Recent progress of chiral three-nucleon forces and applications to nuclei and matter

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Vancouver, March 3, 2020

arXiv:2002.09548

Progress in Ab Initio Techniques in Nuclear Physics

SFB 1245

TECHNISCHE UNIVERSITÄT DARMSTADT

Outline

1. development and implementation of local QMC 3N interactions for harmonic oscillator expansion frameworks
2. application of consistently-evolved nonlocal NN+3N interactions to nuclear matter, comparison with ‘magic’ interactions
3. alternative normal-ordering framework for 3N interactions for applications to medium-mass and heavy nuclei

3NF in different regularization schemes

	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:	$\left\langle \mathbf{p}'\mathbf{q}'\middle\vert V_{3\text{N}}^{\text{reg}}\middle\vert\mathbf{pq}\right\rangle = f_R(\mathbf{p}',\mathbf{q}')\,\langle\mathbf{p}'\mathbf{q}'\vert V_{3\text{N}}\vert\mathbf{pq}\rangle\, f_R(\mathbf{p},\mathbf{q})$	
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:	$\left\langle \mathbf{p}'\mathbf{q}'\middle\vert V_{3\text{N}}^{\text{reg}}\middle\vert\mathbf{pq}\right\rangle = \langle\mathbf{p}'\mathbf{q}'\vert V_{3\text{N}}\vert\mathbf{pq}\rangle\,\prod_i f_R(\mathbf{Q}_i)$	$V_{3\text{N}}^{\pi,\text{reg}}(\mathbf{r}_{ij}) = f_R^{\text{long}}(\mathbf{r}_{ij})V_{3\text{N}}^{\pi}(\mathbf{r}_{ij})$ $\delta^{\text{reg}}(\mathbf{r}_{ij}) = \alpha_n f_R^{\text{short}}(\mathbf{r}_{ij})$
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:	$\left\langle \mathbf{p}'\mathbf{q}'\middle\vert V_{3\text{N}}^{\text{reg},\pi}\middle\vert\mathbf{pq}\right\rangle = f_R^{\text{long}}(\mathbf{Q}_i)\,\langle\mathbf{p}'\mathbf{q}'\vert V_{3\text{N}}\vert\mathbf{pq}\rangle$ $\left\langle \mathbf{p}'\mathbf{q}'\middle\vert V_{3\text{N}}^{\text{reg},\delta}\middle\vert\mathbf{pq}\right\rangle = f_\Lambda^{\text{short}}(\mathbf{p}_\delta')\left\langle\mathbf{p}'\mathbf{q}'\middle\vert V_{3\text{N}}^{\delta}\middle\vert\mathbf{pq}\right\rangle f_\Lambda^{\text{short}}(\mathbf{p}_\delta)$	$V_{3\text{N}}^{\pi,\text{reg}}(\mathbf{r}_{ij}) = f_R^{\text{long}}(\mathbf{r}_{ij})V_{3\text{N}}^{\pi}(\mathbf{r}_{ij})$ $\delta(\mathbf{r}_{ij}) \xrightarrow{FT} V_{3\text{N}}^{\delta}$ $\left\langle \mathbf{p}'\mathbf{q}'\middle\vert V_{3\text{N}}^{\text{reg},\delta}\middle\vert\mathbf{pq}\right\rangle = f_\Lambda^{\text{short}}(\mathbf{p}_\delta')\left\langle\mathbf{p}'\mathbf{q}'\middle\vert V_{3\text{N}}^{\delta}\middle\vert\mathbf{pq}\right\rangle f_\Lambda^{\text{short}}(\mathbf{p}_\delta)$

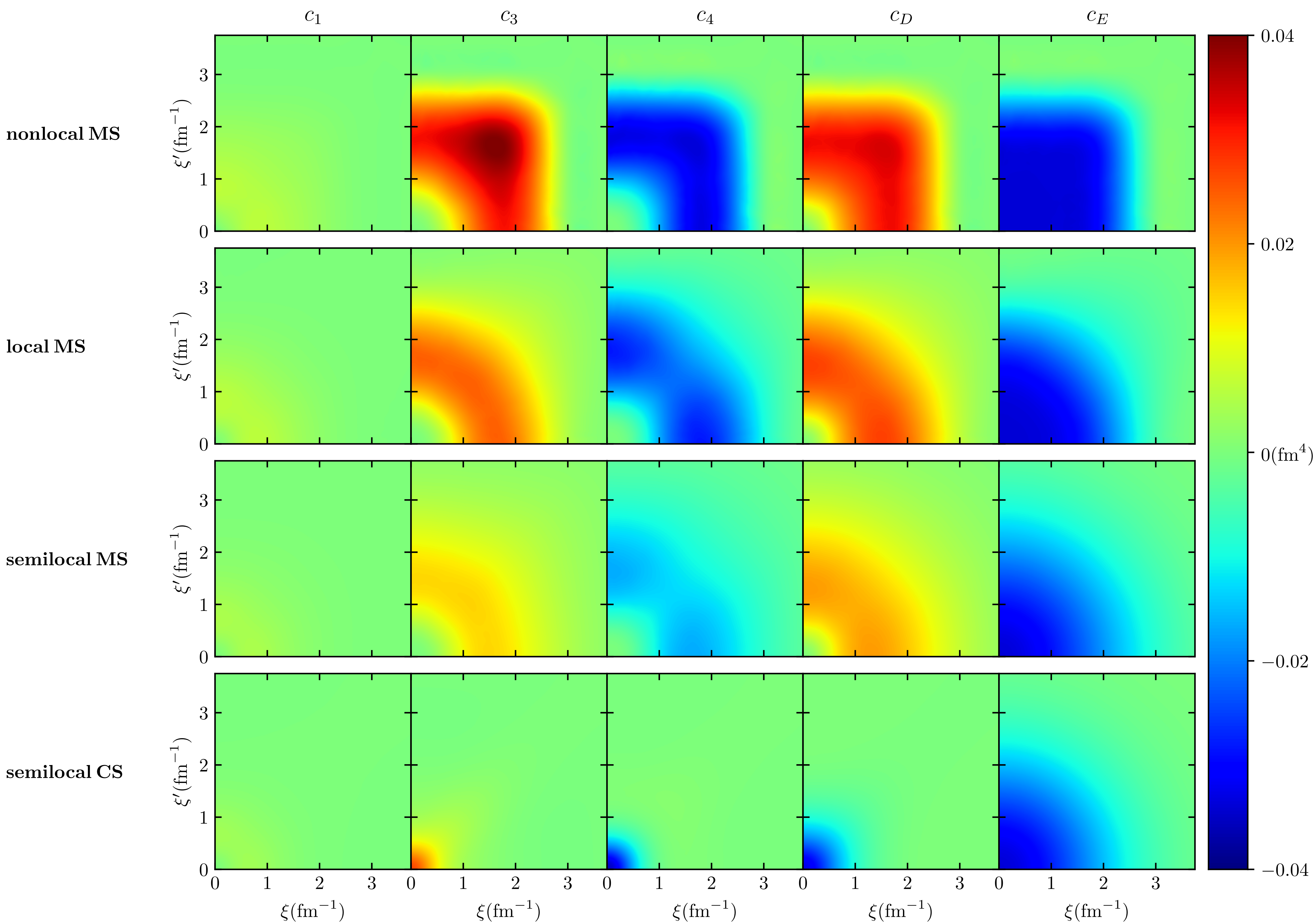
KH, arXiv: 2002.09548 (2020)

3NF in different regularization schemes

	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 $f_R^{\rm long}(\mathbf{r}) = (1 - \exp\left[-r^2/R^2\right])^n$ $f_\Lambda^{\rm short}(\mathbf{p}) = \exp\left[-\mathbf{p}^2/\Lambda^2\right]$ $V_{3N}^{\pi,\rm reg}(\mathbf{r}_{ij}) = f_R^{\rm long}(\mathbf{r}_{ij})V_{3N}^{\pi}(\mathbf{r}_{ij})$ $\delta(\mathbf{r}_{ij}) \xrightarrow{FT} V_{3N}^{\delta}$ $\left\langle \mathbf{p}'\mathbf{q}'\vert V_{3N}^{{\rm reg},\delta}\vert\mathbf{pq}\right\rangle = f_\Lambda^{\rm short}(\mathbf{p}'_\delta)\left\langle \mathbf{p}'\mathbf{q}'\vert V_{3N}^{\delta}\vert\mathbf{pq}\right\rangle f_\Lambda^{\rm short}(\mathbf{p}_\delta)$

KH, arXiv: 2002.09548 (2020)

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, arXiv: 2002.09548 (2020)

3NF in different regularization schemes

<table>
<tr><th></th><th>momentum space</th><th>coordinate space</th></tr>
<tr><td>nonlocal
regulators:
long-range
short-range

regularization:</td><td><u>nonlocal MS</u>
$f_\Lambda^{\text{long}}(\mathbf{p},\mathbf{q}) = \exp\left[-((\mathbf{p}^2 + 3/4\,\mathbf{q}^2)/\Lambda^2)^n\right]$
$f_\Lambda^{\text{short}}(\mathbf{p},\mathbf{q}) = f_\Lambda^{\text{long}}(\mathbf{p},\mathbf{q}) = f_R(\mathbf{p},\mathbf{q})$

