Towards chiral three-nucleon forces in heavy nuclei

Victoria Durant, Kai Hebeler, Achim Schwenk

Nuclear ab initio Theories and Neutrino Physics

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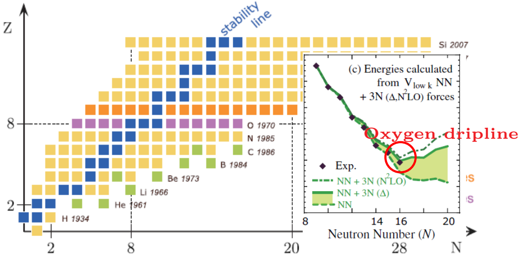
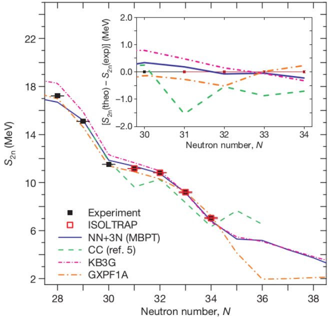
Why three-body forces?

- They are key to explain and predict the nuclear chart
- Medium-mass nuclei properties in good agreement with experiment



Otsuka et al.,PRL 105, 032501 (2010)



Wienholtz et al., Nature 498, (2013)

Why three-body forces?

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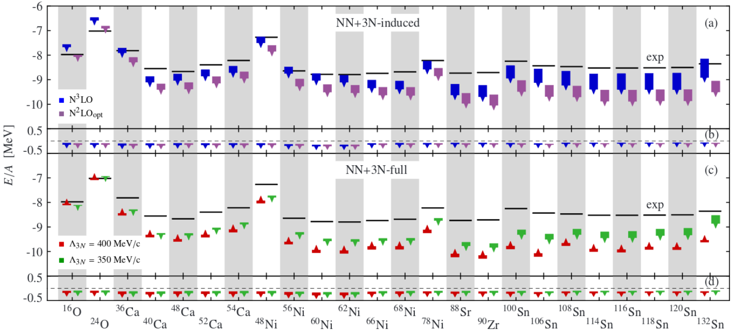

Binder et al., PLB 736, (2014)

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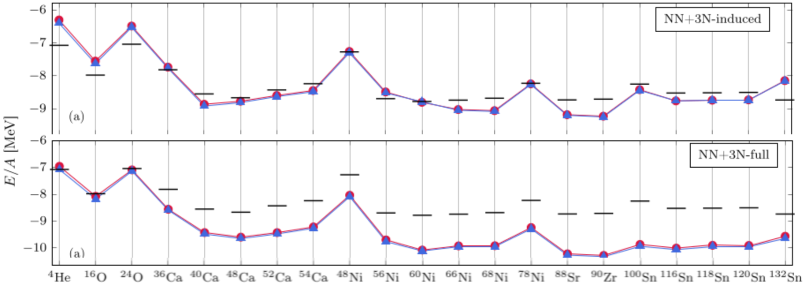
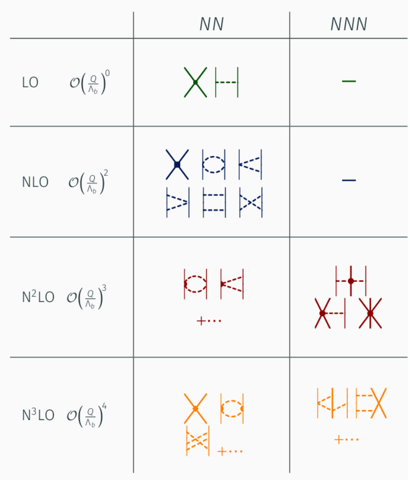


Tichai et al., PLB 756, (2016)

Chiral EFT

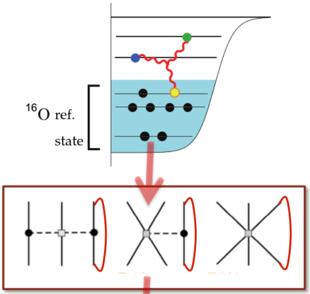


- Chiral EFT: expansion in powers of Q/Λ_b. $Q \sim m_\pi \sim 100$ MeV; $\Lambda_b \sim 500$ MeV
- Long-range physics: given explicitly (no parameters to fit) by pion exchanges.
- Short-range physics: contact interactions with low-energy constants (LECs) fit to πN, NN, 3N, ... data.
- Many-body forces and currents enter systematically.

Chiral EFT

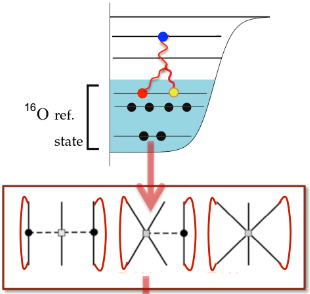
- An effective way to treat 3NF is through normal ordered matrix elements, performed in single-particle basis.

