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

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Outline

Uncertainties related to chiral three-nucleon interactions:

- I. Chiral expansion and different regularization schemes
- II. Fixing of low-energy couplings + SRG evolution
- III. Inclusion of 3NFs in many-body calculations

3NFs in different regularization schemes

	momentum space	coordinate space
nonlocal regulators:	nonlocal MS	
long-range	$\int_{\Lambda}^{\text{long}}(\mathbf{p},\mathbf{q}) = \exp\left[-((\mathbf{p}^2 + 3/4 \mathbf{q}^2)/\Lambda^2)^n\right]$	
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:	$\left\langle \mathbf{p'q'} V_{3N}^{\text{reg}} \mathbf{pq} \right\rangle = f_R(\mathbf{p',q'}) \left\langle \mathbf{p'q'} V_{3N} \mathbf{pq} \right\rangle f_R(\mathbf{p,q})$	
local	local MS	local CS
regulators:	$\left[\left(\mathbf{O}^{2} \right) \right] $	$c\log(n) = 1 \left[(2/p^2)^n \right]$
long-range	$\int_{\Lambda} f_{\Lambda}(\mathbf{Q}_{i}) = \exp\left[-(\mathbf{Q}_{i}^{2}/\Lambda^{2})\right]$	$f_{R}^{+}(\mathbf{r}) = 1 - \exp[-(r^{2}/R^{2})^{T}]$
short-range	$f_{\Lambda}^{\text{short}}(\mathbf{Q}_i) = f_{\Lambda}^{\text{short}}(\mathbf{Q}_i) = f_{\Lambda}(\mathbf{Q}_i)$	$\int_{R}^{\text{short}}(\mathbf{r}) = \exp\left[-(r^2/R^2)^n\right]$
regularization:	$\left\langle \mathbf{p}'\mathbf{q}' V_{3N}^{\text{reg}} \mathbf{p}\mathbf{q}\right\rangle = \left\langle \mathbf{p}'\mathbf{q}' V_{3N} \mathbf{p}\mathbf{q}\right\rangle \prod_{i} f_{R}(\mathbf{Q}_{i})$	$V_{3N}^{\pi,\text{reg}}(\mathbf{r}_{ij}) = f_R^{\text{long}}(\mathbf{r}_{ij})V_{3N}^{\pi}(\mathbf{r}_{ij})$ $\delta^{\text{reg}}(\mathbf{r}_{ij}) = \alpha_n f_R^{\text{short}}(\mathbf{r}_{ij})$
semilocal	semilocal MS	semilocal CS
regulators:		. г ,
long-range	$\int_{\Lambda}^{\text{long}}(\mathbf{Q}_i) = \exp\left[-(\mathbf{Q}_i^2 + m_{\pi}^2)/\Lambda^2\right]$	$\int_{R}^{\text{long}}(\mathbf{r}) = \left(1 - \exp\left[-r^2/R^2\right]\right)^n$
short-range	$\int_{\Lambda}^{\text{short}}(\mathbf{p}) = \exp\left[-\mathbf{p}^2/\Lambda^2\right]$	$f_{\Lambda}^{\text{short}}(\mathbf{p}) = \exp\left[-\mathbf{p}^2/\Lambda^2\right]$
regularization:	$ \left\langle \mathbf{p}'\mathbf{q}' V_{3N}^{\text{reg},\pi} \mathbf{p}\mathbf{q}\right\rangle = f_R^{\text{long}}(\mathbf{Q}_i) \left\langle \mathbf{p}'\mathbf{q}' V_{3N} \mathbf{p}\mathbf{q}\right\rangle \left\langle \mathbf{p}'\mathbf{q}' V_{3N}^{\text{reg},\delta} \mathbf{p}\mathbf{q}\right\rangle = f_\Lambda^{\text{short}}(\mathbf{p}'_\delta) \left\langle \mathbf{p}'\mathbf{q}' V_{3N}^\delta \mathbf{p}\mathbf{q}\right\rangle f_\Lambda^{\text{short}}(\mathbf{p}_\delta) $	$V_{3N}^{\pi,\text{reg}}(\mathbf{r}_{ij}) = f_R^{\text{long}}(\mathbf{r}_{ij}) V_{3N}^{\pi}(\mathbf{r}_{ij})$ $\delta(\mathbf{r}_{ij}) \xrightarrow{FT} V_{3N}^{\delta}$ $\left\langle \mathbf{p'q'} V_{3N}^{\text{reg},\delta} \mathbf{pq} \right\rangle = f_{\Lambda}^{\text{short}}(\mathbf{p}_{\delta}') \left\langle \mathbf{p'q'} V_{3N}^{\delta} \mathbf{pq} \right\rangle f_{\Lambda}^{\text{short}}(\mathbf{p}_{\delta})$