$\left\langle \mathbf{p}'\mathbf{q}'\middle|V_{3\text{N}}^{\text{reg}}\middle|\mathbf{pq}\right\rangle = f_R(\mathbf{p}',\mathbf{q}')\,\langle \mathbf{p}'\mathbf{q}'|V_{3\text{N}}|\mathbf{pq}\rangle\, f_R(\mathbf{p},\mathbf{q})$</td><td></td></tr>
<tr><td>local
regulators:
long-range
short-range

regularization:</td><td><u>local MS</u>
$f_\Lambda^{\text{long}}(\mathbf{Q}_i) = \exp\left[-(\mathbf{Q}_i^2/\Lambda^2)^2\right]$
$f_\Lambda^{\text{short}}(\mathbf{Q}_i) = f_\Lambda^{\text{long}}(\mathbf{Q}_i) = f_\Lambda(\mathbf{Q}_i)$

$\left\langle \mathbf{p}'\mathbf{q}'\middle|V_{3\text{N}}^{\text{reg}}\middle|\mathbf{pq}\right\rangle = \langle \mathbf{p}'\mathbf{q}'|V_{3\text{N}}|\mathbf{pq}\rangle \prod_i f_R(\mathbf{Q}_i)$</td><td><u>local CS</u>
$f_R^{\text{long}}(\mathbf{r}) = 1 - \exp\left[-(r^2/R^2)^n\right]$
$f_R^{\text{short}}(\mathbf{r}) = \exp\left[-(r^2/R^2)^n\right]$

$V_{3\text{N}}^{\pi,\text{reg}}(\mathbf{r}_{ij}) = f_R^{\text{long}}(\mathbf{r}_{ij})V_{3\text{N}}^{\pi}(\mathbf{r}_{ij})$
$\delta^{\text{reg}}(\mathbf{r}_{ij}) = \alpha_n f_R^{\text{short}}(\mathbf{r}_{ij})$

QMC</td></tr>
<tr><td>semilocal
regulators:
long-range
short-range

regularization:</td><td><u>semilocal MS</u>
$f_\Lambda^{\text{long}}(\mathbf{Q}_i) = \exp\left[-(\mathbf{Q}_i^2 + m_\pi^2)/\Lambda^2\right]$
$f_\Lambda^{\text{short}}(\mathbf{p}) = \exp\left[-\mathbf{p}^2/\Lambda^2\right]$

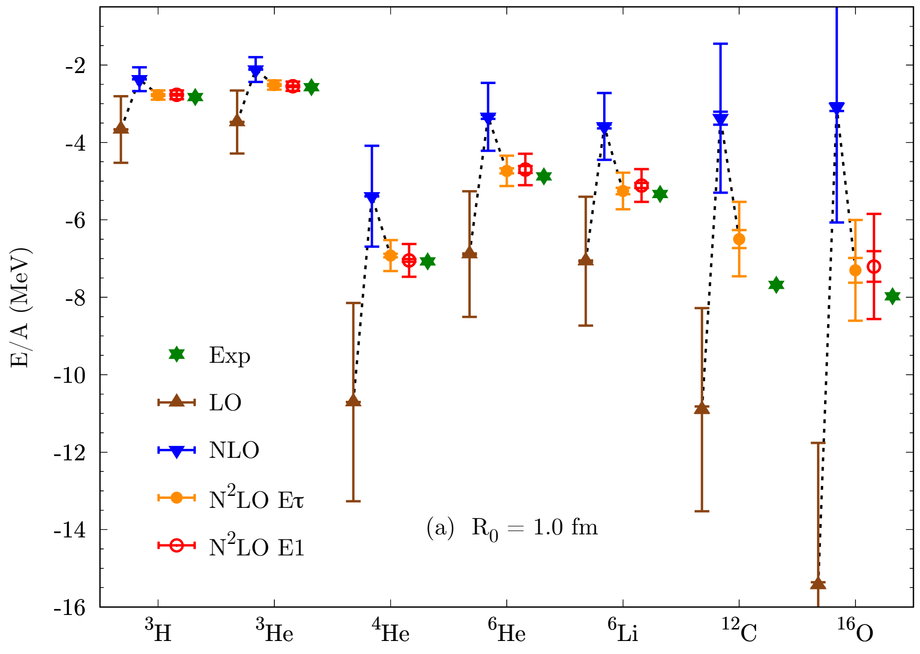
$\left\langle \mathbf{p}'\mathbf{q}'\middle|V_{3\text{N}}^{\text{reg},\pi}\middle|\mathbf{pq}\right\rangle = f_R^{\text{long}}(\mathbf{Q}_i)\,\langle \mathbf{p}'\mathbf{q}'|V_{3\text{N}}|\mathbf{pq}\rangle$
$\left\langle \mathbf{p}'\mathbf{q}'\middle|V_{3\text{N}}^{\text{reg},\delta}\middle|\mathbf{pq}\right\rangle = f_\Lambda^{\text{short}}(\mathbf{p}'_\delta)\left\langle \mathbf{p}'\mathbf{q}'\middle|V_{3\text{N}}^{\delta}\middle|\mathbf{pq}\right\rangle f_\Lambda^{\text{short}}(\mathbf{p}_\delta)$

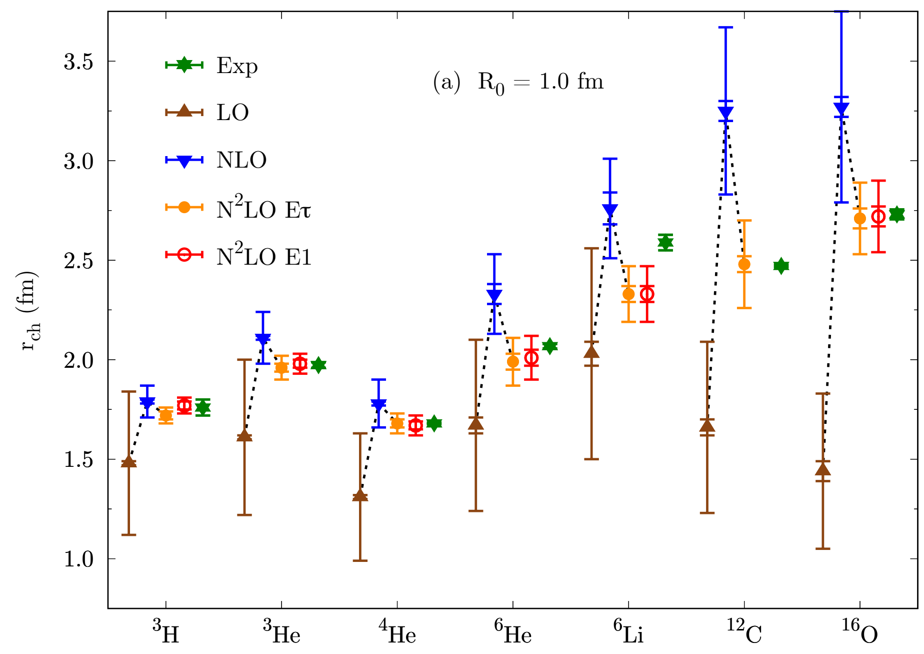
IMSRG,CC,SCGF,MBPT,...</td><td><u>semilocal CS</u>
$f_R^{\text{long}}(\mathbf{r}) = \left(1 - \exp\left[-r^2/R^2\right]\right)^n$
$f_\Lambda^{\text{short}}(\mathbf{p}) = \exp\left[-\mathbf{p}^2/\Lambda^2\right]$

$V_{3\text{N}}^{\pi,\text{reg}}(\mathbf{r}_{ij}) = f_R^{\text{long}}(\mathbf{r}_{ij})V_{3\text{N}}^{\pi}(\mathbf{r}_{ij})$
$\delta(\mathbf{r}_{ij}) \xrightarrow{FT} V_{3\text{N}}^{\delta}$
$\left\langle \mathbf{p}'\mathbf{q}'\middle|V_{3\text{N}}^{\text{reg},\delta}\middle|\mathbf{pq}\right\rangle = f_\Lambda^{\text{short}}(\mathbf{p}'_\delta)\left\langle \mathbf{p}'\mathbf{q}'\middle|V_{3\text{N}}^{\delta}\middle|\mathbf{pq}\right\rangle f_\Lambda^{\text{short}}(\mathbf{p}_\delta)$</td></tr>
</table>

