Status of three-nucleon interactions and a novel normal-ordering framework

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Progress in Ab Initio Techniques in Nuclear Physics

TRIUMF

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TECHNISCHE UNIVERSITÄT DARMSTADT

Outline

1. Status of 3N interactions
   - 3N interactions in different regularization schemes
   - SRG evolution and application of nonlocal NN+3N interactions at N^3LO to matter and nuclei → *also talks by Robert Roth, Achim Schwenk, Thomas Hüther*

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1. Status of 3N interactions
   - 3N interactions in different regularization schemes
   - SRG evolution and application of nonlocal NN+3N interactions at N^3LO to matter and nuclei → *also talks by Robert Roth Achim Schwenk Thomas Hüther*

2. Novel normal-ordering framework for 3N interactions for applications to **medium-mass and heavier nuclei**
   - basic idea and first benchmarks
   - first applications to ^{16}O in IM-SRG

Implementation of 3NF in different regularization schemes (N^2LO) - for N^3LO see next talk by Hermann

	momentum space	coordinate space
nonlocal	**nonlocal MS**	
regulators:		
long-range	$f_\Lambda^{\text{long}}(\mathbf{p},\mathbf{q}) = \exp\left[-((\mathbf{p}^2 + 3/4\,\mathbf{q}^2)/\Lambda^2)^n\right]$	
short-range	$f_\Lambda^{\text{short}}(\mathbf{p},\mathbf{q}) = f_\Lambda^{\text{long}}(\mathbf{p},\mathbf{q}) = f_R(\mathbf{p},\mathbf{q})$	
regularization:	$\left\langle \mathbf{p}'\mathbf{q}'\lvert V_{3N}^{\text{reg}}\rvert\mathbf{pq}\right\rangle = f_R(\mathbf{p}',\mathbf{q}')\,\langle \mathbf{p}'\mathbf{q}'\lvert V_{3N}\rvert\mathbf{pq}\rangle\, f_R(\mathbf{p},\mathbf{q})$	
local	**local MS**	**local CS**
regulators:		
long-range	$f_\Lambda^{\text{long}}(\mathbf{Q}_i) = \exp\left[-(\mathbf{Q}_i^2/\Lambda^2)^2\right]$	$f_R^{\text{long}}(\mathbf{r}) = 1 - \exp\left[-(r^2/R^2)^n\right]$
short-range	$f_\Lambda^{\text{short}}(\mathbf{Q}_i) = f_\Lambda^{\text{long}}(\mathbf{Q}_i) = f_\Lambda(\mathbf{Q}_i)$	$f_R^{\text{short}}(\mathbf{r}) = \exp\left[-(r^2/R^2)^n\right]$
regularization:	$\left\langle \mathbf{p}'\mathbf{q}'\lvert V_{3N}^{\text{reg}}\rvert\mathbf{pq}\right\rangle = \langle \mathbf{p}'\mathbf{q}'\lvert V_{3N}\rvert\mathbf{pq}\rangle \prod_i f_R(\mathbf{Q}_i)$	$V_{3N}^{\pi,\text{reg}}(\mathbf{r}_{ij}) = f_R^{\text{long}}(\mathbf{r}_{ij}) V_{3N}^{\pi}(\mathbf{r}_{ij})$ $\delta^{\text{reg}}(\mathbf{r}_{ij}) = \alpha_n f_R^{\text{short}}(\mathbf{r}_{ij})$
semilocal	**semilocal MS**	**semilocal CS**
regulators:		
long-range	$f_\Lambda^{\text{long}}(\mathbf{Q}_i) = \exp\left[-(\mathbf{Q}_i^2 + m_\pi^2)/\Lambda^2\right]$	$f_R^{\text{long}}(\mathbf{r}) = \left(1 - \exp\left[-r^2/R^2\right]\right)^n$
short-range	$f_\Lambda^{\text{short}}(\mathbf{p}) = \exp\left[-\mathbf{p}^2/\Lambda^2\right]$	$f_\Lambda^{\text{short}}(\mathbf{p}) = \exp\left[-\mathbf{p}^2/\Lambda^2\right]$
regularization:	$\left\langle \mathbf{p}'\mathbf{q}'\lvert V_{3N}^{\text{reg},\pi}\rvert\mathbf{pq}\right\rangle = f_R^{\text{long}}(\mathbf{Q}_i)\,\langle \mathbf{p}'\mathbf{q}'\lvert V_{3N}\rvert\mathbf{pq}\rangle$ $\left\langle \mathbf{p}'\mathbf{q}'\lvert V_{3N}^{\text{reg},\delta}\rvert\mathbf{pq}\right\rangle = f_\Lambda^{\text{short}}(\mathbf{p}_\delta')\left\langle \mathbf{p}'\mathbf{q}'\lvert V_{3N}^{\delta}\rvert\mathbf{pq}\right\rangle f_\Lambda^{\text{short}}(\mathbf{p}_\delta)$	$V_{3N}^{\pi,\text{reg}}(\mathbf{r}_{ij}) = f_R^{\text{long}}(\mathbf{r}_{ij}) V_{3N}^{\pi}(\mathbf{r}_{ij})$ $\delta(\mathbf{r}_{ij}) \xrightarrow{FT} V_{3N}^{\delta}$ $\left\langle \mathbf{p}'\mathbf{q}'\lvert V_{3N}^{\text{reg},\delta}\rvert\mathbf{pq}\right\rangle = f_\Lambda^{\text{short}}(\mathbf{p}_\delta')\left\langle \mathbf{p}'\mathbf{q}'\lvert V_{3N}^{\delta}\rvert\mathbf{pq}\right\rangle f_\Lambda^{\text{short}}(\mathbf{p}_\delta)$

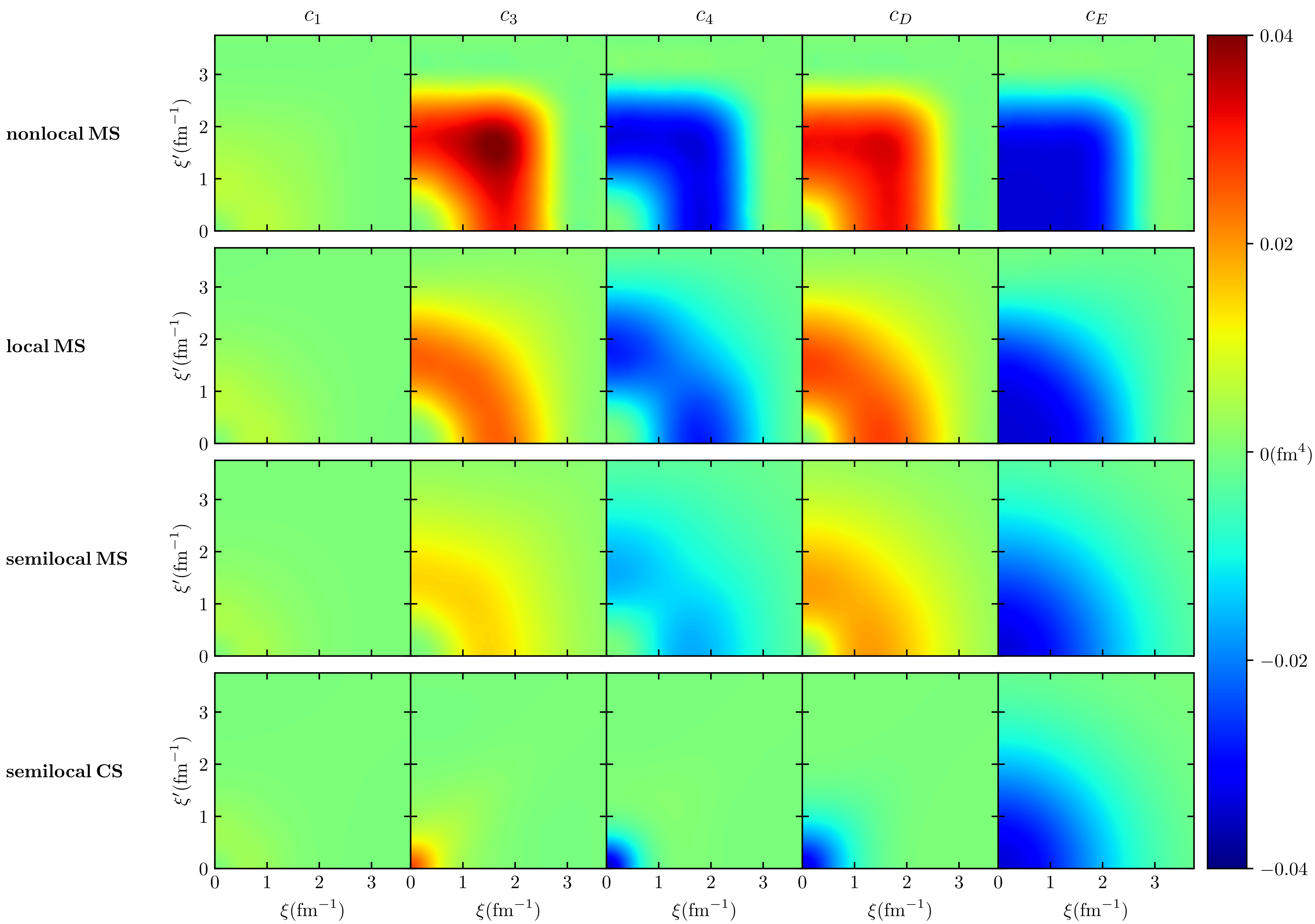
KH, in preparation

Implementation of 3NF in different regularization schemes (N²LO) - for N³LO see next talk by Hermann