KH, Phys. Rept. 890, 1 (2021)

3NFs in different regularization schemes

	momentum space	coordinate space
nonlocal <i>regulators:</i> long-range short-range	$\frac{\text{nonlocal MS}}{f_{\Lambda}^{\text{long}}(\mathbf{p}, \mathbf{q}) = \exp\left[-((\mathbf{p}^2 + 3/4 \mathbf{q}^2)/\Lambda^2)^n\right]}$ $f_{\Lambda}^{\text{short}}(\mathbf{p}, \mathbf{q}) = f_{\Lambda}^{\text{long}}(\mathbf{p}, \mathbf{q}) = f_R(\mathbf{p}, \mathbf{q})$	Violation of chiral symmetry at N3LO? Non-renormalizable? Epelbaum, Krebs
regularization:	$\left\langle \mathbf{p}'\mathbf{q}' V_{3N}^{\text{reg}} \mathbf{p}\mathbf{q}\right\rangle = f_R(\mathbf{p}',\mathbf{q}')\left\langle \mathbf{p}'\mathbf{q}' V_{3N} \mathbf{p}\mathbf{q}\right\rangle f_R(\mathbf{p},\mathbf{q})$	
local regulators:	local MS N ² LO N ³ LO	local CS N ² LO N ³ LO
long-range	$\int_{\Lambda}^{\log}(\mathbf{Q}_i) = \exp\left[-(\mathbf{Q}_i^2/\Lambda^2)^2\right]$	$\int_{R}^{\text{long}}(\mathbf{r}) = 1 - \exp\left[-(r^2/R^2)^n\right]$
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:	$\left\langle \mathbf{p'q'} V_{3N}^{\text{reg}} \mathbf{pq} \right\rangle = \left\langle \mathbf{p'q'} V_{3N} \mathbf{pq} \right\rangle \prod_i f_R(\mathbf{Q}_i)$	$V_{3N}^{\pi, \text{reg}}(\mathbf{r}_{ij}) = f_R^{\text{long}}(\mathbf{r}_{ij}) V_{3N}^{\pi}(\mathbf{r}_{ij})$ $\delta^{\text{reg}}(\mathbf{r}_{ij}) = \alpha_n f_R^{\text{short}}(\mathbf{r}_{ij})$ $\overset{\frown}{\rightarrow} \text{Reduction of cutoff artifacts.}$
semilocal	semilocal MS	semilocal CS
regulators:		
long-range	$\int_{\Lambda}^{\text{long}}(\mathbf{Q}_i) = \exp\left[-(\mathbf{Q}_i^2 + m_{\pi}^2)/\Lambda^2\right]$	$f_R^{\text{long}}(\mathbf{r}) = \left(1 - \exp\left[-r^2/R^2\right]\right)^n$
short-range	$f_{\Lambda}^{\text{short}}(\mathbf{p}) = \exp\left[-\mathbf{p}^2/\Lambda^2\right]$	$f_{\Lambda}^{\text{short}}(\mathbf{p}) = \exp\left[-\mathbf{p}^{2}/\Lambda^{2}\right]$ Derivation of consistently regularised currents at
regularization:	$\begin{pmatrix} \mathbf{p'q'} V_{3N}^{\text{reg},\pi} \mathbf{pq} \rangle = f_R^{\text{long}}(\mathbf{Q}_i) \langle \mathbf{p'q'} V_{3N} \mathbf{pq} \rangle \\ \langle \mathbf{p'q'} V^{\text{reg},\delta} \mathbf{pq} \rangle = f^{\text{short}}(\mathbf{p'}_i) \langle \mathbf{p'q'} V^{\delta} \mathbf{pq} \rangle f^{\text{short}}(\mathbf{p}_s)$	$V_{3N}^{\pi, \text{reg}}(\mathbf{r}_{ij}) = f_R^{\text{long}}(\mathbf{r}_{ij}) V_{3N}^{\pi}(\mathbf{r}_{ij})$ this order very hard, switched to SMS
	Formal derivation 'basically' finished.	$\left\langle \mathbf{p'q'} V_{3N}^{\text{reg},\delta} \mathbf{pq} \right\rangle = f_{\Lambda}^{\text{short}}(\mathbf{p}_{\delta}') \left\langle \mathbf{p'q'} V_{3N}^{\delta} \mathbf{pq} \right\rangle f_{\Lambda}^{\text{short}}(\mathbf{p}_{\delta})$
	Implementation in progress (hard!)	KH, Phys. Rept. 890, 1 (2021)

