tilde{p}, \tilde{q}, \cos\theta)$$

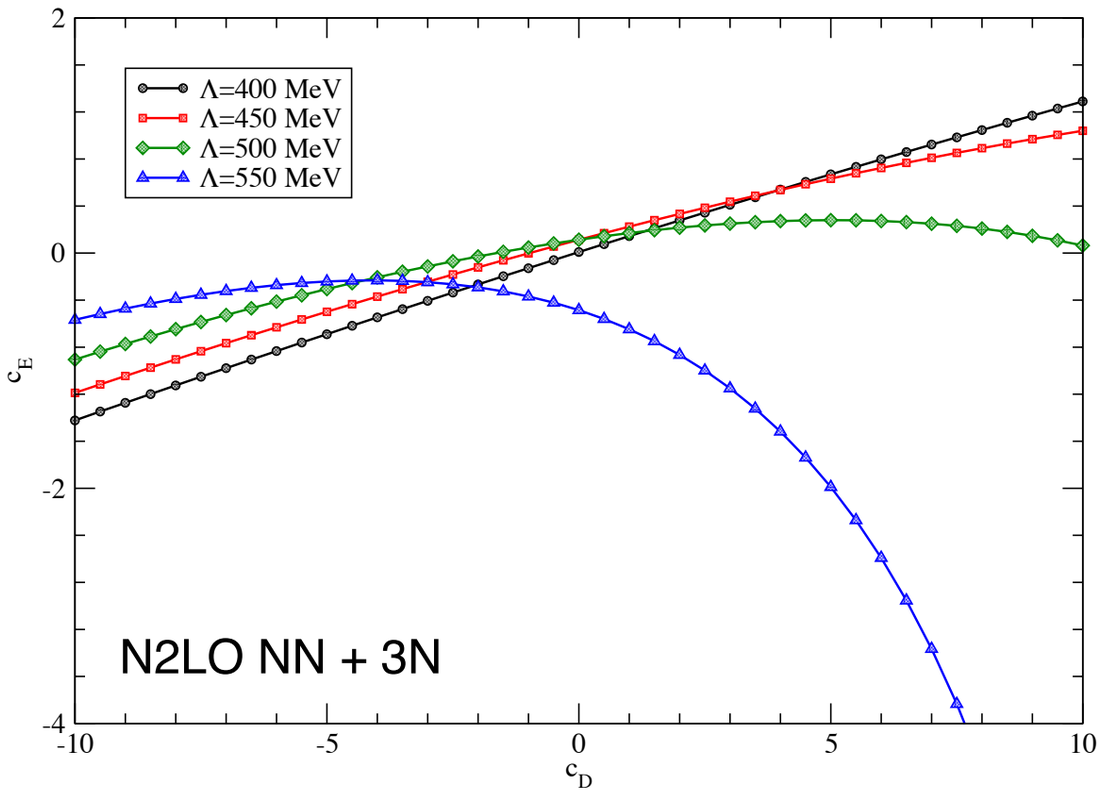
Example:

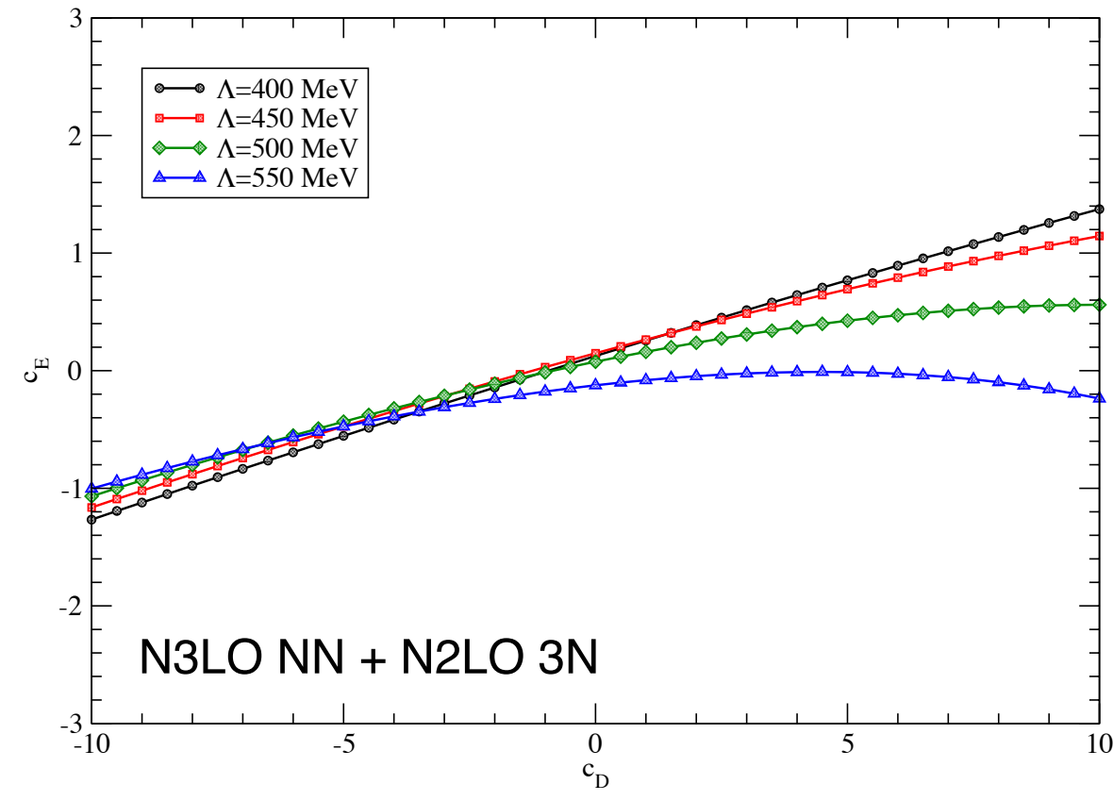
N2LO 2pi topology: $$V_{123}^{2\pi} \sim \frac{1}{(\mathbf{q}_2^2 + m_\pi^2)(\mathbf{q}_2^3 + m_\pi^2)}$$

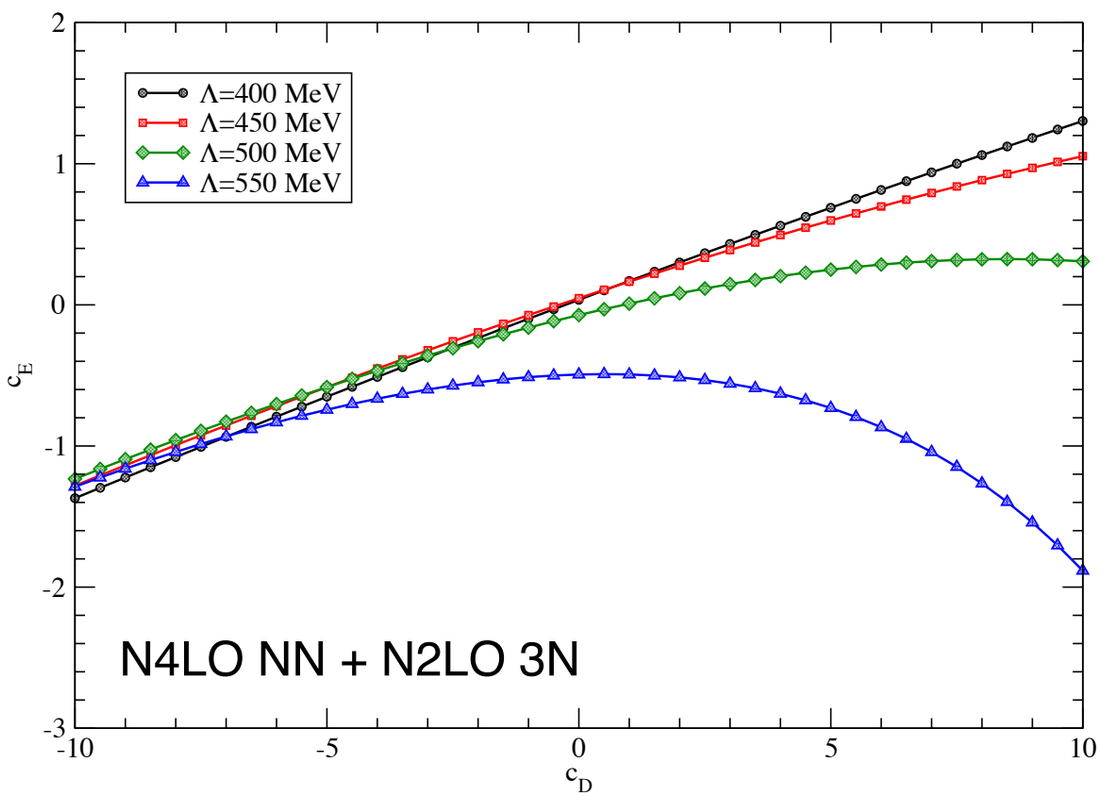
$$= \frac{1}{((\mathbf{p} - \mathbf{q}/2)^2 + m_\pi^2)((\mathbf{p} + \mathbf{q}/2)^2 + m_\pi^2)}$$