	momentum space	coordinate space
nonlocal *regulators:* long-range short-range *regularization:*	**nonlocal MS** N²LO N³LO $f_\Lambda^{\rm long}(\mathbf{p},\mathbf{q}) = \exp\left[-((\mathbf{p}^2 + 3/4\,\mathbf{q}^2)/\Lambda^2)^n\right]$ $f_\Lambda^{\rm short}(\mathbf{p},\mathbf{q}) = f_\Lambda^{\rm long}(\mathbf{p},\mathbf{q}) = f_R(\mathbf{p},\mathbf{q})$ $\left\langle \mathbf{p}'\mathbf{q}' \vert V_{3N}^{\rm reg} \vert \mathbf{pq} \right\rangle = f_R(\mathbf{p}',\mathbf{q}')\,\langle \mathbf{p}'\mathbf{q}' \vert V_{3N} \vert \mathbf{pq}\rangle\, f_R(\mathbf{p},\mathbf{q})$	
local *regulators:* long-range short-range *regularization:*	**local MS** N²LO N³LO $f_\Lambda^{\rm long}(\mathbf{Q}_i) = \exp\left[-(\mathbf{Q}_i^2/\Lambda^2)^2\right]$ $f_\Lambda^{\rm short}(\mathbf{Q}_i) = f_\Lambda^{\rm long}(\mathbf{Q}_i) = f_\Lambda(\mathbf{Q}_i)$ $\left\langle \mathbf{p}'\mathbf{q}' \vert V_{3N}^{\rm reg} \vert \mathbf{pq} \right\rangle = \langle \mathbf{p}'\mathbf{q}' \vert V_{3N} \vert \mathbf{pq}\rangle \prod_i f_R(\mathbf{Q}_i)$	**local CS** N²LO N³LO $f_R^{\rm long}(\mathbf{r}) = 1 - \exp\left[-(r^2/R^2)^n\right]$ $f_R^{\rm short}(\mathbf{r}) = \exp\left[-(r^2/R^2)^n\right]$ $V_{3N}^{\pi,{\rm reg}}(\mathbf{r}_{ij}) = f_R^{\rm long}(\mathbf{r}_{ij}) V_{3N}^{\pi}(\mathbf{r}_{ij})$ $\delta^{\rm reg}(\mathbf{r}_{ij}) = \alpha_n f_R^{\rm short}(\mathbf{r}_{ij})$
semilocal *regulators:* long-range short-range *regularization:*	**semilocal MS** N²LO N³LO $f_\Lambda^{\rm long}(\mathbf{Q}_i) = \exp\left[-(\mathbf{Q}_i^2 + m_\pi^2)/\Lambda^2\right]$ $f_\Lambda^{\rm short}(\mathbf{p}) = \exp\left[-\mathbf{p}^2/\Lambda^2\right]$ $\left\langle \mathbf{p}'\mathbf{q}' \vert V_{3N}^{{\rm reg},\pi} \vert \mathbf{pq} \right\rangle = f_R^{\rm long}(\mathbf{Q}_i)\,\langle \mathbf{p}'\mathbf{q}' \vert V_{3N} \vert \mathbf{pq}\rangle$ $\left\langle \mathbf{p}'\mathbf{q}' \vert V_{3N}^{{\rm reg},\delta} \vert \mathbf{pq} \right\rangle = f_\Lambda^{\rm short}(\mathbf{p}'_\delta) \left\langle \mathbf{p}'\mathbf{q}' \vert V_{3N}^{\delta} \vert \mathbf{pq} \right\rangle f_\Lambda^{\rm short}(\mathbf{p}_\delta)$	**semilocal CS** N²LO N³LO $f_R^{\rm long}(\mathbf{r}) = (1 - \exp\left[-r^2/R^2\right])^n$ $f_\Lambda^{\rm short}(\mathbf{p}) = \exp\left[-\mathbf{p}^2/\Lambda^2\right]$ $V_{3N}^{\pi,{\rm reg}}(\mathbf{r}_{ij}) = f_R^{\rm long}(\mathbf{r}_{ij}) V_{3N}^{\pi}(\mathbf{r}_{ij})$ $\delta(\mathbf{r}_{ij}) \overset{FT}{\rightarrow} V_{3N}^{\delta}$ $\left\langle \mathbf{p}'\mathbf{q}' \vert V_{3N}^{{\rm reg},\delta} \vert \mathbf{pq} \right\rangle = f_\Lambda^{\rm short}(\mathbf{p}'_\delta) \left\langle \mathbf{p}'\mathbf{q}' \vert V_{3N}^{\delta} \vert \mathbf{pq} \right\rangle f_\Lambda^{\rm short}(\mathbf{p}_\delta)$

KH, in preparation

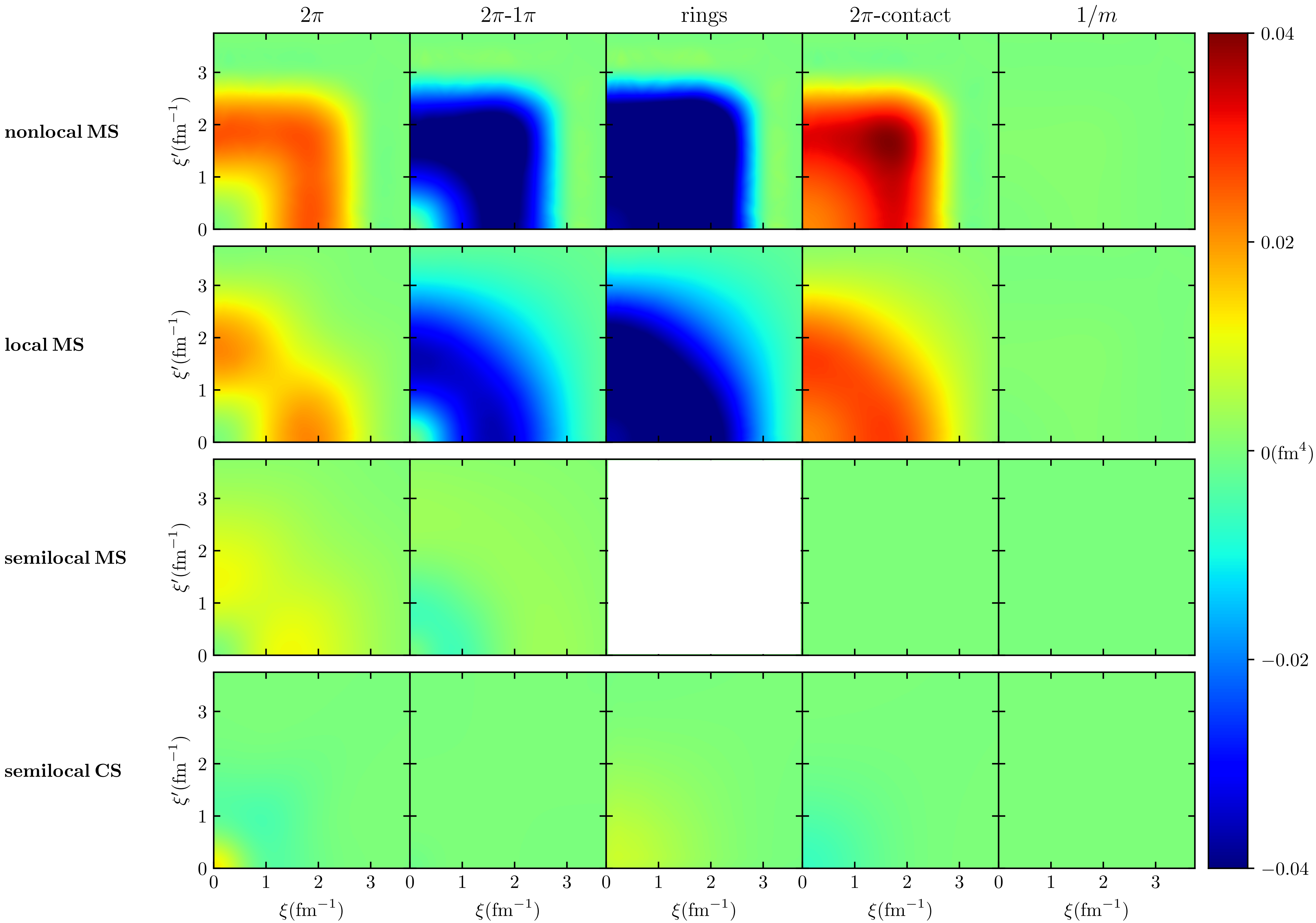
Illustration of 3NF in different regularization schemes



$$\xi^2 = p^2 + 3/4q^2 \quad \tan\theta = p/(\sqrt{3}/2q) = \frac{\pi}{4}$$

KH, in preparation

Illustration of 3NF in different regularization schemes



$$\xi^2 = p^2 + 3/4q^2 \qquad \tan\theta = p/(\sqrt{3}/2q) = \frac{\pi}{4}$$

KH, in preparation

3NF in different regularization schemes (N2LO)

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semilocal	**semilocal MS**	**semilocal CS**

Fits to 3H (plus another observable):