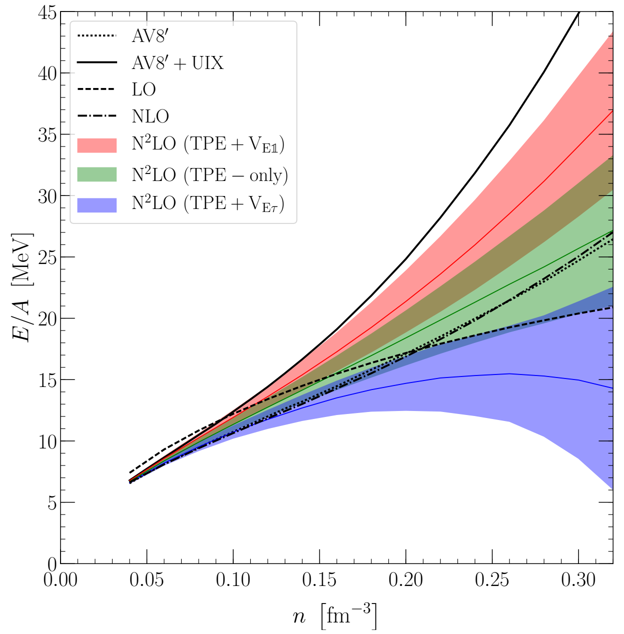
KH, arXiv: 2002.09548 (2020)

New chiral 3N interactions for QMC frameworks





Lonardoni et al., PRC 97, 044381 (2018)



Tews, Carlson, Gandolfi, Reddy, ApJ 860, 149 (2018)

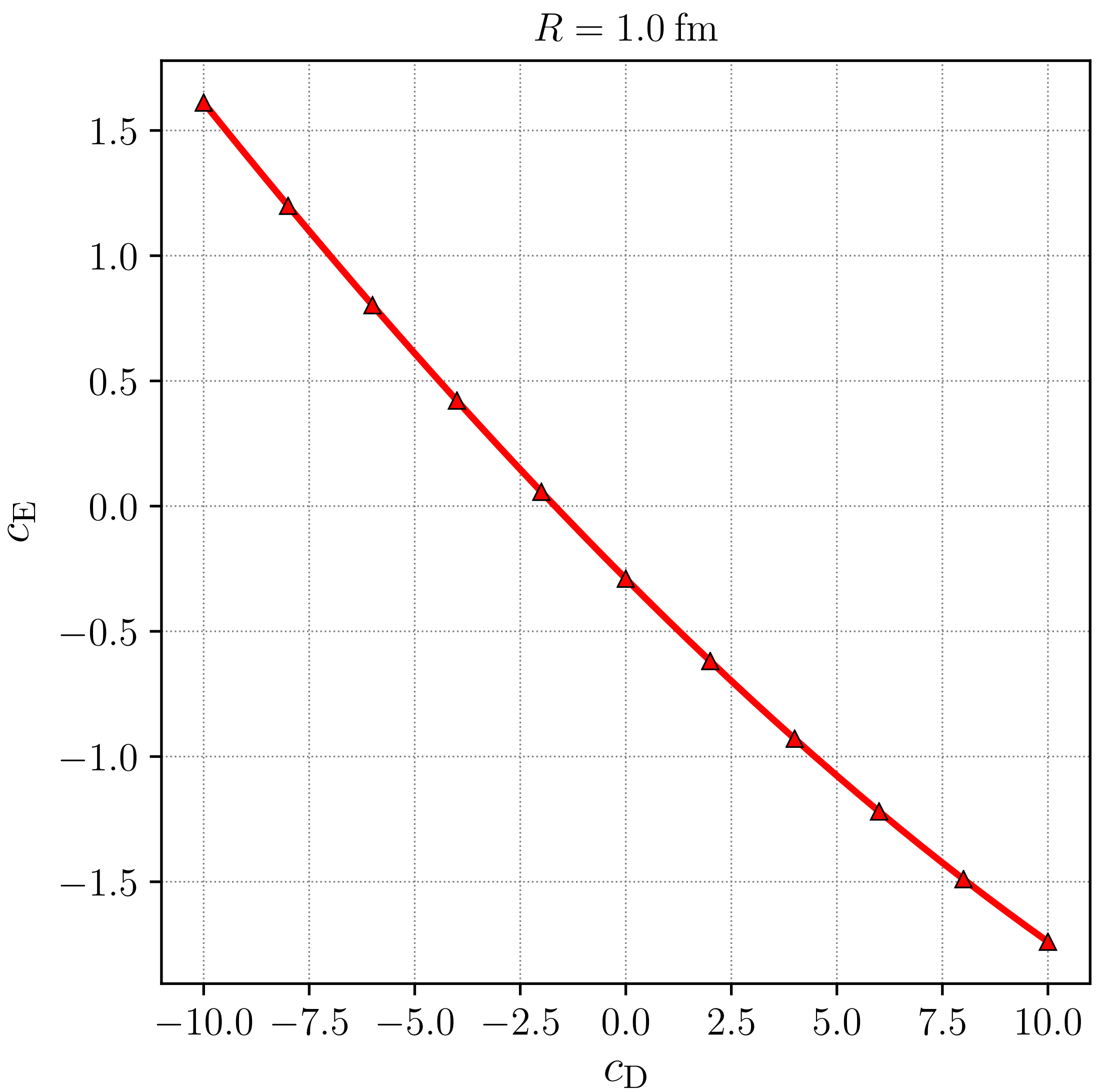
Development of novel local CS NN+3N interactions (Tews, Londardoni)

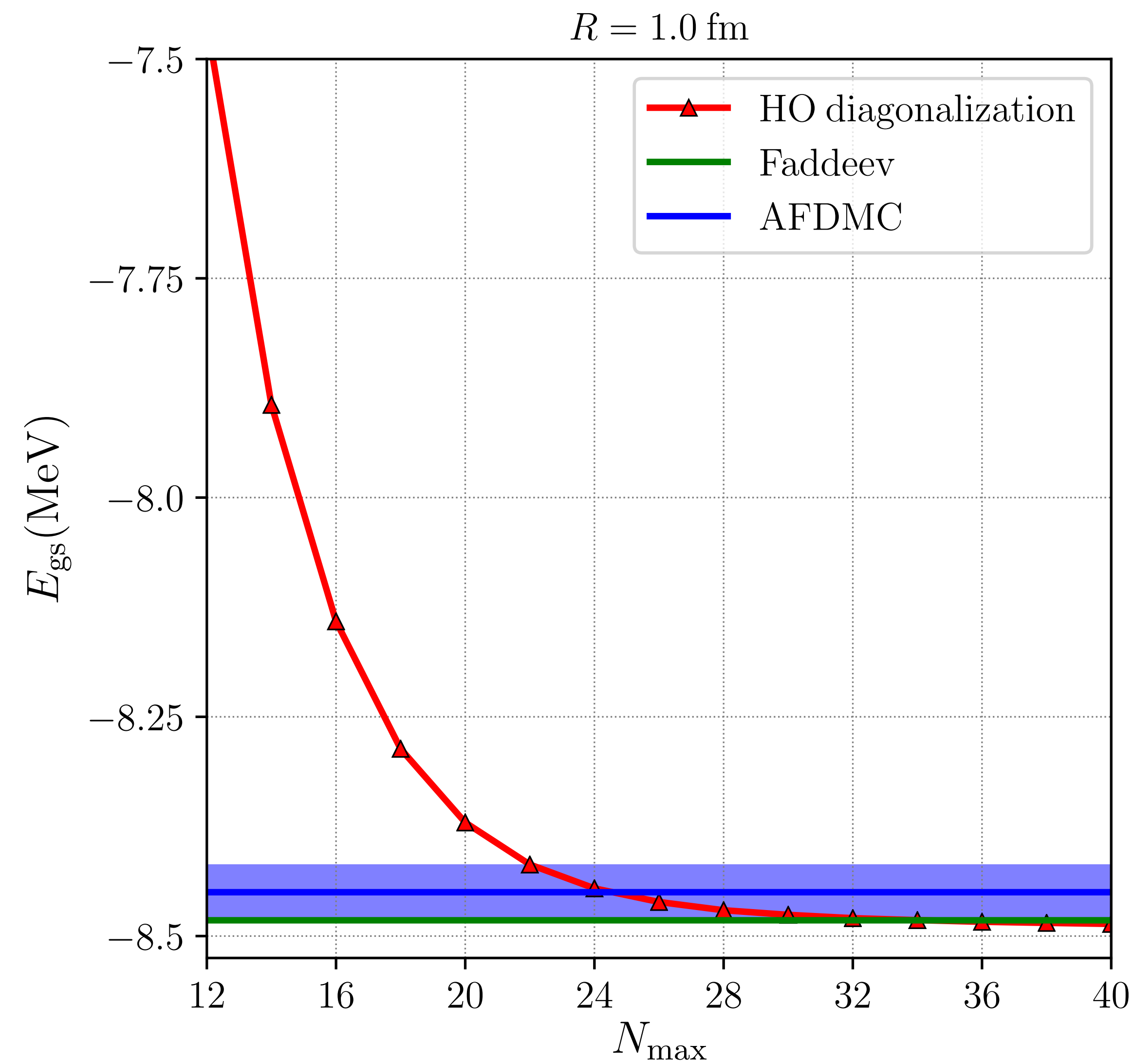
- wider range of cutoff values, reduced cutoff artifacts
- cutoff form that allows easier generalization to N^3LO

In progress (virtually finished):
Calculation of momentum space and HO matrix elements for applications to HO-based many-body frameworks