→ $$V_{123}^{2\pi,reg} \sim \frac{f_{\rm LR}(\mathbf{q}_2) f_{\rm LR}(\mathbf{q}_3)}{(\mathbf{q}_2^2 + m_\pi^2)(\mathbf{q}_2^3 + m_\pi^2)}$$

Fits of N2LO 3NF (semi-local momentum space) to 3H binding energy







- currently exploring behaviour of NN+3N interactions in many-body systems
- Which set of observables for fixing 3NF couplings cD and cE?

Determination of LECs: Uncertainties from triton beta decay

$$(1+\delta_R)t = \frac{K/G_V^2}{f_V \langle \mathrm{F} \rangle^2 + f_A\, g_A^2 \langle \mathrm{GT} \rangle^2}$$

$$\langle \mathrm{F} \rangle = \langle {}^3\mathrm{He} \| \sum_{i=1}^{3} \tau_i^+ \| {}^3\mathrm{H} \rangle \qquad \langle \mathrm{GT} \rangle = \frac{1}{g_A} \langle {}^3\mathrm{He} \| \sum_{i=1}^{3} \mathbf{J}_{i,1\mathrm{b}}^+ + \sum_{i<j} \mathbf{J}_{ij,2\mathrm{b}}^+ \| {}^3\mathrm{H} \rangle$$

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$$\mathbf{J}^+_{i,1\mathrm{b}} = g_A \tau_i^+ \sigma_i$$

$$\begin{aligned}
\mathbf{J}^+_{12,2\mathrm{b}} = -\frac{g_A}{2F_\pi^2}\frac{1}{\mathbf{k}^2+m_\pi^2}\Big[& 4c_3 \mathbf{k}\,\mathbf{k}\cdot(\tau_1^+\sigma_1 + \tau_2^+\sigma_2) \\
& + \Big(c_4 + \frac{1}{4m_N}\Big)(\tau_1\times\tau_2)^+\,\mathbf{k}\times[(\sigma_1\times\sigma_2)\times\mathbf{k}] \\
& - \frac{i}{8m_N}(\tau_1\times\tau_2)^+(\mathbf{p}_1+\mathbf{p}_1'-\mathbf{p}_2-\mathbf{p}_2')(\sigma_1-\sigma_2)\cdot\mathbf{k}\Big] \\
& - 2id_1(\tau_1^+\sigma_1+\tau_2^+\sigma_2) - id_2(\tau_1\times\tau_2)^+(\sigma_1\times\sigma_2)
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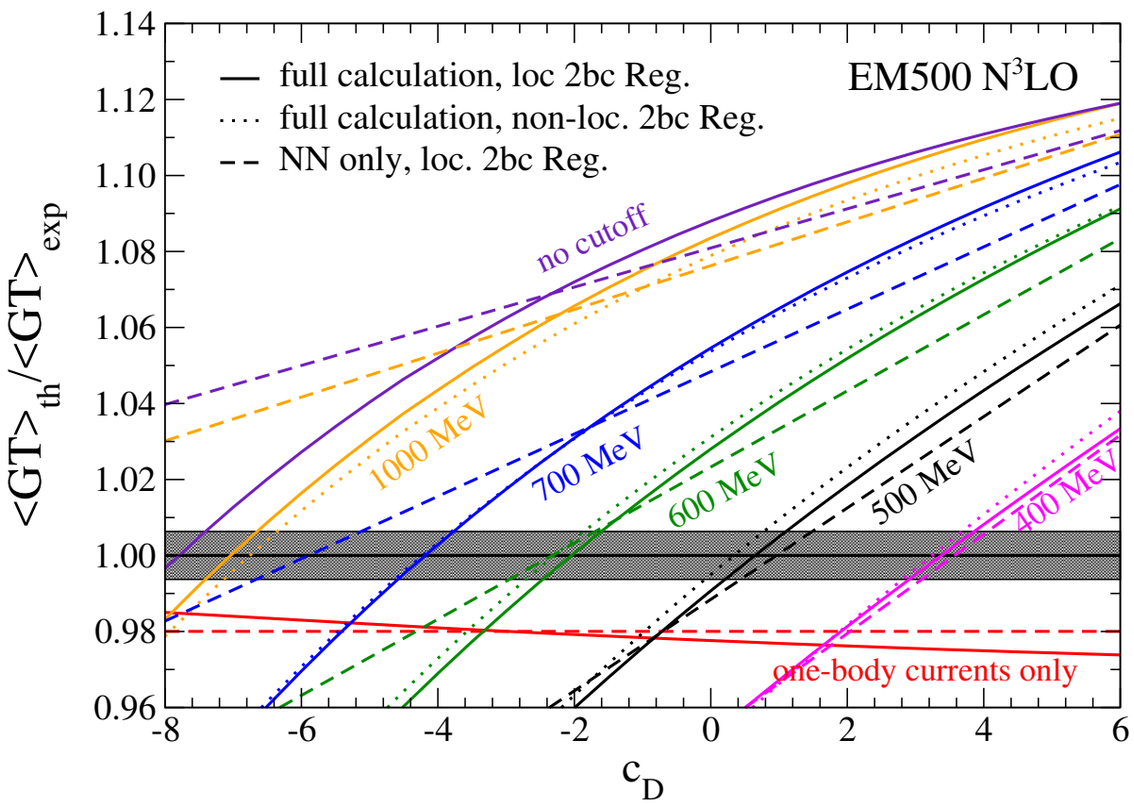
\end{aligned}$$