Illustration of 3NFs in different regularization schemes



Uncertainty II: Fitting of low-energy couplings + SRG evolution

- choice of observables
- separate or simultaneous fits of NN and 3N LECs?
- using few-body and/or many-body observables?
- using bare or low-resolution interactions for fits?
- low resolution interactions:
 - evolve NN interactions to lower scales via the RG
 - * fit the 3N LECs at a low cutoff scale ($\Lambda_{3N}\sim 2\,{\rm fm}^{-1})$
 - * e.g., use ³H binding energy and ⁴He radius to fix c_D and c_E

	$V_{\mathrm{low}\ k}$		SRG	
$\Lambda \text{ or } \lambda / \Lambda_{3\mathrm{NF}} \ [\mathrm{fm}^{-1}]$	c_D	c_E	c_D	c_E
$1.8/2.0 \ (\text{EM} \ c_i\text{'s})$	+1.621	-0.143	+1.264	-0.120
$2.0/2.0 ~({ m EM}~c_i{ m 's})$	+1.705	-0.109	+1.271	-0.131
$2.0/2.5 ~({ m EM}~c_i{ m 's})$	+0.230	-0.538	-0.292	-0.592
$2.2/2.0 \ ({ m EM} \ c_i{ m 's})$	+1.575	-0.102	+1.214	-0.137
$2.8/2.0 ~({ m EM}~c_i{ m 's})$	+1.463	-0.029	+1.278	-0.078
$2.0/2.0~(\mathrm{EGM}~c_i\mathrm{'s})$	-4.381	-1.126	-4.828	-1.152
$2.0/2.0~(\mathrm{PWA}~c_i\mathrm{`s})$	-2.632	-0.677	-3.007	-0.686

PRC 83, 031301 (2011)



Low-resolution fits versus consistent NN+3N evolution



		NN+3N SRG evolution		
$\lambda_{\rm SRG} ({\rm fm}^{-1})$	$\Lambda_{3\rm NF}~({\rm fm}^{-1})$	$E_{^{3}\mathrm{H}}$ (MeV)	$r_{^{3}\mathrm{H}}(\mathrm{fm})$	$E_{^{4}\mathrm{He}}$ (MeV)
00	2.0	-8.482	1.601	-28.64(4)
2.8	2.0 [116]	-8.482	1.605	-28.72(2)
2.6	2.0	-8.481	1.606	-28.73(2)
2.4	2.0	-8.481	1.608	-28.73(2)
2.2	2.0 [116]	-8.480	1.611	-28.74(2)
2.0	2.0 [116]	-8.479	1.615	-28.75(2)
1.8	2.0 [116]	-8.478	1.622	-28.76(2)
1.6	2.0	-8.476	1.635	-28.79(2)
∞	2.5	-8.482	1.604	-28.65(4)
2.8	2.5	-8.482	1.608	-28.75(2)
2.6	2.5	-8.482	1.609	-28.76(2)
2.4	2.5	-8.482	1.610	-28.77(2)
2.2	2.5	-8.481	1.613	-28.77(2)
2.0	2.5 [116]	-8.481	1.617	-28.77(2)
1.8	2.5	-8.480	1.625	-28.77(2)
1.6	2.5	-8.478	1.638	-28.77(2)

pure neutron matter (\mathbf{PNM})