New chiral 3N interactions for QMC frameworks

three-body tests and three-body fits complete:

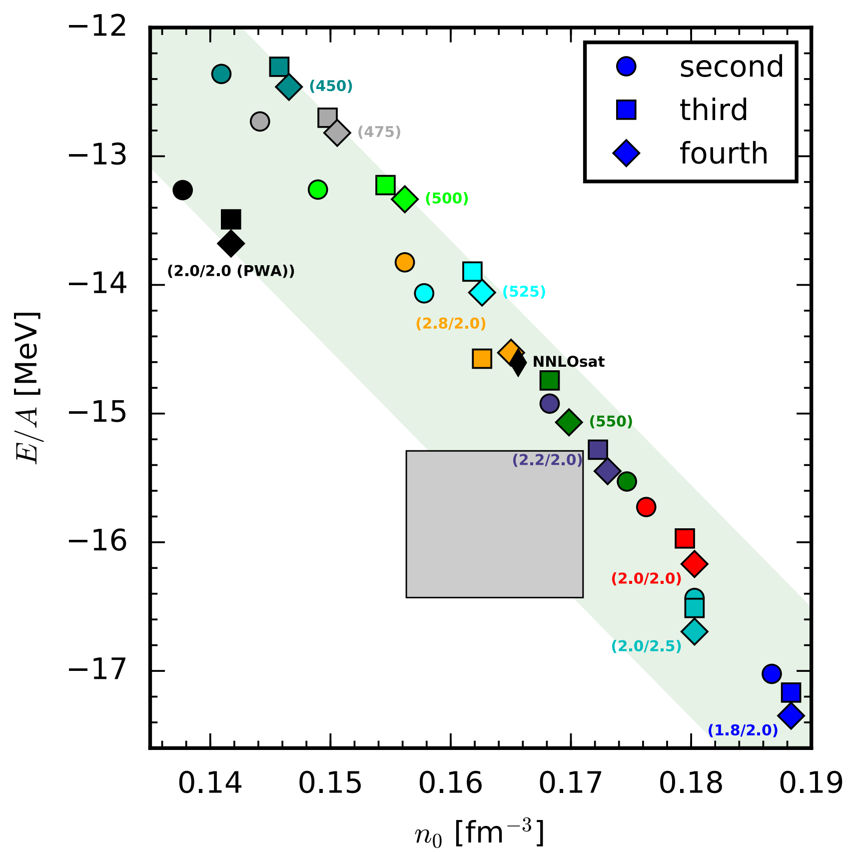




Work in progress in collaboration with Ingo and Diego:

- exploration of different fitting strategies for 3NF
- N_{max} convergence in HO basis for heavier systems

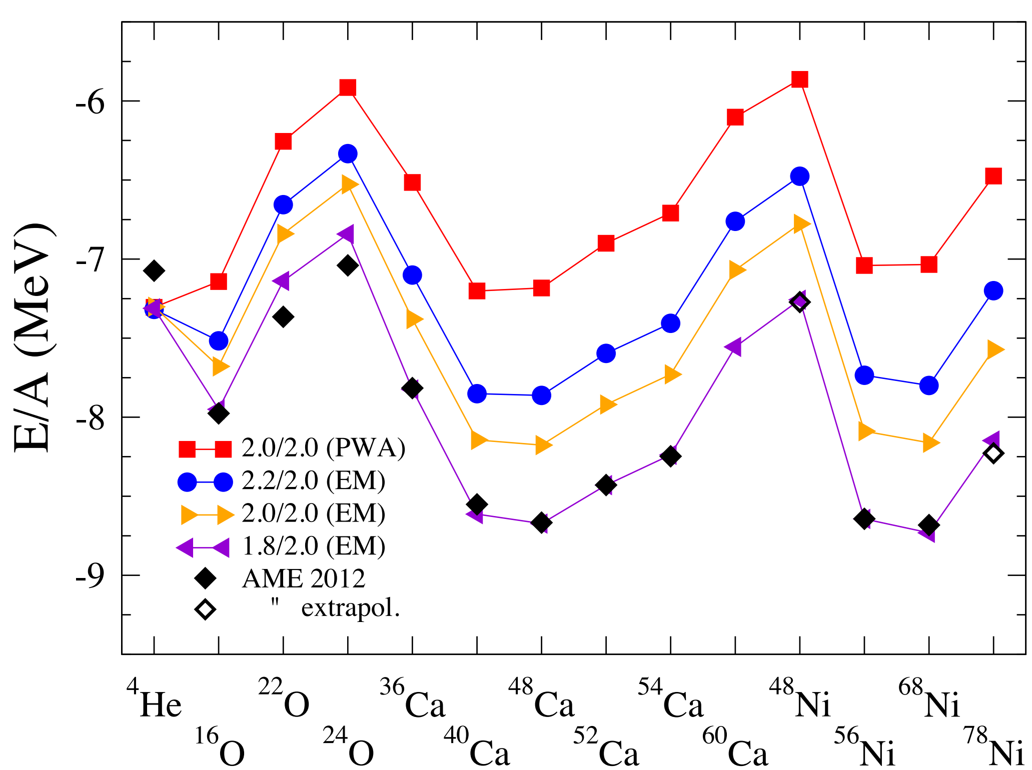
Consistent NN+3N evolutions versus low-resolution fits

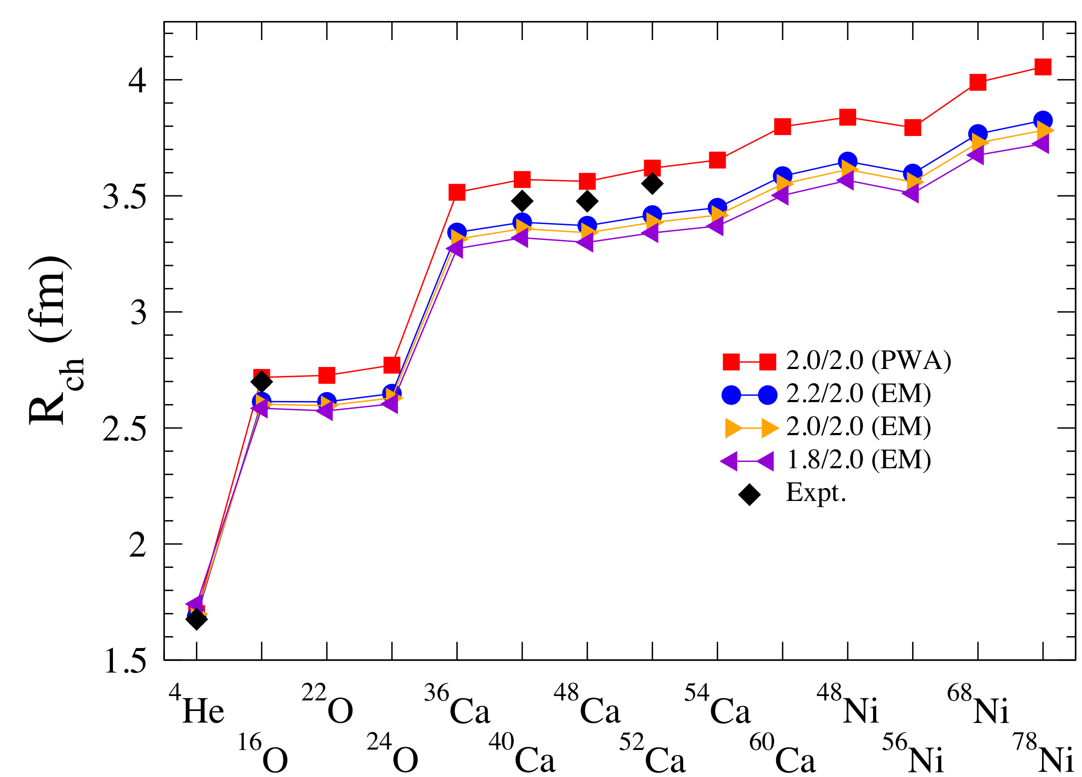


Drischler, KH, Schwenk, PRL 122, 042501 (2019)

	NN SRG evolution + 3N fits				
$\lambda_{\rm SRG}$ (fm^{-1})	$\Lambda_{\rm 3NF}$ (fm^{-1})	c_D	c_E	$r_{^3\rm H}$ (fm)	$E_{^4\rm He}$ (MeV)
∞	2.0	+1.5	0.114	1.601	−28.64(4)
2.8	2.0 [116]	+1.278	−0.078	1.604	−28.75(2)
2.6	2.0	+1.26	−0.099	1.605	−28.77(2)
2.4	2.0	+1.265	−0.115	1.606	−28.80(2)
2.2	2.0 [116]	+1.214	−0.137	1.608	−28.86(2)
2.0	2.0 [116]	+1.271	−0.131	1.612	−28.95(2)
1.8	2.0 [116]	+1.264	−0.120	1.617	−29.11(2)
1.6	2.0	+1.25	−0.075	1.626	−29.42(2)
∞	2.5	−1.45	−0.633	1.604	−28.65(4)
2.8	2.5	−1.35	−0.735	1.606	−28.84(2)
2.6	2.5	−1.2	−0.75	1.606	−28.85(2)
2.4	2.5	−1.0	−0.725	1.607	−28.89(2)
2.2	2.5	−0.7	−0.675	1.609	−28.95(2)
2.0	2.5 [116]	−0.292	−0.592	1.612	−29.05(2)
1.8	2.5	0.05	−0.503	1.617	−29.21(2)
1.6	2.5	0.55	−0.353	1.626	−29.48(2)