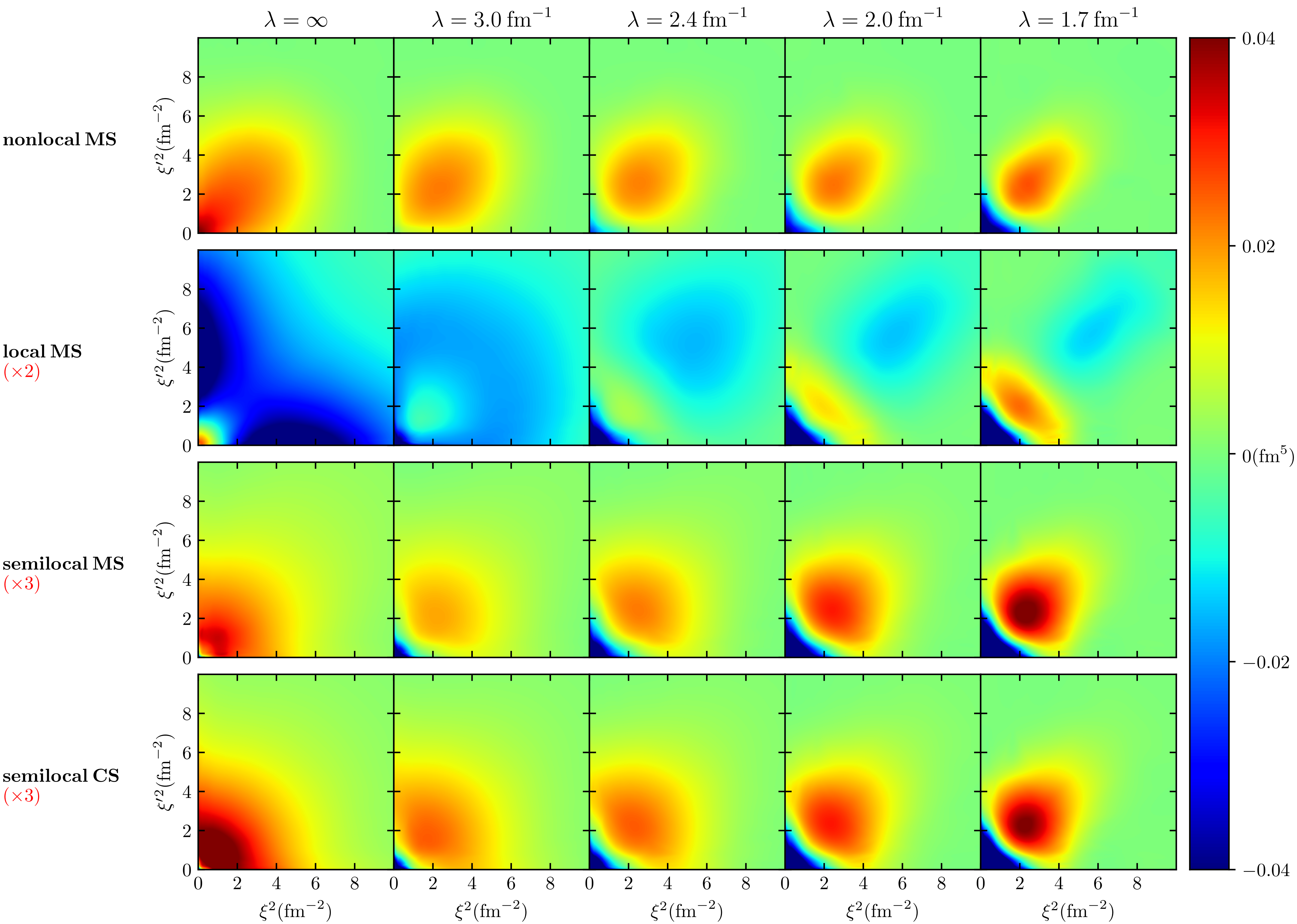
regularization	c_1 [GeV $^{-1}$]	c_3 [GeV $^{-1}$]	c_4 [GeV $^{-1}$]	c_D	c_E
nonlocal MS	-0.74	-3.61	2.44	−1.5	-0.61
local MS	-0.81	-3.2	5.4	0.83	-0.052
semilocal MS	-0.74	-3.61	2.44	2.0	0.23
semilocal CS	-0.81	-4.69	3.4	1.0	-0.25

Drischler et al., PRL 122, 042501 (2019)

Gazit et al., PRL 122, 029901(E) (2019)

Epelbaum et al., arXiv:1807.02848
accepted for publication in PRC

Momentum space SRG evolution of 3NF in different regularization schemes

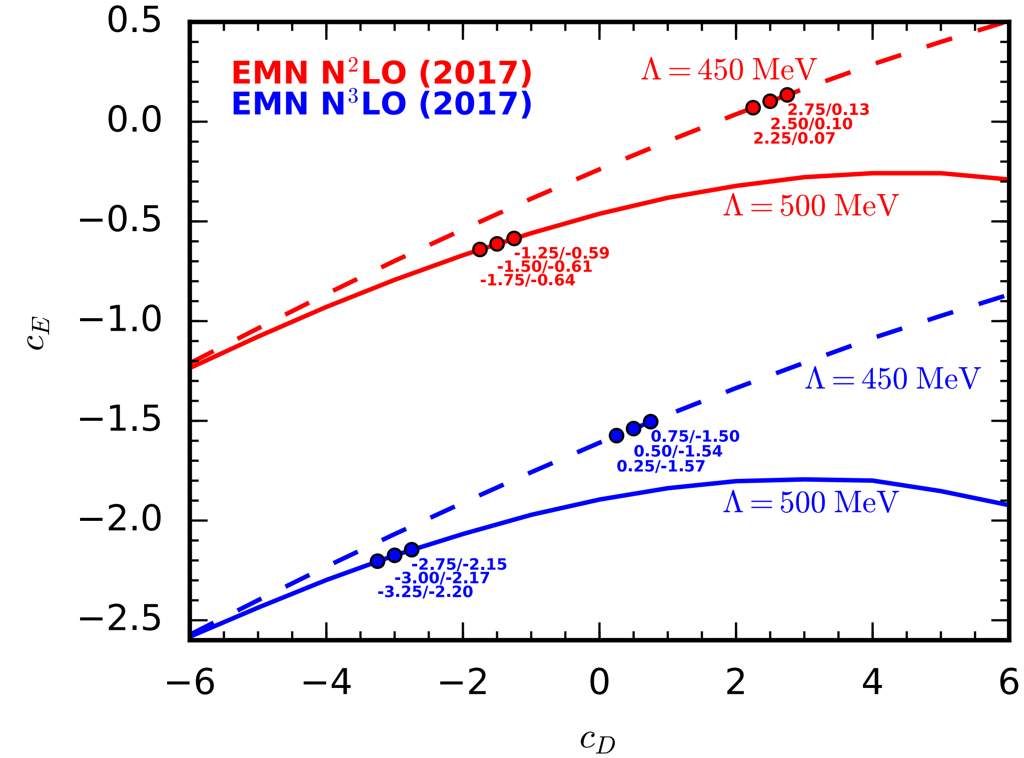


KH, in preparation

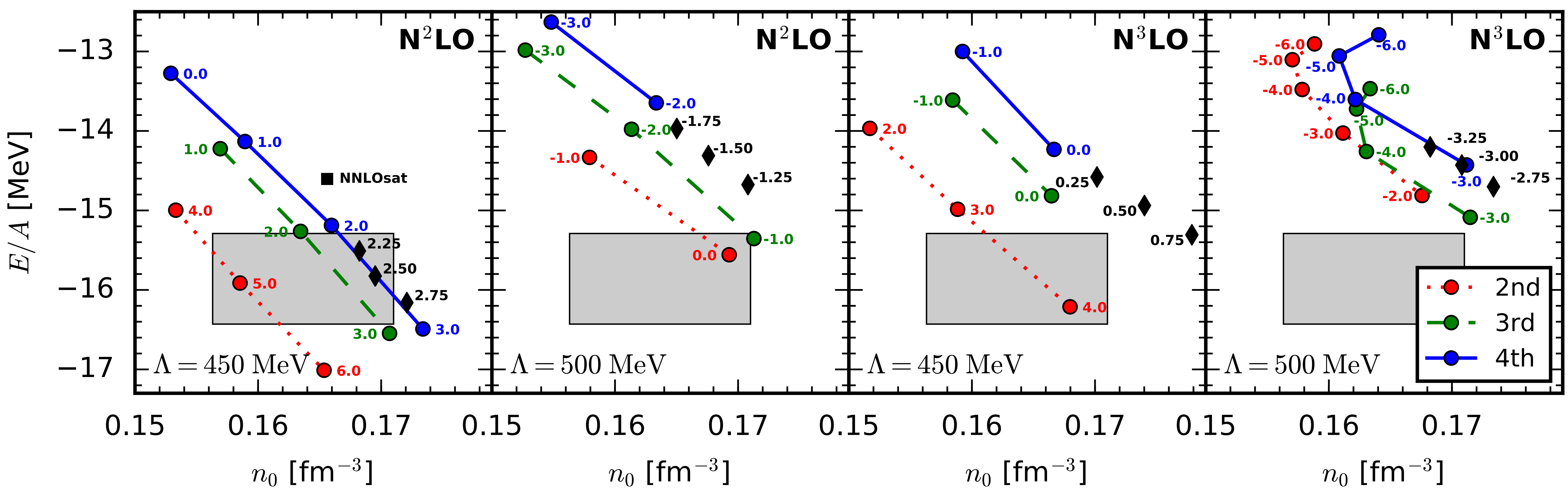
Fits of 3N interactions to saturation properties of nuclear matter

fits for 3NF at N^2LO and N^3LO to ^3H and matter for new family of NN forces by Entem, Machleidt and Nosyk:

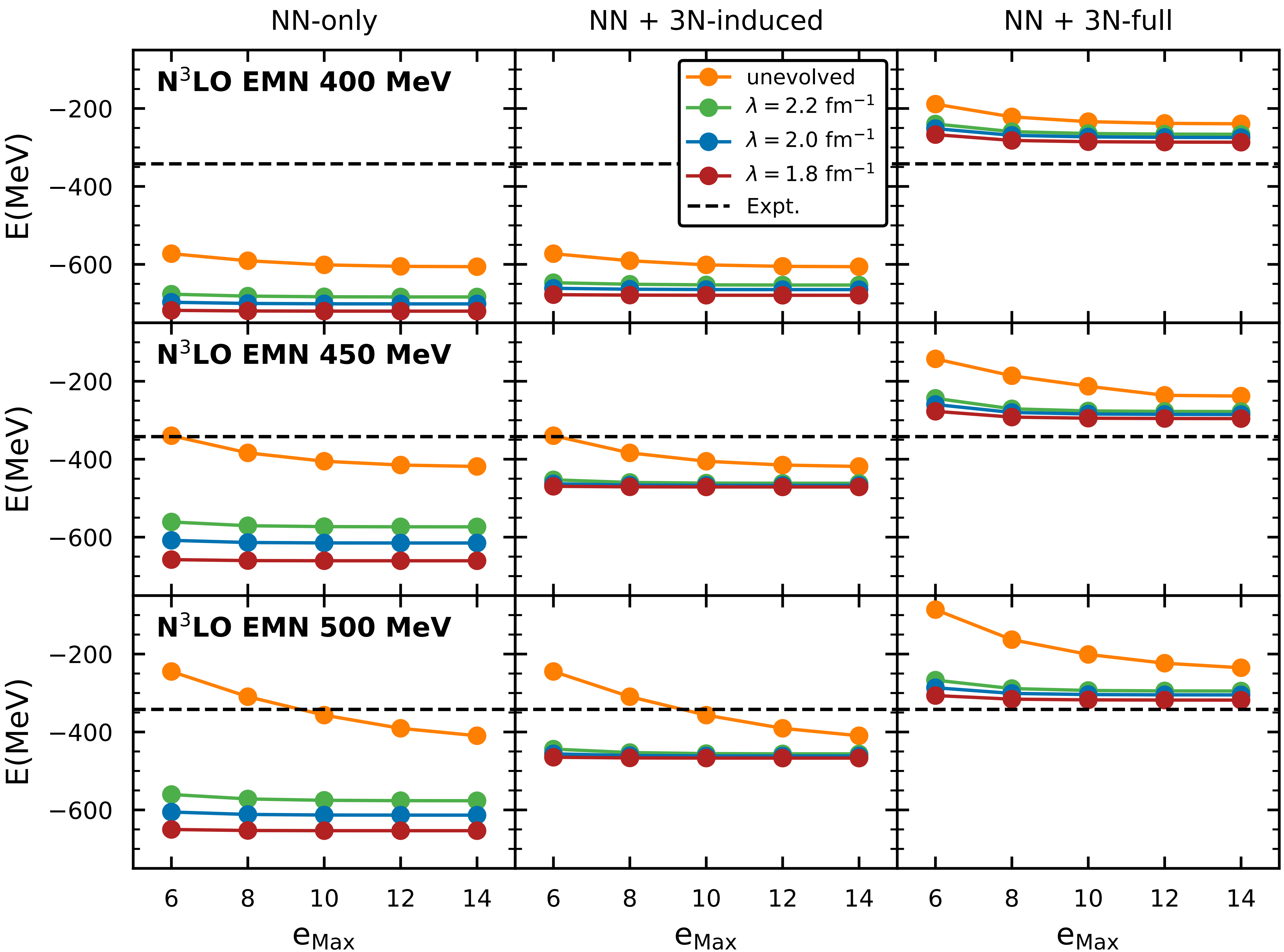
Entem et al. PRC 96, 024004 (2017)