Low-resolution fits versus consistent NN+3N evolution





New and improved 'magic' interactions

Arthuis, KH, Schwenk, arXiv:2401.06675



- Fit to c_D and c_E to ³H energy and **both** binding energies and radius of ¹⁶O using EM500 and NNLO_{sim} 550 low-resolution NN interactions
- Simultaneous reproduction of experimental binding energies and charge radii see talk by Achim for more details and results

New and improved 'magic' interactions





- Fit to c_D and c_E to ³H energy and **both** binding energies and radius of ¹⁶O using EM500 and NNLO_{sim} 550 low-resolution NN interactions
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Uncertainty III: Inclusion of 3NF in many-body calculations

A general Hamiltonian consisting of kinetic energy, NN and 3N interactions:

$$\hat{H} = \hat{T}_{rel} + \hat{V}_{NN} + \hat{V}_{3N}$$

$$\hat{T}_{rel} = \sum_{ij} \langle i|T|j \rangle \hat{a}_i^{\dagger} \hat{a}_j,$$

$$\hat{V}_{NN} = \frac{1}{(2!)^2} \sum_{ijkl} \langle ij|V_{NN}^{as}|kl\rangle \hat{a}_i^{\dagger} \hat{a}_j^{\dagger} \hat{a}_l \hat{a}_k,$$

$$\hat{V}_{3N} = \frac{1}{(3!)^2} \sum_{ijklmn} \langle ijk|V_{3N}^{as}|lmn\rangle \hat{a}_i^{\dagger} \hat{a}_j^{\dagger} \hat{a}_k^{\dagger} \hat{a}_n \hat{a}_m \hat{a}_l$$

can be exactly rewritten in a normal-ordered form:

$$\begin{split} \Gamma_{\rm HF}^{(0)} &= \sum_{i} n_{i} \langle i|T|i \rangle + \frac{1}{2} \sum_{ij} n_{i} n_{j} \langle ij|V_{\rm NN}^{\rm as}|ij \rangle + \frac{1}{6} \sum_{ijk} n_{i} n_{j} n_{k} \langle ijk|V_{\rm 3N}^{\rm as}|ijk \rangle, \\ \hat{\Gamma}_{\rm HF}^{(1)} &= \sum_{ij} \left[\langle i|T|j \rangle + \sum_{k} n_{k} \langle ik|V_{\rm NN}^{\rm as}|jk \rangle + \frac{1}{2} \sum_{kl} n_{k} n_{l} \langle ikl|V_{\rm 3N}^{\rm as}|jkl \rangle \right] N(\hat{a}_{i}^{\dagger}\hat{a}_{j}), \\ \hat{\Gamma}_{\rm HF}^{(2)} &= \sum_{ijkl} \left[\langle ij|V_{\rm NN}^{\rm as}|kl \rangle + \sum_{m} n_{m} \langle ijm|V_{\rm 3N}^{\rm as}|klm \rangle \right] N(\hat{a}_{i}^{\dagger}\hat{a}_{j}^{\dagger}\hat{a}_{l}\hat{a}_{k}), \\ \hat{\Gamma}_{\rm HF}^{(3)} &= \sum_{ijklmn} \langle ijk|V_{\rm 3N}^{\rm as}|lmn \rangle N(\hat{a}_{i}^{\dagger}\hat{a}_{j}^{\dagger}\hat{a}_{k}^{\dagger}\hat{a}_{n}\hat{a}_{m}\hat{a}_{l}). \end{split}$$