KH, Bogner, Furnstahl, Nogga, Schwenk, PRC 83, 031301(2011)
KH, arXiv: 2002.09548 (2020)





Simonis, Stroberg, KH, Holt, Schwenk, PRC 96, 014303 (2017)

Consistent NN+3N evolutions versus low-resolution fits

	NN SRG evolution + 3N fits					NN+3N SRG evolution		
λ_{SRG} (fm^{-1})	Λ_{3NF} (fm^{-1})	c_D	c_E	$r_{^3\text{H}}$ (fm)	$E_{^4\text{He}}$ (MeV)	$E_{^3\text{H}}$ (MeV)	$r_{^3\text{H}}$ (fm)	$E_{^4\text{He}}$ (MeV)
∞	2.0	+1.5	0.114	1.601	−28.64(4)	−8.482	1.601	−28.64(4)
2.8	2.0 [116]	+1.278	−0.078	1.604	−28.75(2)	−8.482	1.605	−28.72(2)
2.6	2.0	+1.26	−0.099	1.605	−28.77(2)	−8.481	1.606	−28.73(2)
2.4	2.0	+1.265	−0.115	1.606	−28.80(2)	−8.481	1.608	−28.73(2)
2.2	2.0 [116]	+1.214	−0.137	1.608	−28.86(2)	−8.480	1.611	−28.74(2)
2.0	2.0 [116]	+1.271	−0.131	1.612	−28.95(2)	−8.479	1.615	−28.75(2)
1.8	2.0 [116]	+1.264	−0.120	1.617	−29.11(2)	−8.478	1.622	−28.76(2)
1.6	2.0	+1.25	−0.075	1.626	−29.42(2)	−8.476	1.635	−28.79(2)
∞	2.5	−1.45	−0.633	1.604	−28.65(4)	−8.482	1.604	−28.65(4)
2.8	2.5	−1.35	−0.735	1.606	−28.84(2)	−8.482	1.608	−28.75(2)
2.6	2.5	−1.2	−0.75	1.606	−28.85(2)	−8.482	1.609	−28.76(2)
2.4	2.5	−1.0	−0.725	1.607	−28.89(2)	−8.482	1.610	−28.77(2)
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1.8	2.5	0.05	−0.503	1.617	−29.21(2)	−8.480	1.625	−28.77(2)
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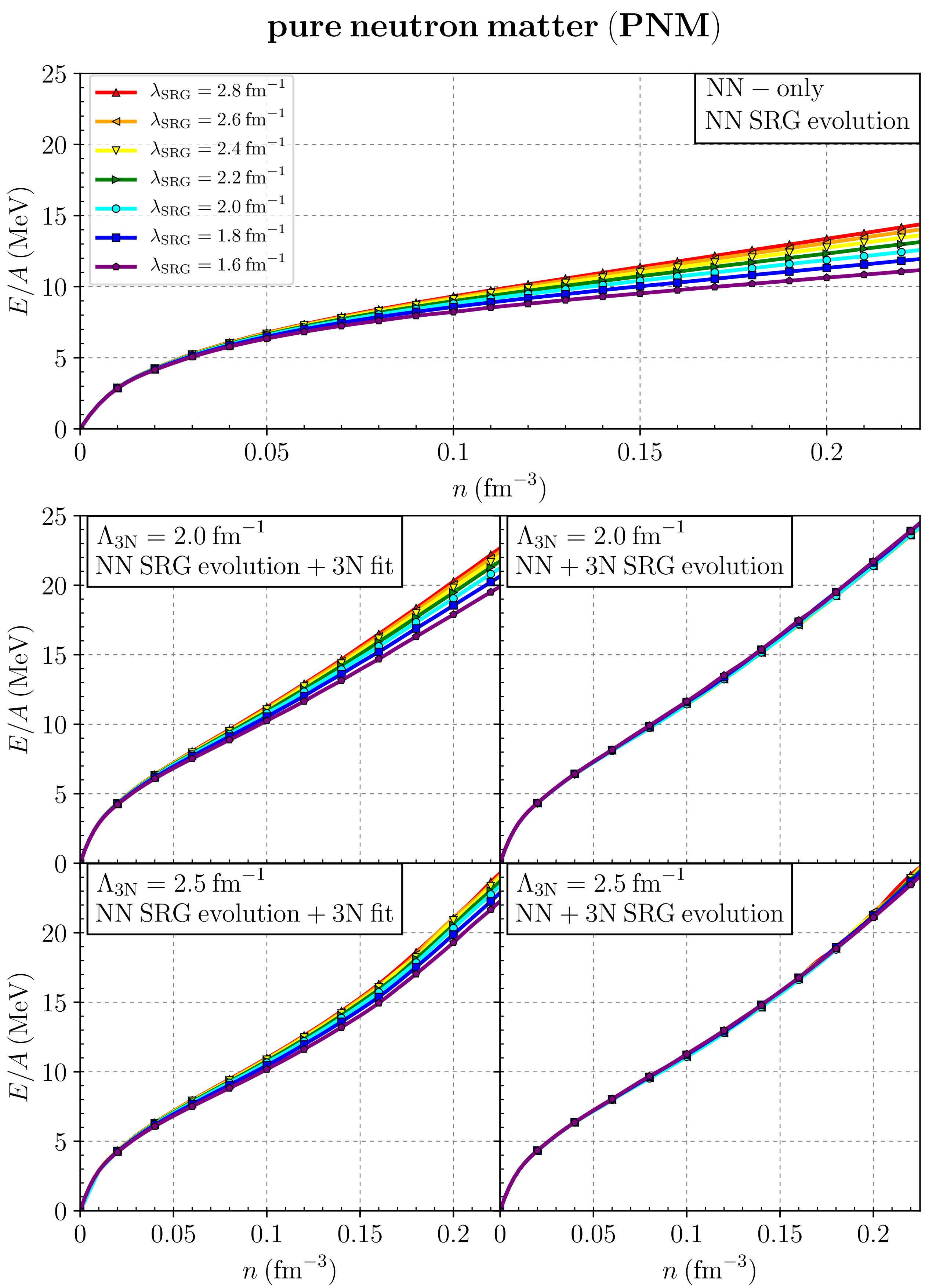
KH, arXiv: 2002.09548 (2020)

Consistent NN+3N evolutions versus low-resolution fits



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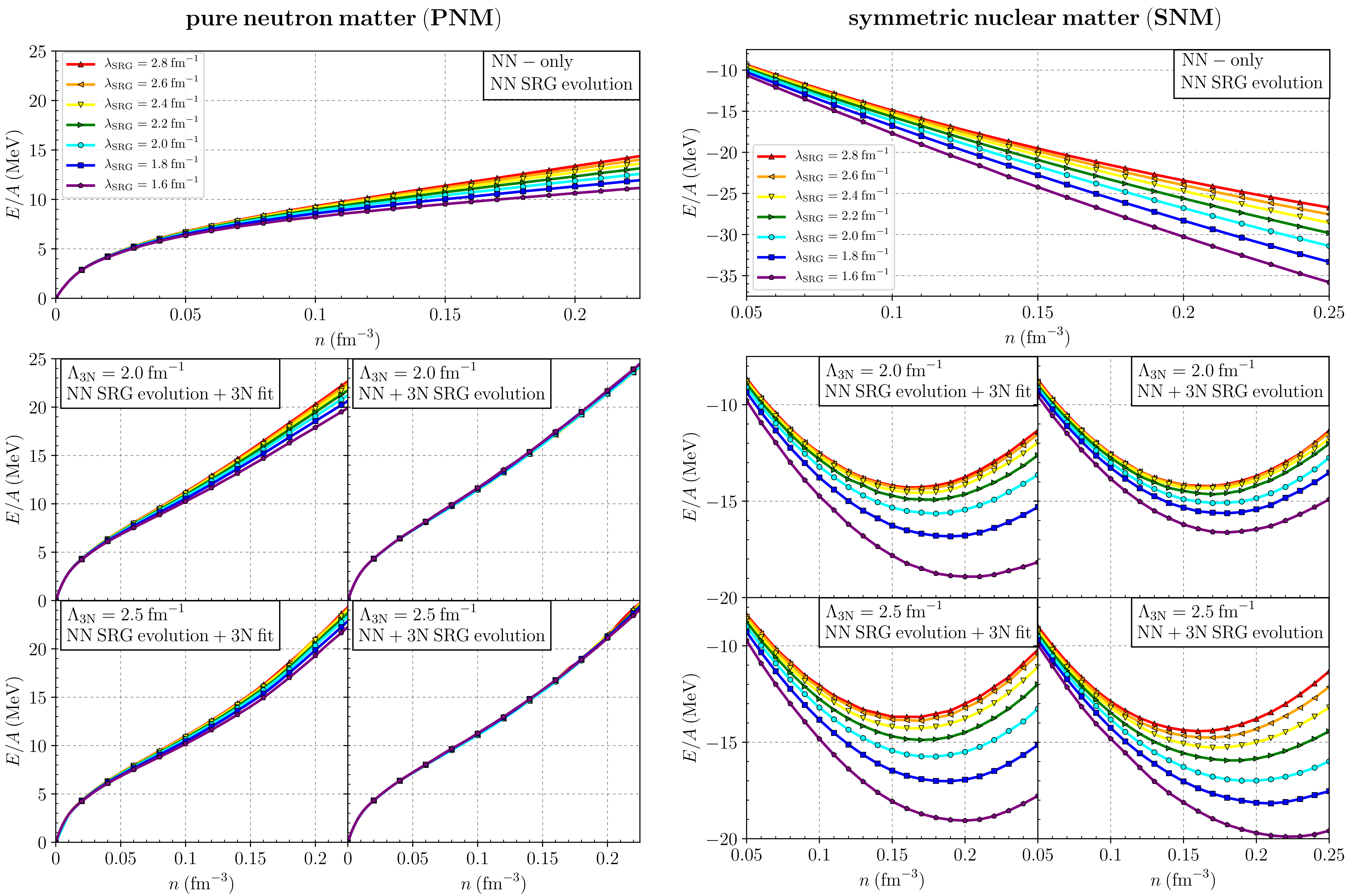
Consistent NN+3N evolutions versus low-resolution fits