Drischler et al., PRL 122, 042501 (2019)



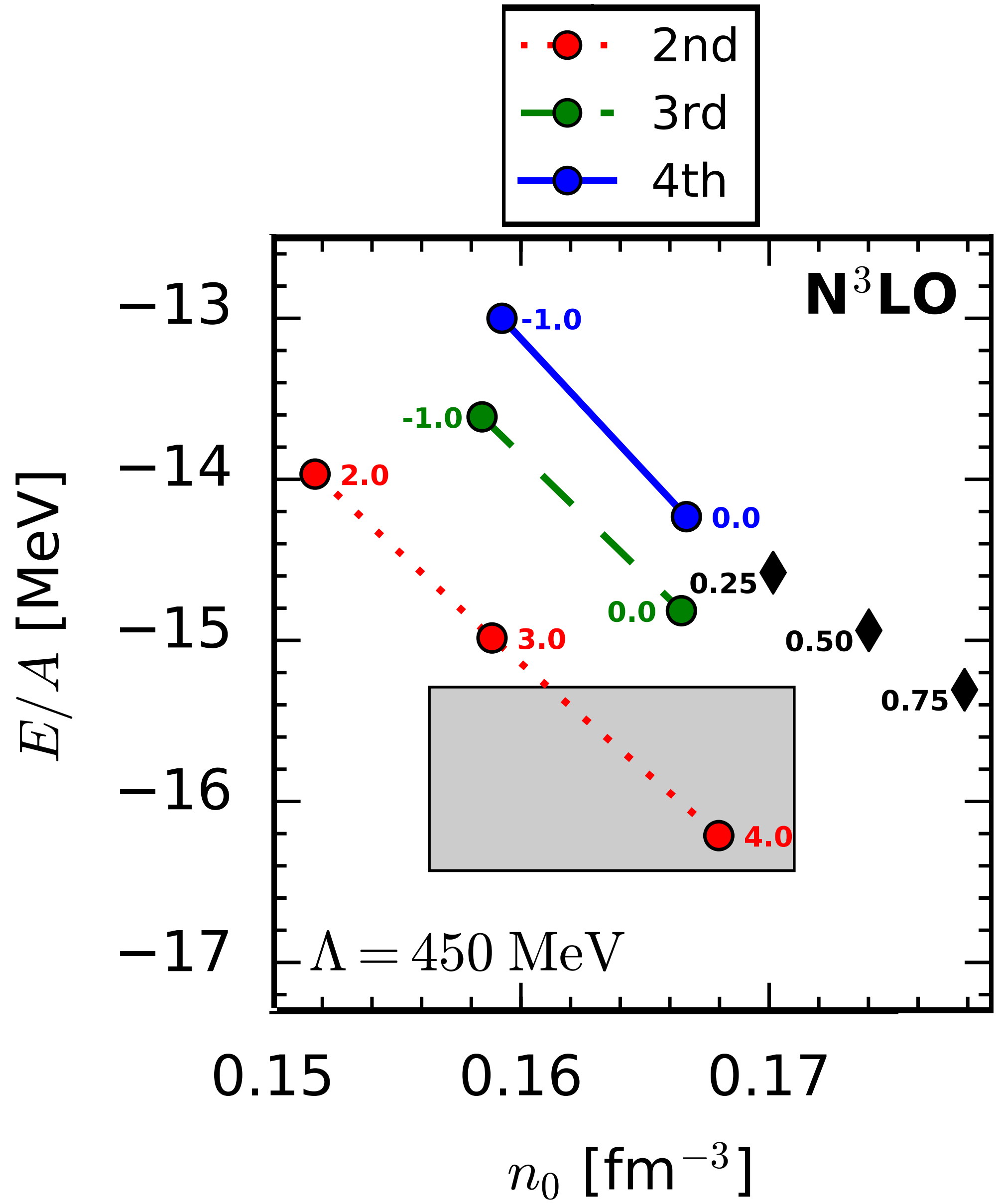
First applications to ^{40}Ca



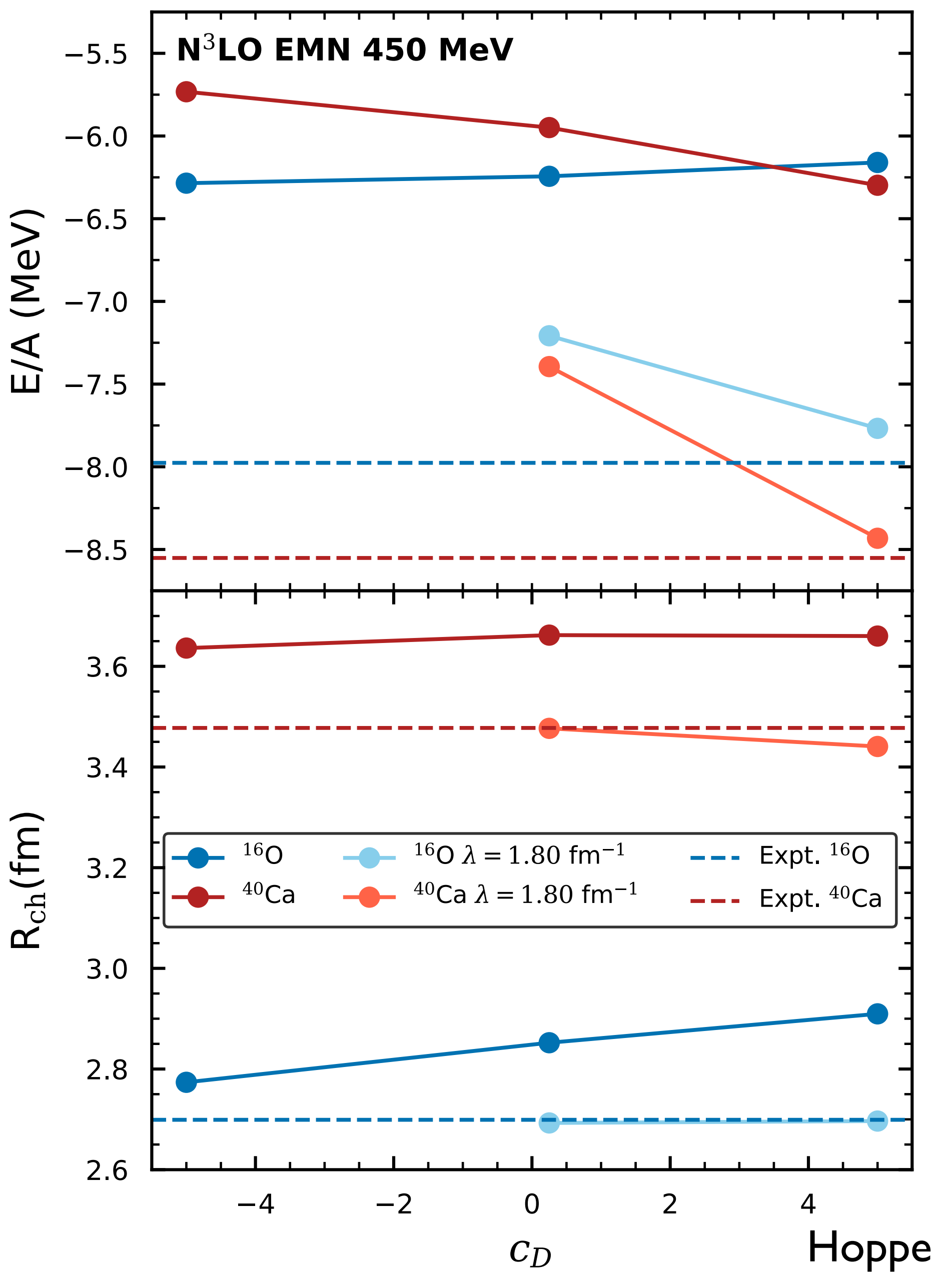
Jan Hoppe

Hoppe at al., in preparation

Comparing systematics of results for matter and nuclei



Drischler et al., PRL 122, 042501 (2019)



Jan Hoppe

Hoppe at al., in preparation

- connection between results for matter and nuclei still not fully understood
- role of higher-body forces in SRG evolution?