 $\hat{H} = \Gamma_{\rm HF}^{(0)} + \hat{\Gamma}_{\rm HF}^{(1)} + \hat{\Gamma}_{\rm HF}^{(2)} + \hat{\Gamma}_{\rm HF}^{(3)}$

Traditional normal ordering framework for 3N interactions

I. transformation to Jacobi HO basis plus antisymmetrization $\langle p'q'\alpha'|V_{3N}^{(i),reg}|pq\alpha\rangle \rightarrow \langle N'n'\alpha'|V_{3N}^{(as,reg}|Nn\alpha\rangle$

2. transformation to single particle basis

 $\left\langle N'n'\alpha'|V_{3\mathrm{N}}^{\mathrm{as, reg}}|Nn\alpha
ight
angle
ightarrow \left\langle 1'2'3'|V_{3\mathrm{N}}^{\mathrm{as, reg}}|123
ight
angle$

3. Normal ordering with respect to some reference state

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

- severe memory limitations for handling of single-particle matrix elements with increasing E3max
- Significant optimisations possible when storing only those matrix elements needed for normal ordering Miyagi at al., PRC 105, 1 (2022)



Roth at al., PRC 90 024325 (2014)

Novel normal ordering framework for 3N interactions

I. Use momentum space and expand reference state in HO basis:

$$\begin{split} \left\langle \mathbf{k}_{1}'\mathbf{k}_{2}'|\overline{V}|\mathbf{k}_{1}\mathbf{k}_{2}\right\rangle &= \sum_{n_{3}l_{3}m_{3}} \overline{n}_{3}\left\langle \mathbf{k}_{1}'\mathbf{k}_{2}'\gamma_{3}|V_{3\mathrm{N}}^{\mathrm{as}}|\mathbf{k}_{1}\mathbf{k}_{2}\gamma_{3}\right\rangle \\ &= \int d\mathbf{k}_{3}d\mathbf{k}_{3}'\left\langle \mathbf{k}_{1}'\mathbf{k}_{2}'\mathbf{k}_{3}'|V_{3\mathrm{N}}^{\mathrm{as}}|\mathbf{k}_{1}\mathbf{k}_{2}\mathbf{k}_{3}\right\rangle \sum_{n_{3}l_{3}m_{3}} \overline{n}_{3}\left\langle \gamma_{3}|\mathbf{k}_{3}'\right\rangle \left\langle \mathbf{k}_{3}|\gamma_{3}\right\rangle \end{split}$$

2. Rewrite interaction in Jacobi momentum basis:

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

3. Decomposition in Jacobi partial wave momentum states:

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

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

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

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

4. transform matrix elements to Jacobi HO basis

$$\langle p'P'L'M'L'_{cm}M'_{cm}|\overline{V}|pPLML_{cm}M_{cm}\rangle \rightarrow \langle n'_pN'_PL'M'L'_{cm}M'_{cm}|\overline{V}|n_pN_PLML_{cm}M_{cm}\rangle$$

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

Novel normal ordering framework for 3N interactions



- at no stage single-particle 3N HO matrix elements needed
- N_{max} can be increased straightforwardly
- \bullet basis size and storage space determined by J_{max} and $L_{\text{cm},\text{max},}$

Novel normal ordering framework for 3N interactions





Singular value decomposition of NN interactions



 excellent agreement with full results for phase shifts and binding energies for very low number of ranks (= number of retained singular values)

(Randomized) singular value decomposition of 3N interactions

Tichai et al., arXiv:2307.15572



 again good agreement with full results for binding energies and charge radii for very low number of ranks (NN interactions not SVD-decomposed)

(Randomized) singular value decomposition of 3N interactions

Tichai et al., arXiv:2307.15572



 again good agreement with full results for binding energies and charge radii for very low number of ranks (NN interactions not SVD-decomposed) Which contributions should a comprehensive uncertainty estimate contain?

- I. Power counting scheme
- II. Chiral expansion
- III. Regularization schemes
- IV. Different fitting strategies for low-energy couplings
- V. Truncation in many-body expansions/SRG evolution
- VI. Basis truncations
- VII....?