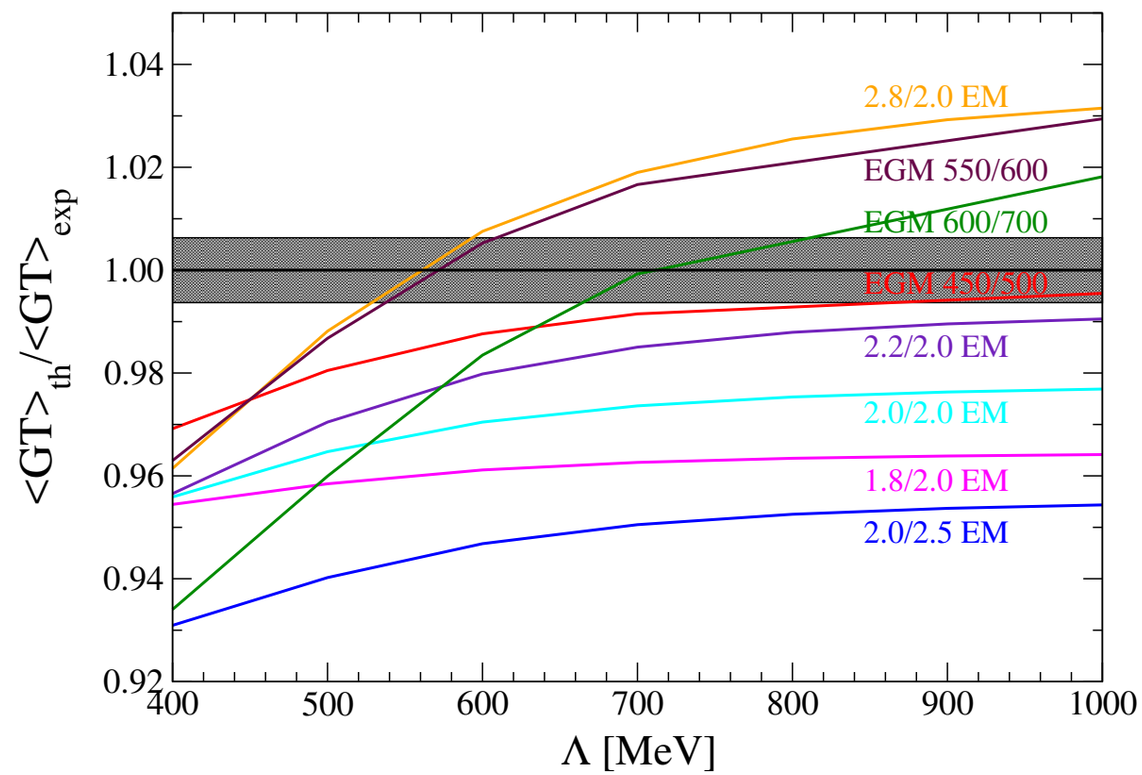
Question:

How should the current be regularized when computing <F> and <GT>?
What are the uncertainties related to this choice?