KH, arXiv: 2002.09548 (2020)

Novel normal ordering framework for 3N interactions

traditional approach:

1. transformation to Jacobi HO basis plus antisymmetrization

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

Novel normal ordering framework for 3N interactions

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

2. transformation to single particle basis

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

Novel normal ordering framework for 3N interactions

traditional approach:

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

2. transformation to single particle basis

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

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

traditional approach:

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2. transformation to single particle basis

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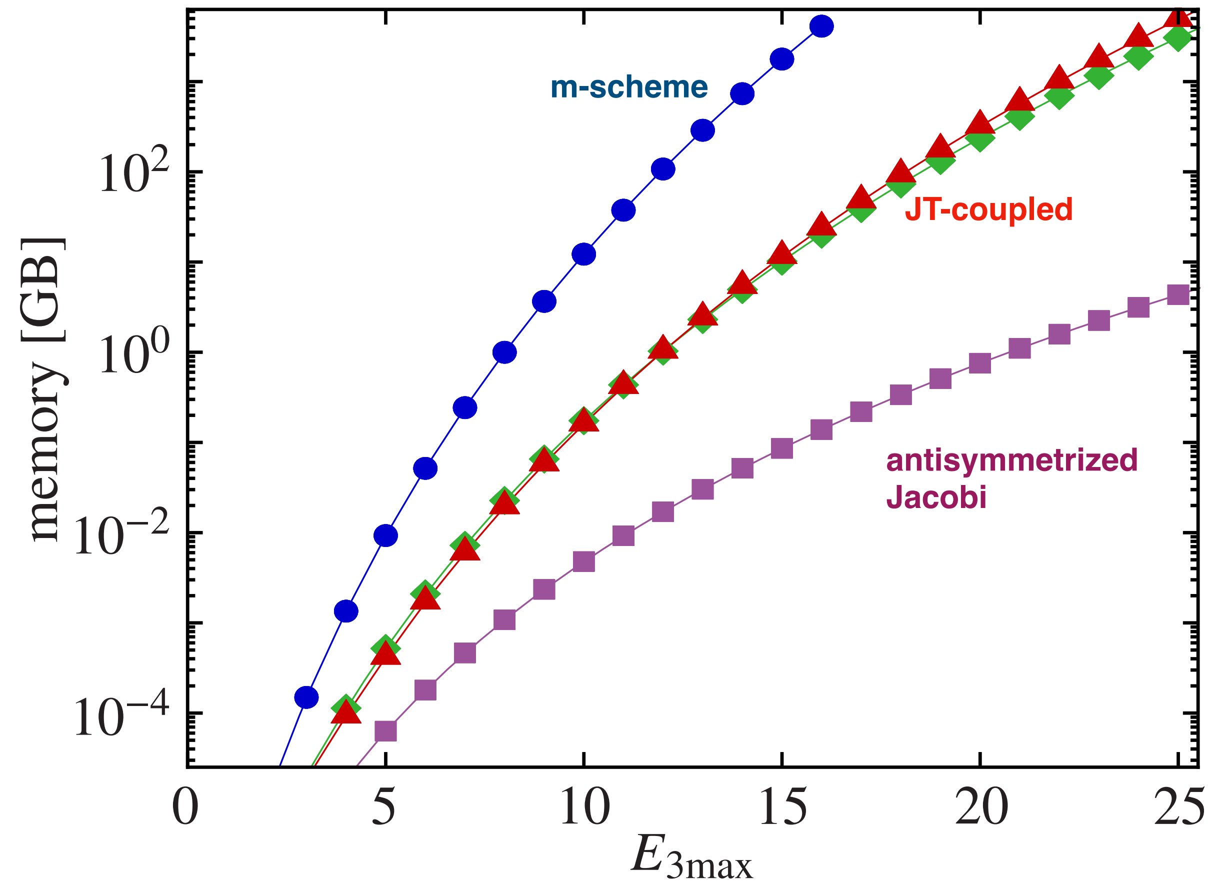
3. Normal ordering with respect to some reference state

$$\langle 1'2'|\overline{V}|12\rangle = \sum_3 \bar{n}_3 \langle 1'2'3|V_{3N}^{\mathrm{as}}|123\rangle$$

- 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

new approach:

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

Novel normal ordering framework for 3N interactions

new approach:

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

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

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

2. Rewrite interaction in Jacobi momentum basis:

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

Novel normal ordering framework for 3N interactions

new approach:

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

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

2. Rewrite interaction in Jacobi momentum basis:

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

3. Decomposition in 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:

4. transform matrix elements to Jacobi HO basis

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

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

Novel normal ordering framework for 3N interactions

new approach:

4. transform matrix elements to Jacobi HO basis

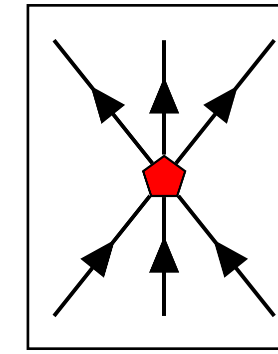
$$\langle p' P' L' M' L'_{cm} M'_{cm} | \overline{V} | p P L M L_{cm} M_{cm} \rangle$$
$$\rightarrow \langle n'_p N'_P L' M' L'_{cm} M'_{cm} | \overline{V} | n_p N_P L M L_{cm} M_{cm} \rangle$$

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

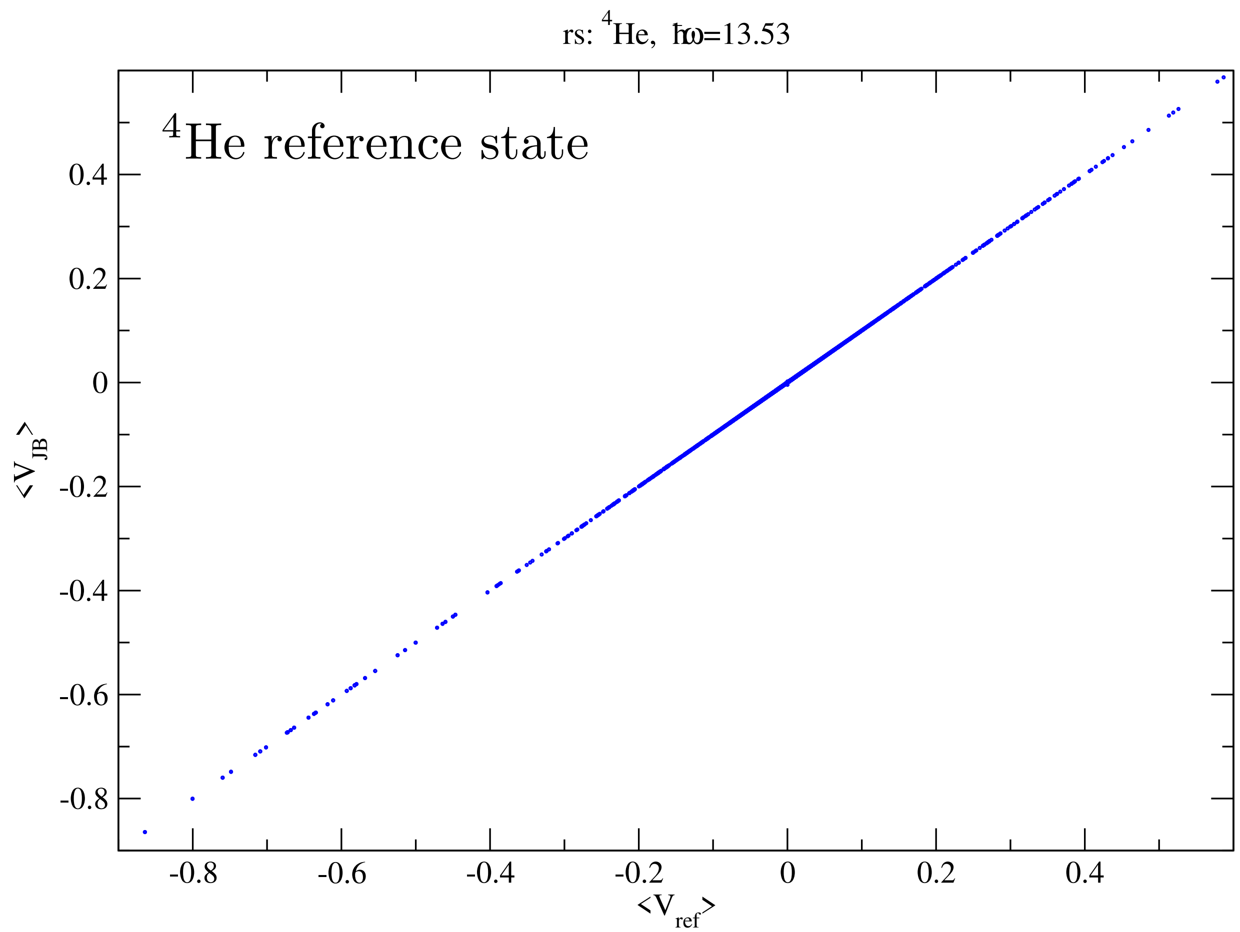
- at no stage single-particle 3N HO matrix elements needed
- straightforward generalization to spin-dependent 3N interactions (already implemented)
- significant recent improvements and optimizations (thanks Alex! :))
- N_{max} can be increased straightforwardly