→ *more in Achim's talk*

Novel normal ordering framework for 3N interactions

traditional approach:

1. transformation to Jacobi HO basis plus antisymmetrization

$$\langle p'q'\alpha'|V_{3\mathrm{N}}^{(i),\mathrm{reg}}|pq\alpha\rangle \rightarrow \langle N'n'\alpha'|V_{3\mathrm{N}}^{(\mathrm{as},\mathrm{reg}}|Nn\alpha\rangle$$

Novel normal ordering framework for 3N interactions

traditional approach:

1. transformation to Jacobi HO basis plus antisymmetrization

$$\langle p'q'\alpha'|V_{3N}^{(i),\mathrm{reg}}|pq\alpha\rangle \rightarrow \langle N'n'\alpha'|V_{3N}^{(\mathrm{as,reg}}|Nn\alpha\rangle$$

2. transformation to single particle basis

$$\langle N'n'\alpha'|V_{3N}^{\mathrm{as,\ reg}}|Nn\alpha\rangle \rightarrow \langle 1'2'3'|V_{3N}^{\mathrm{as,\ reg}}|123\rangle$$

Novel normal ordering framework for 3N interactions

traditional approach:

1. transformation to Jacobi HO basis plus antisymmetrization

$$\langle p'q'\alpha'|V_{3N}^{(i),\mathrm{reg}}|pq\alpha\rangle \rightarrow \langle N'n'\alpha'|V_{3N}^{(\mathrm{as},\mathrm{reg}}|Nn\alpha\rangle$$

2. transformation to single particle basis

$$\langle N'n'\alpha'|V_{3N}^{\mathrm{as},\ \mathrm{reg}}|Nn\alpha\rangle \rightarrow \langle 1'2'3'|V_{3N}^{\mathrm{as},\ \mathrm{reg}}|123\rangle$$

3. Normal ordering with respect
to some reference state

$$\langle 1'2'|\overline{V}|12\rangle = \sum_{3} \bar{n}_3 \langle 1'2'3|V_{3N}^{\mathrm{as}}|123\rangle$$

Novel normal ordering framework for 3N interactions

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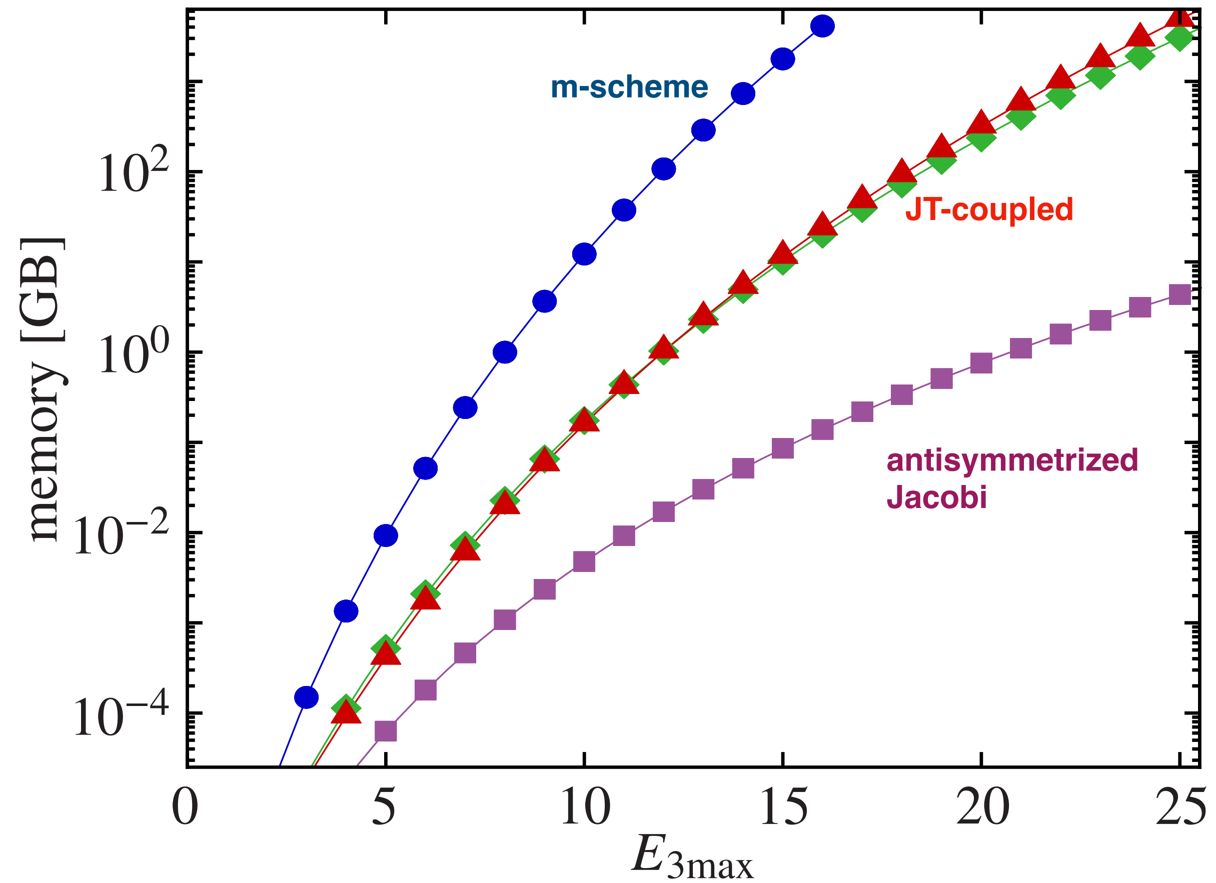
3. Normal ordering with respect to some reference state

$$\langle 1'2'|\overline{V}|12\rangle = \sum_{3} \bar{n}_3 \langle 1'2'3|V_{3N}^{\mathrm{as}}|123\rangle$$

- severe memory limitations for handling of single-particle matrix elements with increasing E_{3max}
- convergence in heavier systems?



Roth at al., PRC 90 024325

Novel normal ordering framework for 3N interactions

Victoria Durant

new approach:

1. Express effective interaction in momentum space and expand reference state in HO basis:

$$\langle \mathbf{k}_1' \mathbf{k}_2' | \overline{V} | \mathbf{k}_1 \mathbf{k}_2 \rangle = \sum_{n_3 l_3 m_3} \overline{n}_3 \langle \mathbf{k}_1' \mathbf{k}_2' \gamma_3 | V_{3\mathrm{N}}^{\mathrm{as}} | \mathbf{k}_1 \mathbf{k}_2 \gamma_3 \rangle$$

$$= \int d\mathbf{k}_3 d\mathbf{k}_3' \langle \mathbf{k}_1' \mathbf{k}_2' \mathbf{k}_3' | V_{3\mathrm{N}}^{\mathrm{as}} | \mathbf{k}_1 \mathbf{k}_2 \mathbf{k}_3 \rangle \sum_{n_3 l_3 m_3} \overline{n}_3 \langle \gamma_3 | \mathbf{k}_3' \rangle \langle \mathbf{k}_3 | \gamma_3 \rangle$$

Novel normal ordering framework for 3N interactions

new approach:

Victoria Durant

1. Express effective interaction in momentum space and expand reference state in HO basis:

$$\langle \mathbf{k}_1'\mathbf{k}_2'|\overline{V}|\mathbf{k}_1\mathbf{k}_2\rangle = \sum_{n_3 l_3 m_3} \overline{n}_3 \langle \mathbf{k}_1'\mathbf{k}_2'\gamma_3|V_{3\mathrm{N}}^{\mathrm{as}}|\mathbf{k}_1\mathbf{k}_2\gamma_3\rangle$$

$$= \int d\mathbf{k}_3 d\mathbf{k}_3' \langle \mathbf{k}_1'\mathbf{k}_2'\mathbf{k}_3'|V_{3\mathrm{N}}^{\mathrm{as}}|\mathbf{k}_1\mathbf{k}_2\mathbf{k}_3\rangle \sum_{n_3 l_3 m_3} \overline{n}_3 \langle \gamma_3|\mathbf{k}_3'\rangle\langle \mathbf{k}_3|\gamma_3\rangle$$

2. Rewrite interaction in Jacobi momentum basis:

$$\langle \mathbf{p}'\mathbf{P}'|\overline{V}|\mathbf{p}\mathbf{P}\rangle = \int d\mathbf{k}_3 d\mathbf{k}_3' \langle \mathbf{p}'\mathbf{q}'|V_{3\mathrm{N}}^{\mathrm{as}}|\mathbf{p}\mathbf{q}\rangle \delta(\mathbf{P}+\mathbf{k}_3-\mathbf{P}'-\mathbf{k}_3') \sum_{n_3 l_3 m_3} \bar{n}_3 \langle \gamma_3|\mathbf{k}_3'\rangle\langle \mathbf{k}_3|\gamma_3\rangle$$

Novel normal ordering framework for 3N interactions

new approach:


Victoria Durant

1. Express effective interaction in momentum space and expand reference state in HO basis:

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$$= \int d\mathbf{k}_3 d\mathbf{k}_3' \langle \mathbf{k}_1'\mathbf{k}_2'\mathbf{k}_3'|V_{3\mathrm{N}}^{\mathrm{as}}|\mathbf{k}_1\mathbf{k}_2\mathbf{k}_3\rangle \sum_{n_3 l_3 m_3} \overline{n}_3 \langle \gamma_3|\mathbf{k}_3'\rangle\langle \mathbf{k}_3|\gamma_3\rangle$$

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3. Decomposition in generalized Jacobi partial wave momentum states:

$$\langle p'P'L'M'L_{cm}'M_{cm}'|\overline{V}|pPLML_{cm}M_{cm}\rangle$$

$$= \int d\hat{\mathbf{p}} d\hat{\mathbf{P}} d\hat{\mathbf{p}}' d\hat{\mathbf{P}}' Y^*_{L_{cm}'M_{cm}'}(\hat{\mathbf{P}}') Y^*_{L'M'}(\hat{\mathbf{p}}') \langle \mathbf{p}'\mathbf{P}'|\overline{V}|\mathbf{p}\mathbf{P}\rangle Y_{L_{cm}M_{cm}}(\hat{\mathbf{P}}) Y_{LM}(\hat{\mathbf{p}})$$

$$= \int d\hat{\mathbf{P}} d\hat{\mathbf{P}}' Y^*_{L_{cm}'M_{cm}'}(\hat{\mathbf{P}}') Y_{L_{cm}M_{cm}}(\hat{\mathbf{P}}) \int d\mathbf{k}_3 d\mathbf{k}_3' \sum_{l,l'} \sum_{m,m'} Y^*_{l'm'}(\hat{\mathbf{q}}') Y_{lm}(\hat{\mathbf{q}})$$

$$\times \delta(\mathbf{P}+\mathbf{k}_3-\mathbf{P}'-\mathbf{k}_3') \sum_{n_3,l_3} \overline{n}_3 R_{n_3 l_3}(k_3) R_{n_3 l_3}(k_3') \frac{2l_3+1}{4\pi} P_{l_3}(\hat{\mathbf{k}}_3 \cdot \hat{\mathbf{k}}_3') \langle p'q'L'M'l'm'|V_{3\mathrm{N}}^{\mathrm{as}}|pqLMlm\rangle$$