Determination of LECs: Uncertainties from triton beta decay

Using for the 2b-currents: $f_\Lambda^{\rm loc}(\mathbf{p},\mathbf{p}') = \exp\left[-(\mathbf{p}-\mathbf{p}')^4/\Lambda^4\right]$ Gazit et al., PRL103, 102502 (2009)





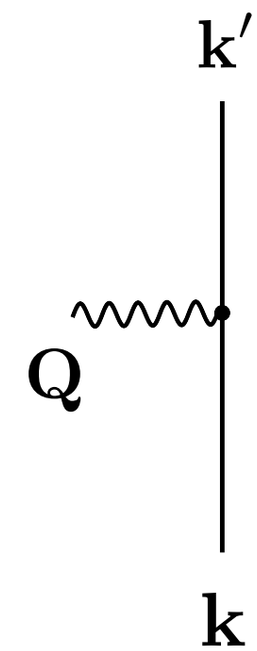
Klos et al., EPJA A53, 168 (2018), EPJA A54, 76 (2018) [erratum]

- varying Lambda in current leads to a significant range in cD
- how to choose the cutoffs consistently in currents and interaction (continuity equation?)

Implementation of nuclear current operators for applications in few- and many-body frameworks

Warmup problem: single-nucleon point charge operator

$$\langle \mathbf{k}_i' | \rho | \mathbf{k}_i \rangle = \left[G_E^p \frac{(1+\tau_z)}{2} + G_E^n \frac{(1-\tau_z)}{2} \right] \delta(\mathbf{k}_i' - \mathbf{k}_i - \mathbf{Q})$$