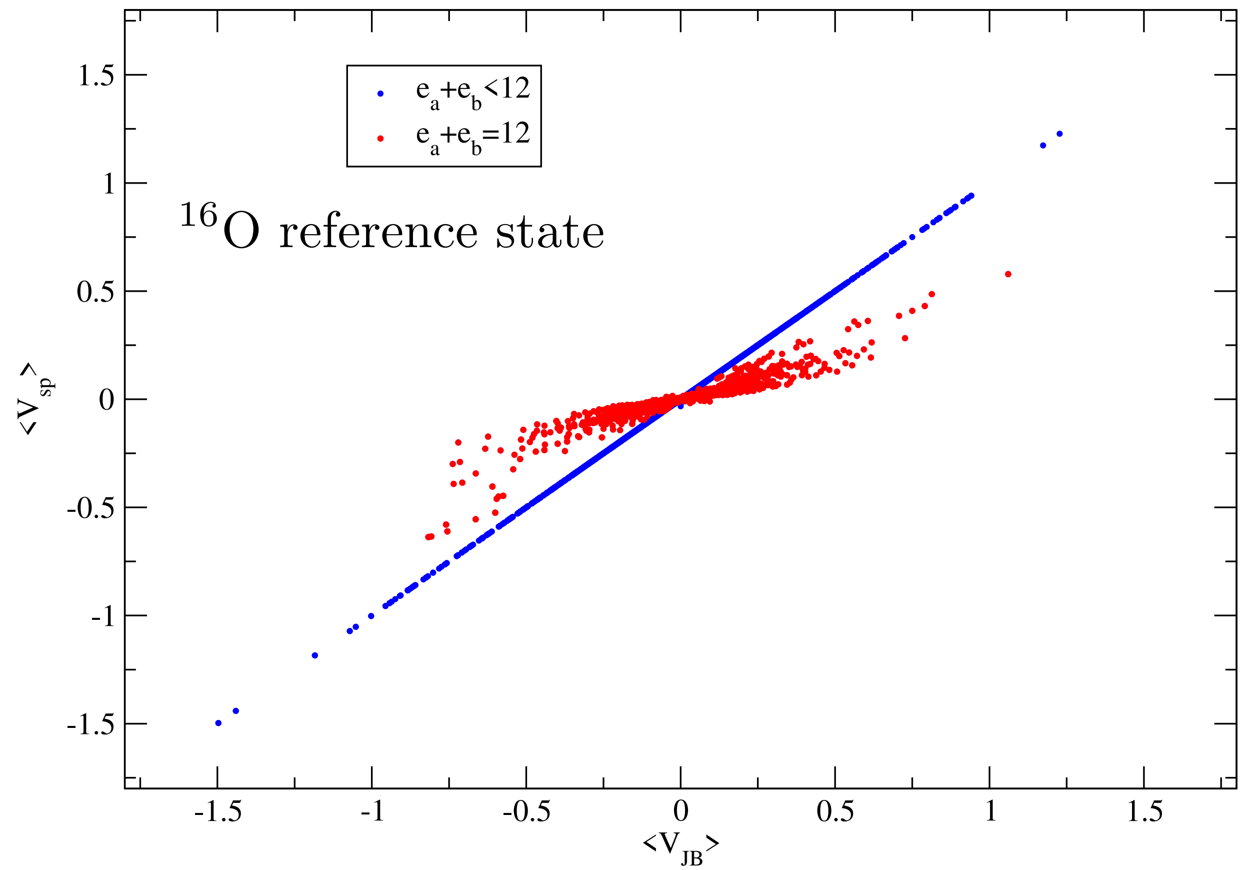
- number of partial waves grows quickly with increasing L and L_{cm}, further optimizations and benchmarks needed
- currently implemented for HO reference state, generalization work in progress

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



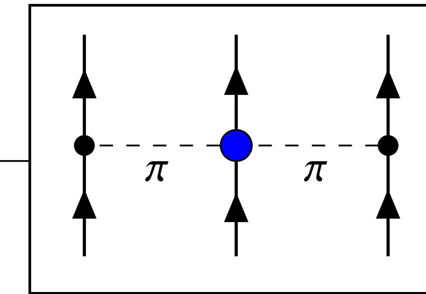
only configurations with L=L'=0 contribute:

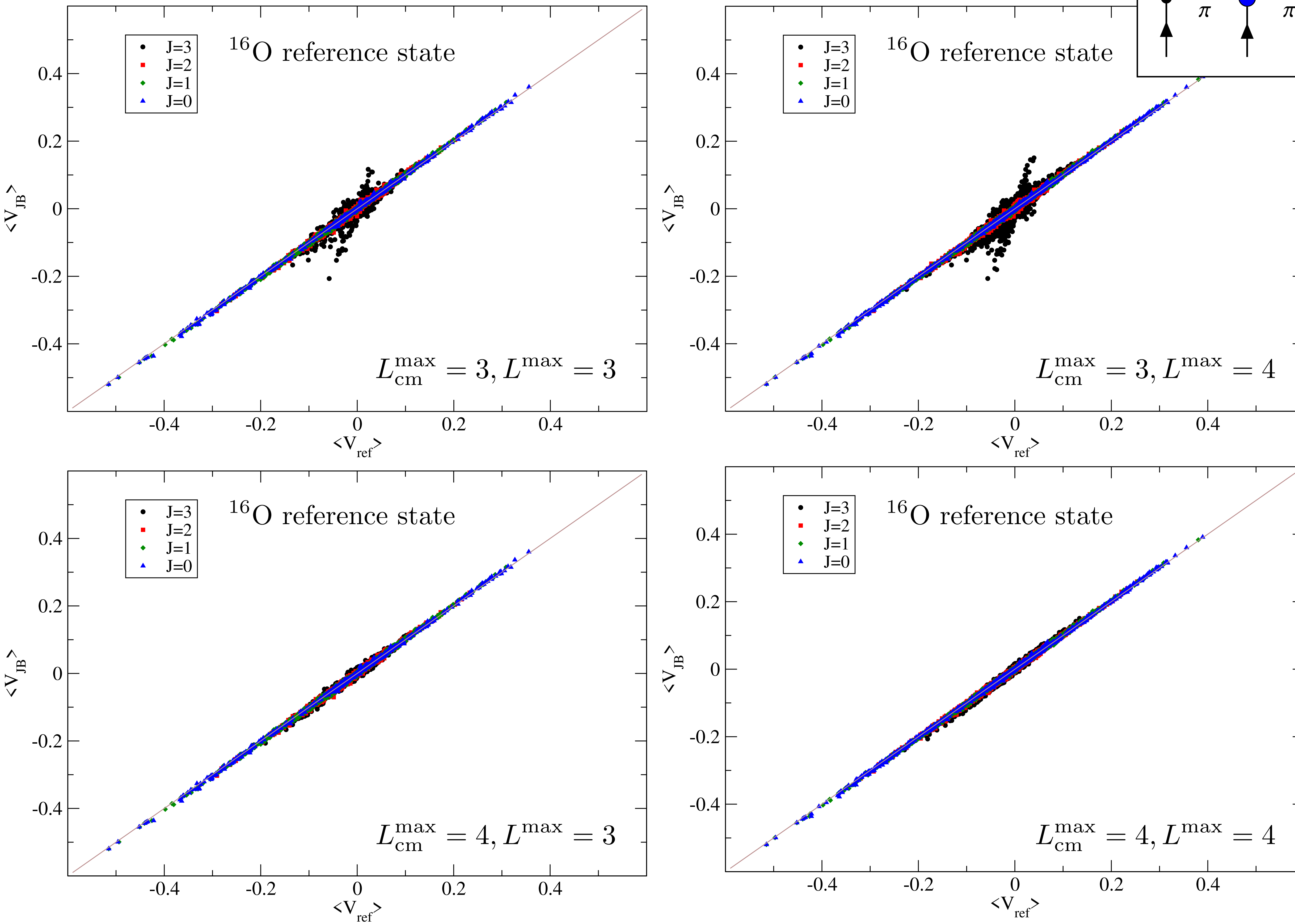




perfect agreement between results from both approaches up to given model space

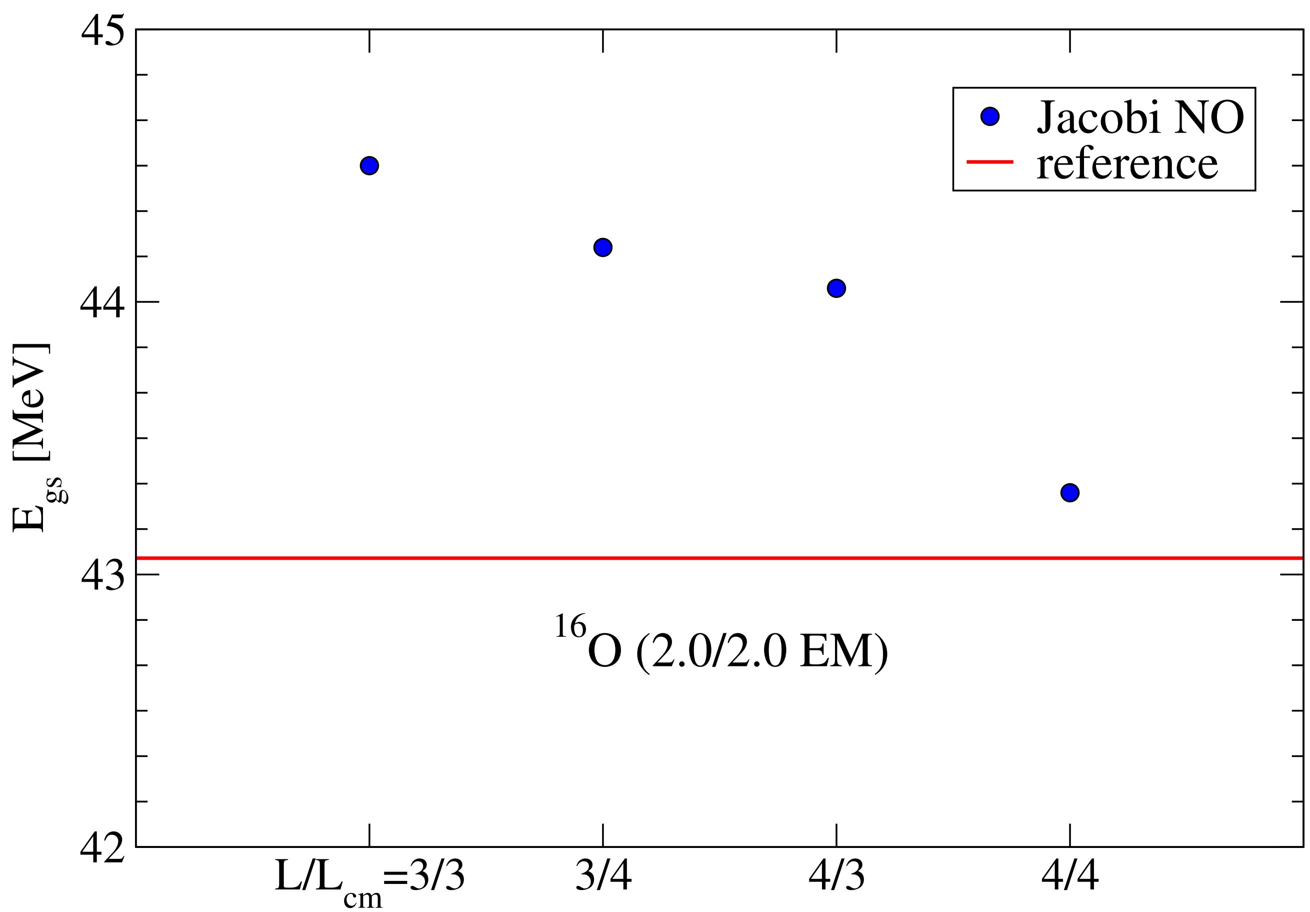
Novel normal ordering framework for 3N interactions: Long-range 2pi interaction (c_3)

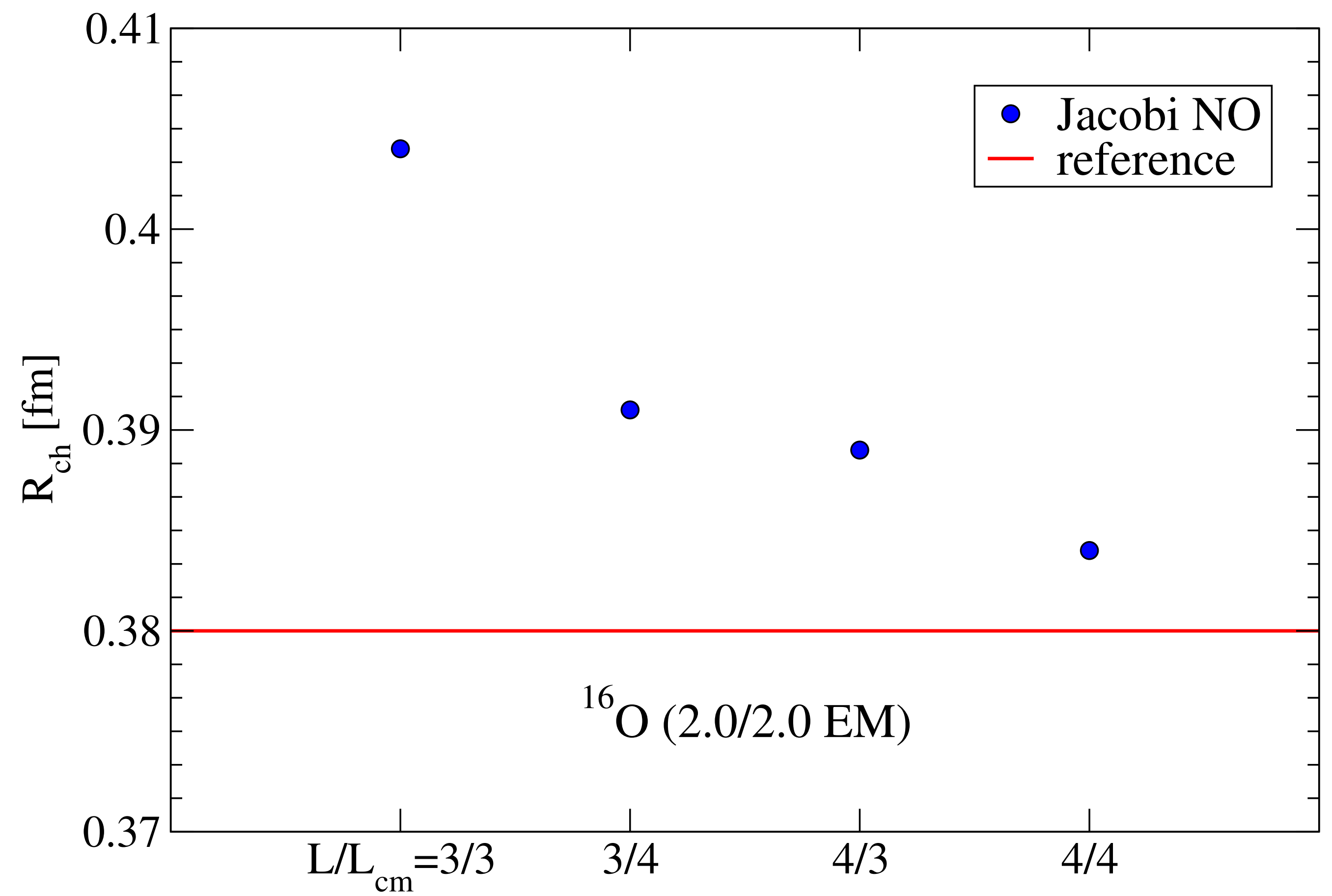




Novel normal ordering framework for 3N interactions
First benchmark calculations for ^{16}O

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





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 used in QMC frameworks, new cross-benchmarks and extended applications?

First calculations of nuclear matter based on consistently SRG-evolved NN+3N interactions, comparison with ‘magic’ interactions

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

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Thank you!