Novel normal ordering framework for 3N interactions

new approach:

Victoria Durant

4. transform matrix elements to Jacobi HO basis

$$\langle n'_p N'_P L' M' L'_{cm} M'_{cm} | \overline{V} | n_p N_P L M L_{cm} M_{cm} \rangle$$

5. transformation to single-particle HO basis via generalized Talmi transformation (taking into account L_{cm} dependence)

Novel normal ordering framework for 3N interactions

Victoria Durant

new approach:

4. transform matrix elements to Jacobi HO basis

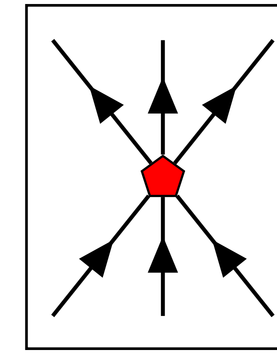
$$\langle n_p' N_P' L' M' L_{cm}' M_{cm}' | \overline{V} | n_p N_P L M L_{cm} M_{cm} \rangle$$

5. transformation to single-particle HO basis via generalized Talmi transformation (taking into account L_{cm} dependence)

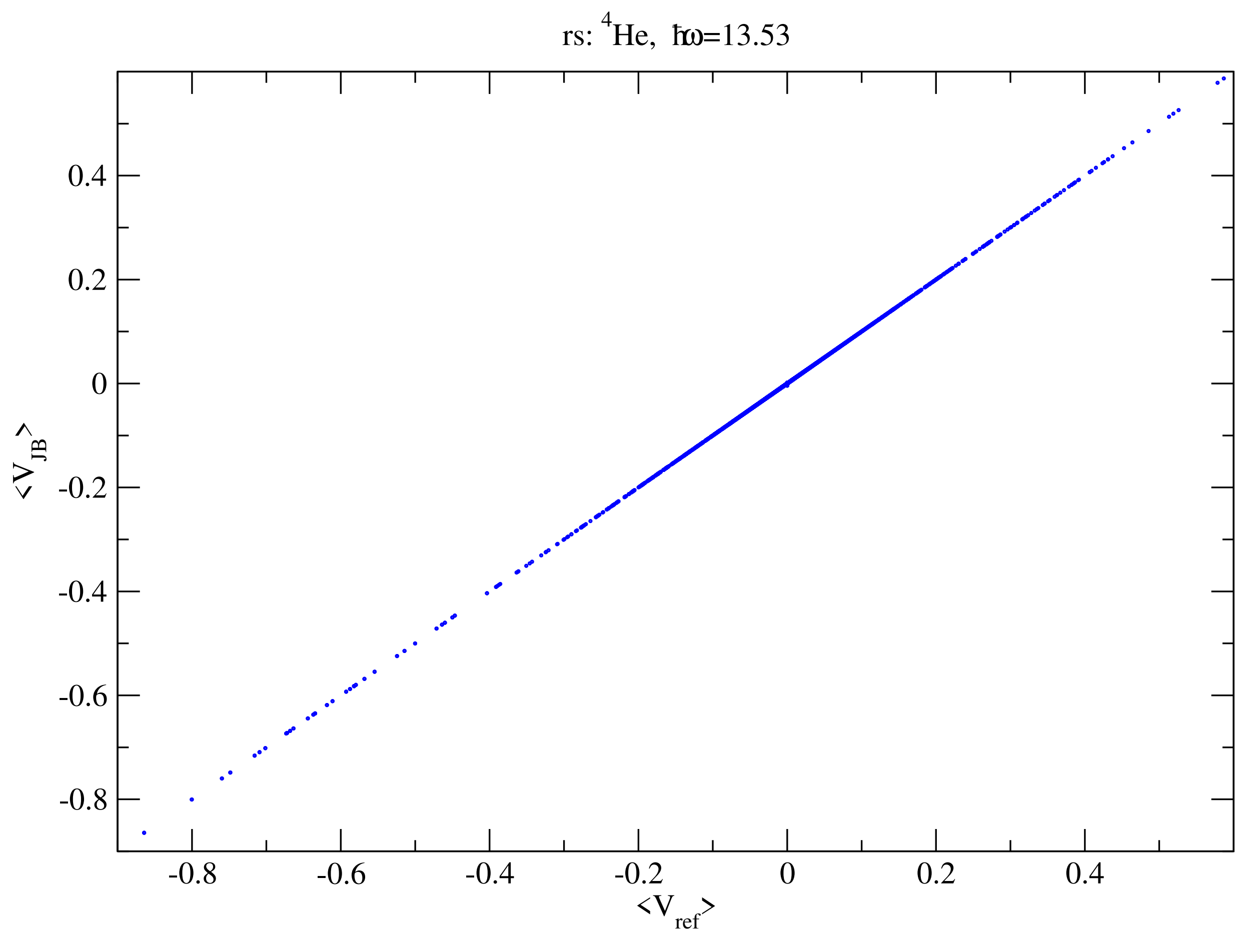
- single-particle 3N matrix elements are not needed at any point
- generalization to general spin-dependent 3N interactions straightforward and already implemented
- N_{max} can be increased easily

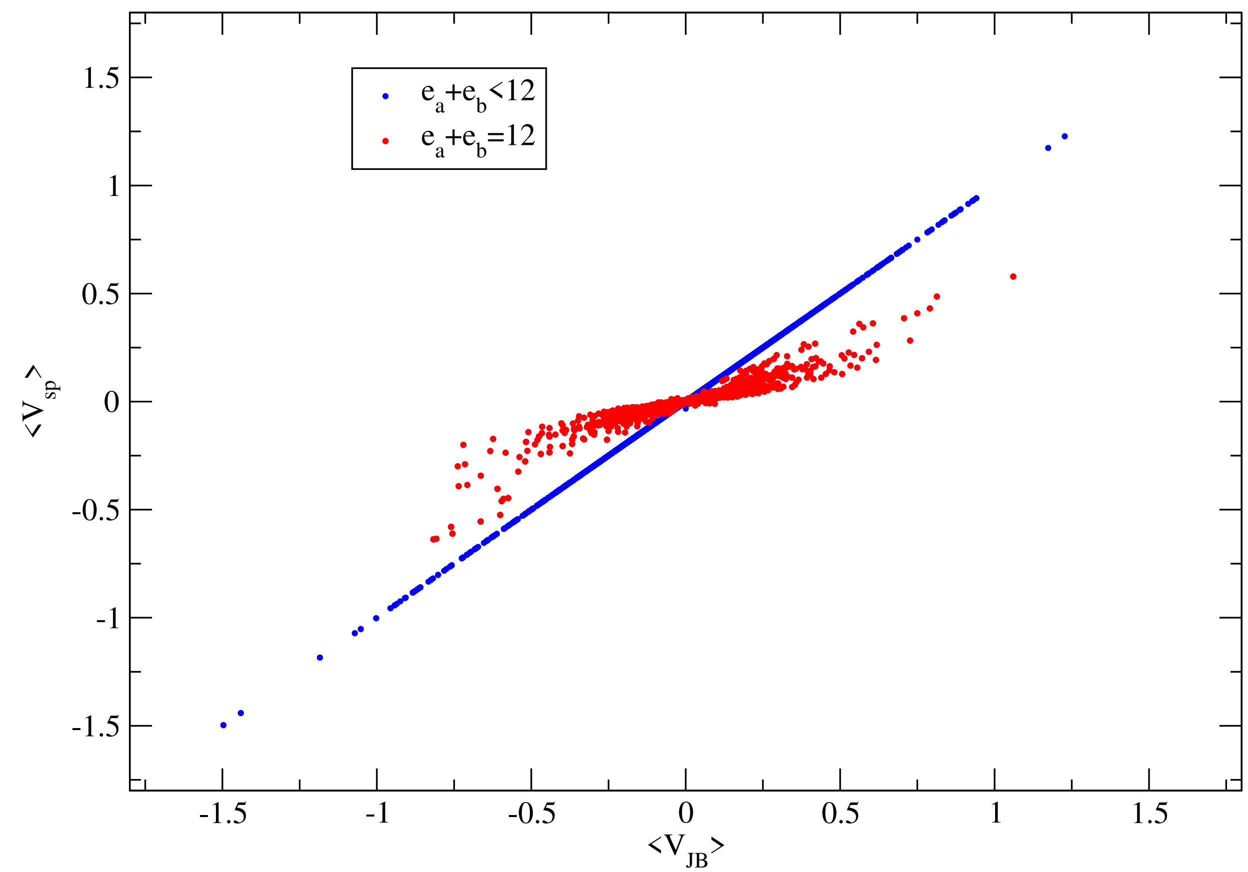
- number of partial waves grows quickly with increasing L and L_{cm}
- model space limitations governed by in L_{max} resp. J_{max}
- currently implemented for HO reference state, HF reference state work in progress