with $G_E^p = 1$ and $G_E^n = 0$

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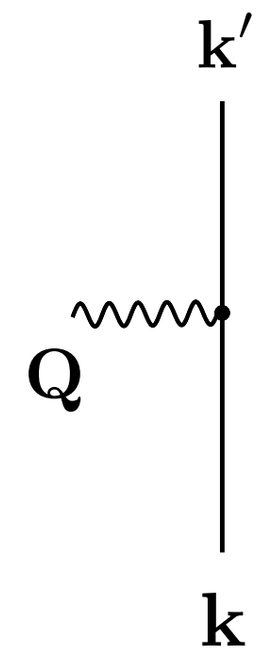
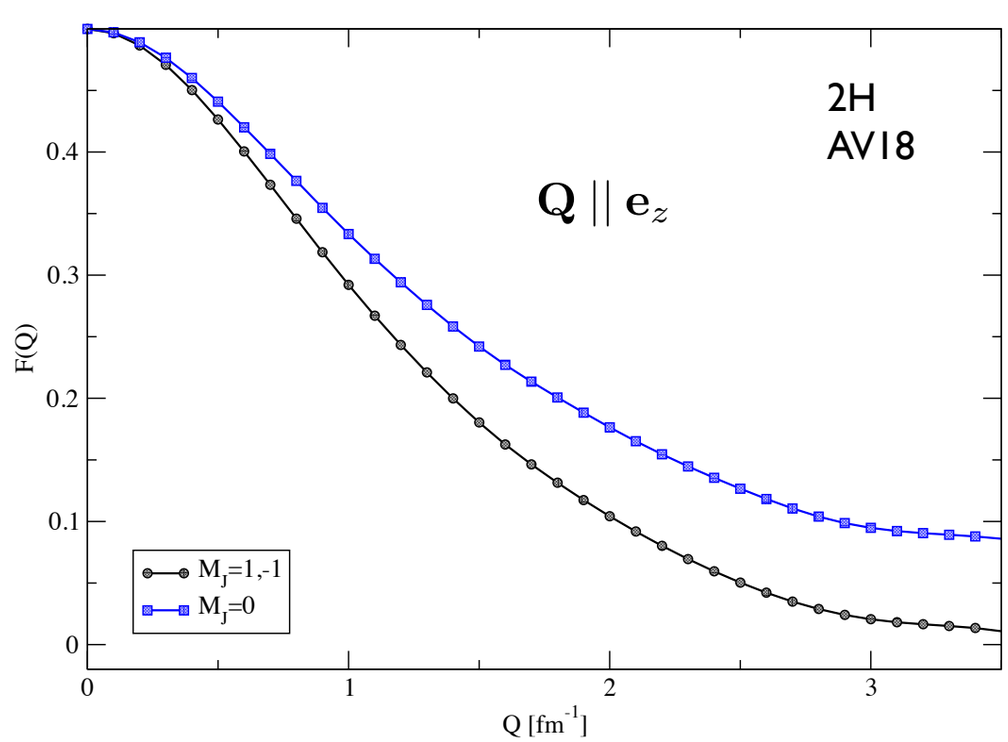
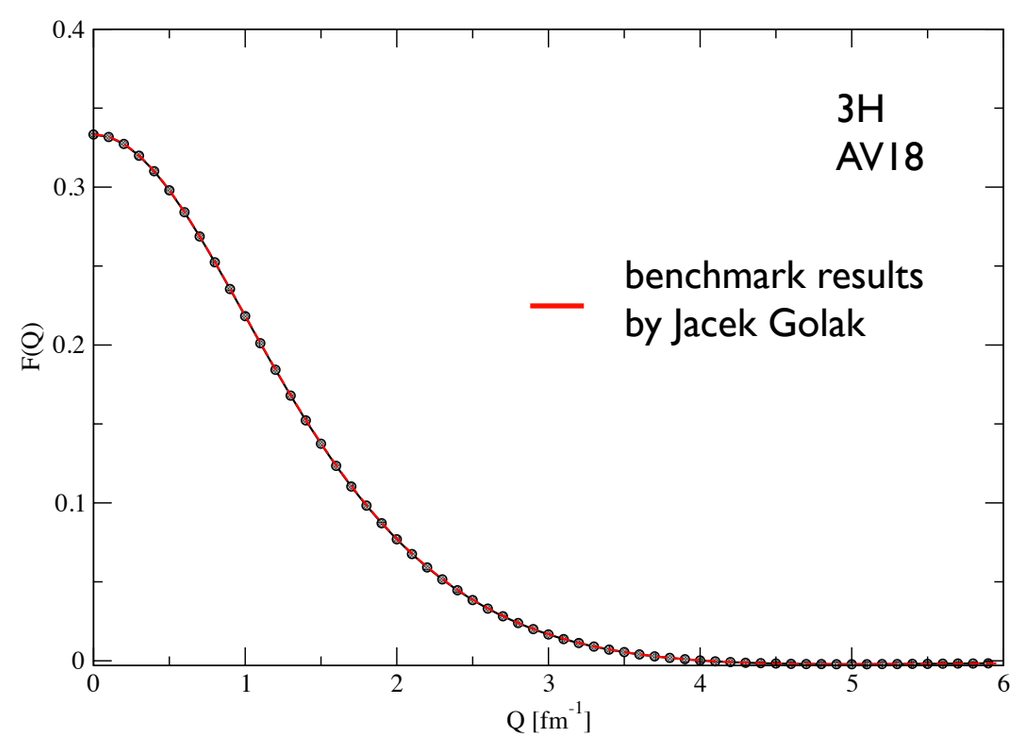


with $G_E^p = 1$ and $G_E^n = 0$

charge form factors of 2H and 3H:

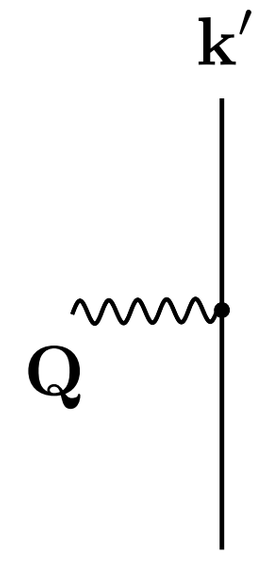




Implementation of nuclear current operators for applications in few- and many-body frameworks