Novel normal ordering framework for 3N interactions: Pure contact 3N interaction



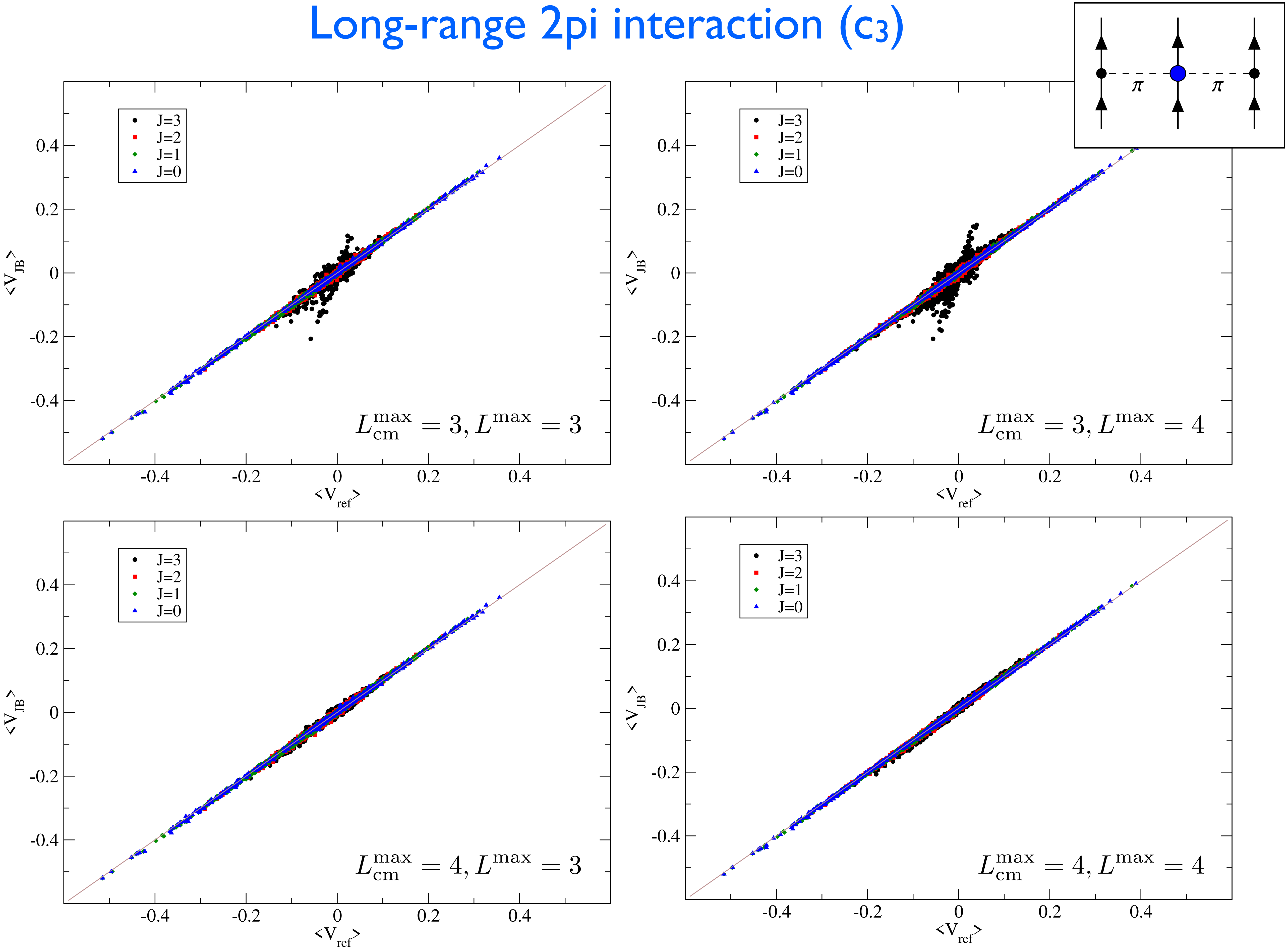
only configurations with L=L'=0 contribute:





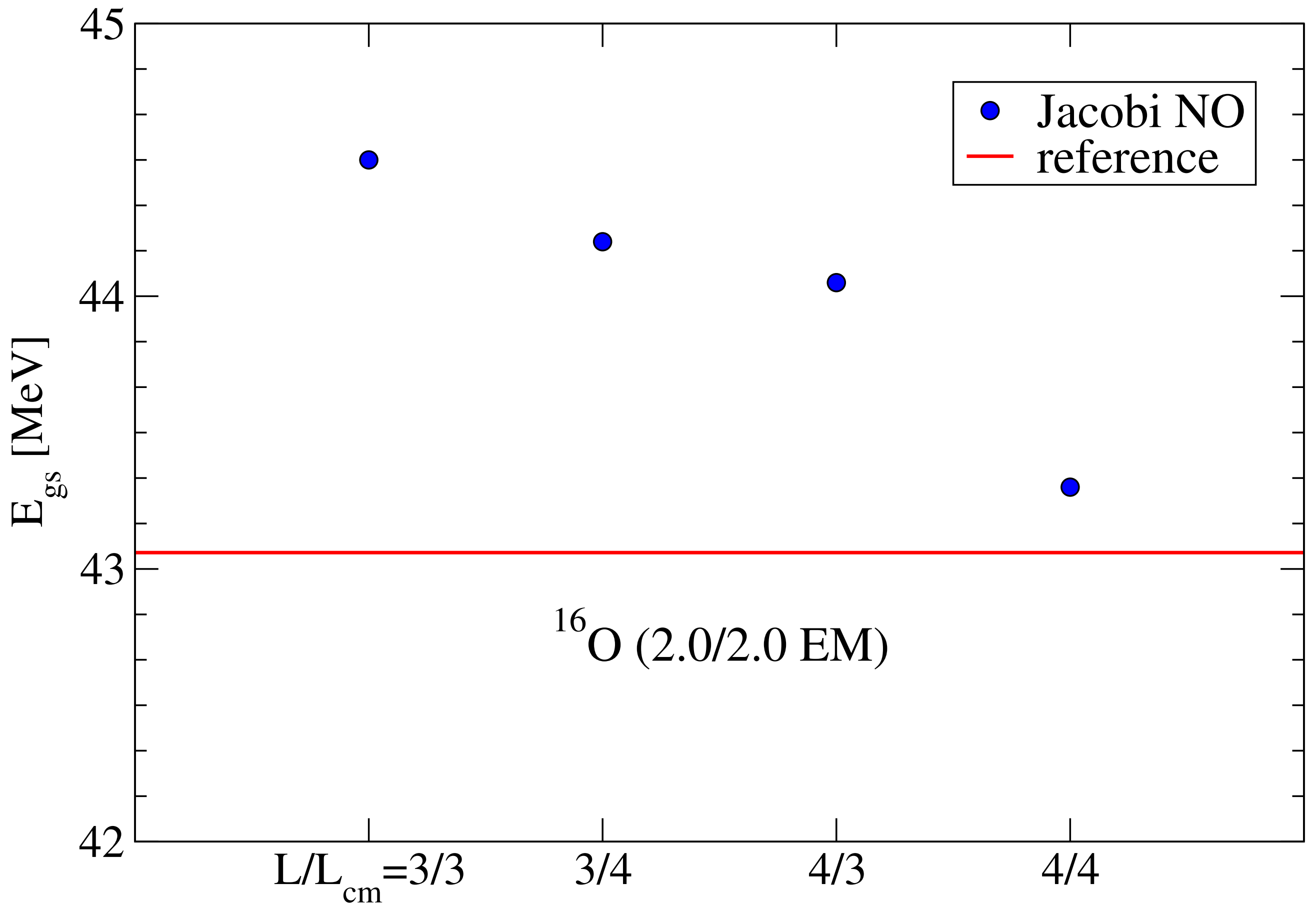
perfect agreement between results from both approaches up to given model space

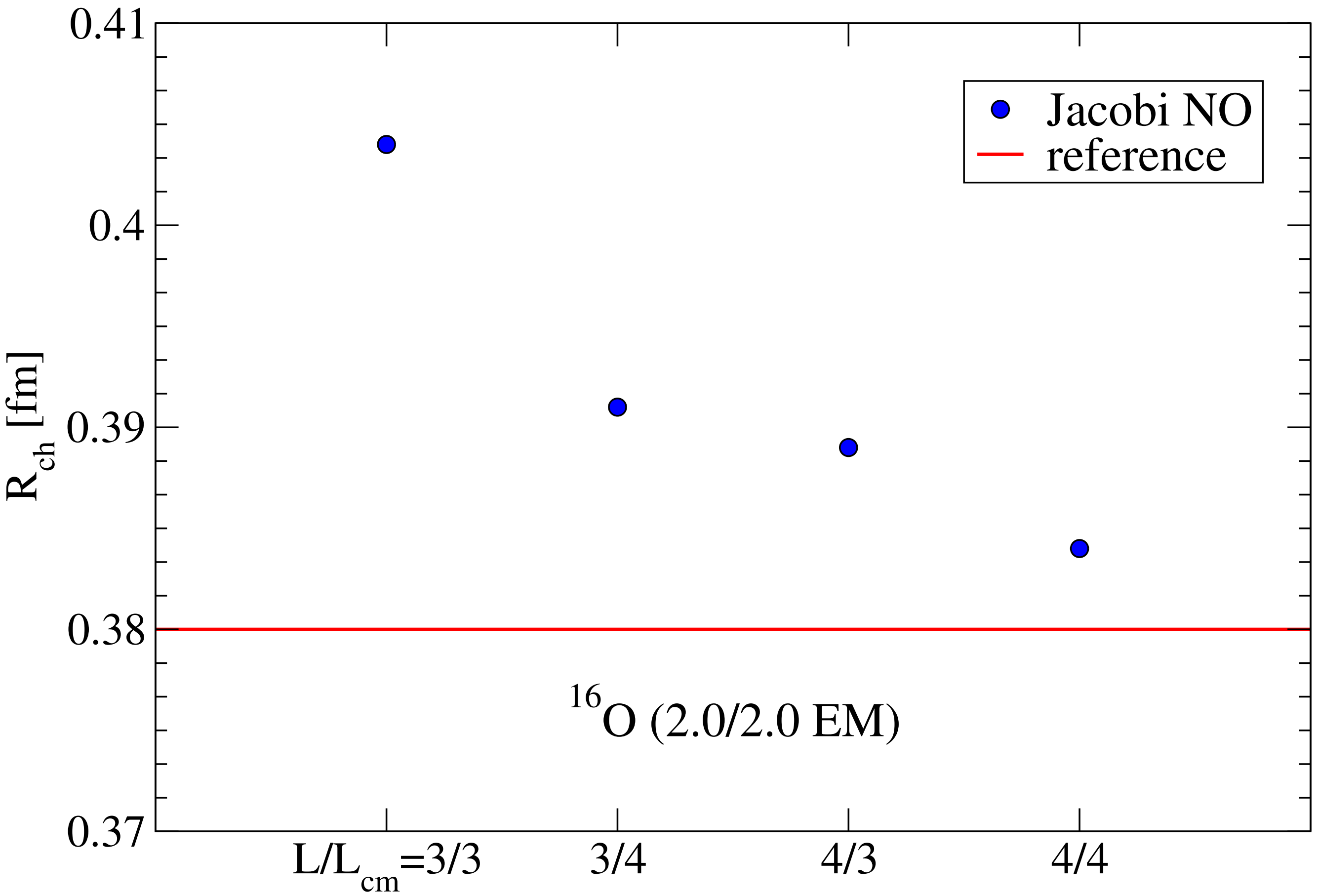
Novel normal ordering framework for 3N interactions: Long-range 2pi interaction (c_3)



Novel normal ordering framework for 3N interactions
First benchmark calculations for ^{16}O

comparison of 3N contributions to the energy (left) and charge radius (left):





systematic convergence towards results based on traditional normal ordering approach with increasing L/L_{cm}

Summary and Outlook

Development and calculation of 3N matrix elements in progress, size and structure of matrix elements sensitive to regularization
n → next talk by Hermann

First calculations of nuclei and matter based on nonlocal interactions up to N^3LO → talks by Achim, Robert, Thomas (plus poster)

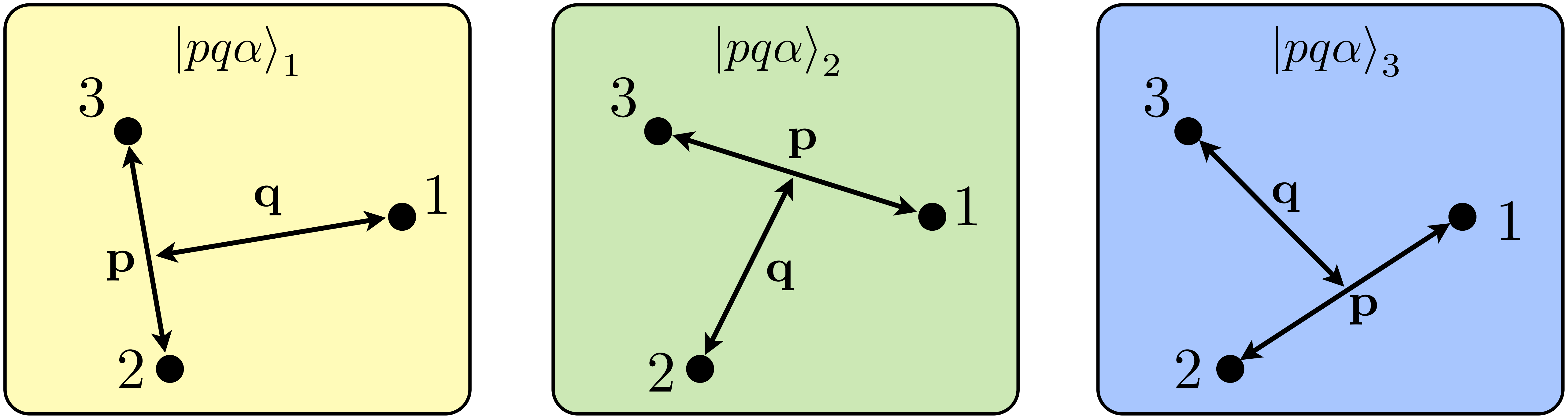
Novel normal ordering framework for 3NF that avoids the need to represent 3NF in single-particle coordinates, first benchmarks promising - further tests and optimizations in progress

Thank you!

Backup slides

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.

$$N_p \simeq N_q \simeq 15$$
$$N_\alpha \simeq 30 - 180$$
$$\longrightarrow \quad \dim[\langle pq\alpha|V_{123}|p'q'\alpha'\rangle] \simeq 10^7 - 10^{10}$$

A ‘new’ algorithm allows efficient calculation.

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

Novel efficient many-body framework for nuclear matter (and other problems?)

Main code developer:
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Problem:

Evaluation of MBPT diagrams beyond second order in perturbation theory becomes complicated and tedious in partial wave representation.

Present frameworks too inefficient for including matter properties in force fits.

Strategy:

Implementation of NN and 3N forces without partial wave decomposition.

Calculate MBPT diagrams in vector basis

$$|12...n\rangle = |\mathbf{k}_1 m_{s_1} m_{t_1}\rangle \otimes |\mathbf{k}_2 m_{s_2} m_{t_2}\rangle \otimes ... \otimes |\mathbf{k}_n m_{s_n} m_{t_n}\rangle$$

using Monte-Carlo techniques. Implementation efficient and very transparent.

Drischler et al. arXiv:1710.08220 (2017)

Status:

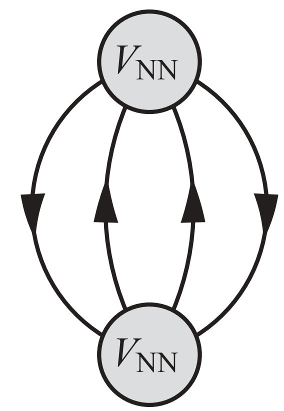
Implementation of nonlocal NN plus 3N forces up to N3LO complete.

Implemented MBPT diagrams up to 4th order for state-of-the-art interactions.

Entem et al. PRC 96, 024004 (2017)

Example: Second order diagram in MBPT

$$E^{(2)}_{\rm NN+3N,eff} = \frac{1}{4}\left[\prod_{i=1}^{4} {\rm Tr}_{\sigma_i}\int \frac{d\mathbf{k}_i}{(2\pi)^3}\right]\left|\langle 12|V^{(2)}_{\rm as}|34\rangle\right|^2 \times \frac{n_{\mathbf{k}_1}n_{\mathbf{k}_2}(1-n_{\mathbf{k}_3})(1-n_{\mathbf{k}_4})}{\varepsilon_{\mathbf{k}_1}+\varepsilon_{\mathbf{k}_2}-\varepsilon_{\mathbf{k}_3}-\varepsilon_{\mathbf{k}_4}}(2\pi)^3 \times \delta(\mathbf{k}_1+\mathbf{k}_2-\mathbf{k}_3-\mathbf{k}_4).$$



Partial wave representation:

$$\sum_{S,M_S,M'_S}\left|\langle \mathbf{k}SM_S|V^{(2)}_{\rm as}|\mathbf{k}'SM'_S\rangle\right|^2 = \sum_L P_L(\cos\theta_{\mathbf{k},\mathbf{k}'})\sum_{J,l,l',S}\sum_{\tilde{J},\tilde{l},\tilde{l}'}(4\pi)^2 i^{(l-l'+\tilde{l}-\tilde{l}')}(-1)^{\tilde{l}+l'+L} \times \mathcal{C}^{L0}_{l0\tilde{l}'0}\mathcal{C}^{L0}_{l'0\tilde{l}0}\sqrt{(2l+1)(2l'+1)(2\tilde{l}+1)(2\tilde{l}'+1)} \times (2J+1)(2\tilde{J}+1)\begin{Bmatrix} l & S & J \\ \tilde{J} & L & \tilde{l}'\end{Bmatrix}\begin{Bmatrix} J & S & l' \\ \tilde{l} & L & \tilde{J}\end{Bmatrix} \times \langle k|V^{(2)}_{Sl'lJ}|k'\rangle\langle k'|V^{(2)}_{S\tilde{l}'\tilde{l}\tilde{J}}|k\rangle[1-(-1)^{l+S+1}] \times [1-(-1)^{\tilde{l}+S+1}],$$

e.g., KH, Schwenk PRC 82, 014314 (2013)

- hard to automatize and generalize to higher order diagrams
- prone to mistakes

Single-particle vector representation:

$$\frac{E^{(2)}_{\rm NN}}{V} = +\frac{1}{4}\sum_{\substack{ij\\ab}}\frac{\langle ij|\mathscr{A}_{12}V_{\rm NN}|ab\rangle\,\langle ab|\mathscr{A}_{12}V_{\rm NN}|ij\rangle}{D_{ijab}}$$

- each diagram a compact single line of code
- straightforward to automatize code generation
- adaptive evaluation of integrals using Monte-Carlo techniques

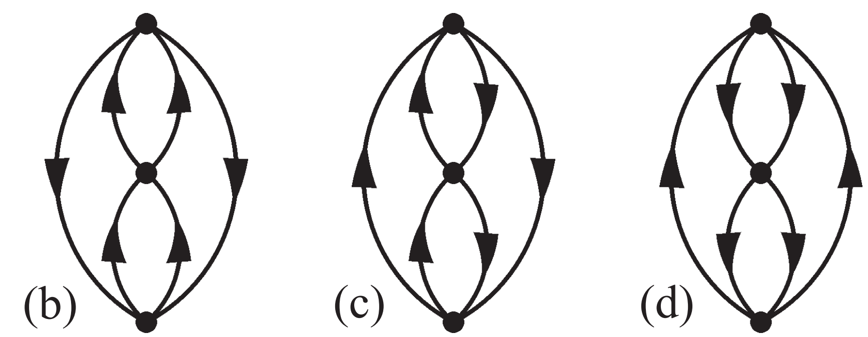
Higher-order contributions

example: third order (particle-particle, hole-hole, particle-hole)

$$\frac{E_1^{(3)}}{V} = +\frac{1}{8}\sum_{\substack{ijkl\\ab}} \frac{\langle ij|\mathscr{A}_{12}V_{\text{NN}}|ab\rangle \langle kl|\mathscr{A}_{12}V_{\text{NN}}|ij\rangle \langle ab|\mathscr{A}_{12}V_{\text{NN}}|kl\rangle}{D_{ijab}D_{klab}},$$

$$\frac{E_2^{(3)}}{V} = +\sum_{\substack{ijk\\abc}} \frac{\langle ij|\mathscr{A}_{12}V_{\text{NN}}|ab\rangle \langle ak|\mathscr{A}_{12}V_{\text{NN}}|ic\rangle \langle bc|\mathscr{A}_{12}V_{\text{NN}}|jk\rangle}{D_{ijab}D_{jkbc}},$$

$$\frac{E_3^{(3)}}{V} = +\frac{1}{8}\sum_{\substack{ij\\abcd}} \frac{\langle ij|\mathscr{A}_{12}V_{\text{NN}}|ab\rangle \langle ab|\mathscr{A}_{12}V_{\text{NN}}|cd\rangle \langle cd|\mathscr{A}_{12}V_{\text{NN}}|ij\rangle}{D_{ijab}D_{ijcd}}.$$



Status:

- implemented all NN diagrams up to fourth order in MBPT, 3N interactions up to third order
- implemented all NN and 3N interactions (nonlocal) up to N3LO
- possible to also use NN matrix elements stored in partial wave basis by partial wave resummation
- interaction interface suitable for all many-body frameworks that require matrix elements in a momentum vector single-particle basis

Proof of principle:
Fits of 3N interactions to saturation properties of nuclear matter

- incorporation of saturation properties in fits was not possible so far due to insufficient efficiency of many-body calculations

- performed calculations up to 4th order for set of presently used NN interactions, natural convergence pattern   Drischler et al., arXiv:1710.08220 (2017)