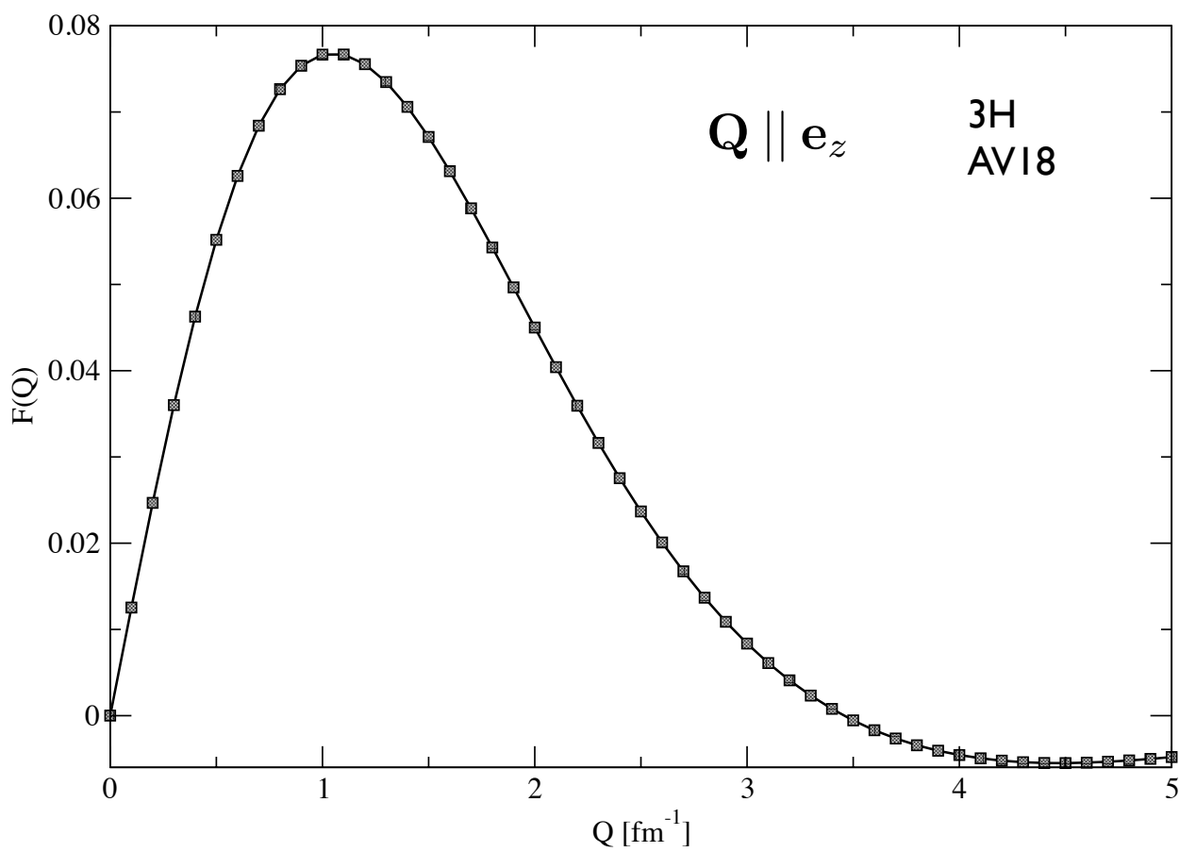
Spin vector current

$$\langle \mathbf{k}_i' | \mathbf{j} | \mathbf{k}_i \rangle = \frac{1}{2M} G_M \left[i\boldsymbol{\sigma} \times \mathbf{Q} \right] \, \delta(\mathbf{k}_i' - \mathbf{k}_i - \mathbf{Q})$$



Spin form factors 3H:

$$\langle \psi, M_J = 1/2 | j_+ | \psi, M_J = -1/2 \rangle = \langle \psi, M_J = -1/2 | j_- | \psi, M_J = 1/2 \rangle$$



Summary

- **power counting** in 3NF sector sensitively depends on regularization scheme

- developed efficient framework to compute **general 3NF** for basically **arbitrary regulators** in coordinate or momentum space

- adaption of framework to calculation of **general one- and two-body nuclear currents** (benchmarks finished for first simple test cases)

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- developed efficient framework to compute **general 3NF** for basically **arbitrary regulators** in coordinate or momentum space

- adaption of framework to calculation of **general one- and two-body nuclear currents** (benchmarks finished for first simple test cases)

Open Questions

- more systematic study of power counting $\longrightarrow$ uncertainty estimates in fits?
- how to avoid fine tuning/cancellations in fits at N3LO?
- inclusion of new observables in fitting frameworks
  - ⋆ identify relevant nuclear currents
  - ⋆ regularization of currents?