Normal ordered two-body



$$\langle ab|\, V_{3N,\mathrm{eff}}\, |a'b'\rangle = \sum_{\alpha = core} \langle \alpha ab|\, V_{3N}\, |\alpha a'b'\rangle$$

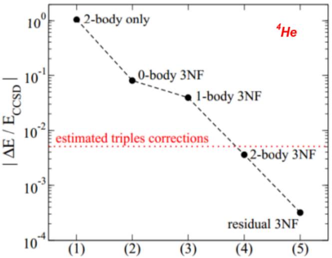
Normal ordered one-body



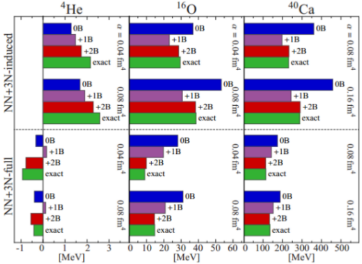
$$\langle a|\, V_{3N,\mathrm{eff}}\, |a'\rangle = \frac{1}{2} \sum_{\alpha\beta = core} \langle \alpha\beta a|\, V_{3N}\, |\alpha\beta a'\rangle$$

Chiral EFT

- An effective way to treat 3NF is through normal ordered matrix elements, performed in single-particle basis.
  $\rightarrow$ Residual three-body forces are small.



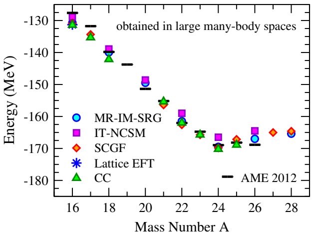
Hagen et al., Phys. Rev. C 76,034302 (2007)

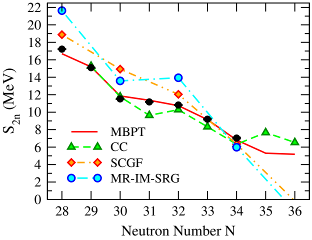


Roth et al., Phys. Rev. Lett. 109, 052501 (2012)

Chiral EFT

- An effective way to treat 3NF is through normal ordered matrix elements, performed in single-particle basis.
- Very good agreement for different methods in medium-mass nuclei and with experiment.





Hebeler et al., Ann. Rev. Nucl. Part. Sci. 65, 457 (2015)

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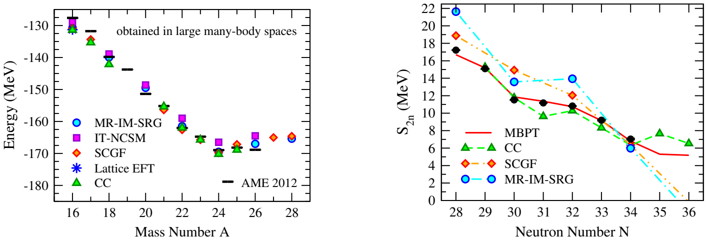
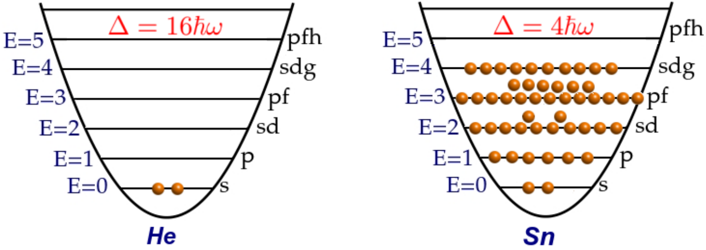


Hebeler et al., Ann. Rev. Nucl. Part. Sci. 65, 457 (2015)

- Challenges to overcome:
  → improvement of the Hamiltonian.
  → expansion of the reachable many-body space.

Many-body space

- $E_1 + E_2 + E_3 \leq E_{3\max}$ $\rightarrow$ Currently $E_{3\max} \approx 16\,\hbar\omega$

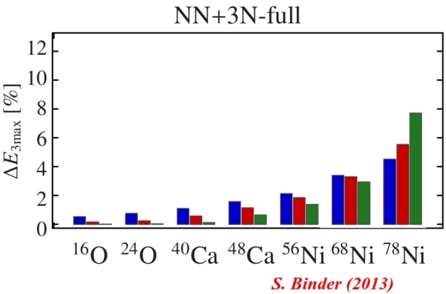


$$\Delta = E_{3\max} - 3E_{\mathrm{occ}}$$

- The space of interaction between three particles is reduced for heavy nuclei!

Many-body space

- Difference of relative errors for $E_{3\max} = 12\hbar\omega$ and $E_{3\max} = 14\hbar\omega$ in ground state energies (ΔE_{3max})



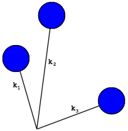
$\alpha = 0.02$ fm^4, $\alpha = 0.04$ fm^4, $\alpha = 0.08$ fm^4

- ΔE_{3max} grows with A. Convergence is challenging for heavy nuclei.

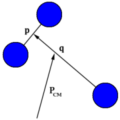
Normal ordered matrix elements

- To determine the normal-ordered interaction, we need the matrix elements evaluated at single-particle coordinates.

$$\left\langle ab|V_{eff}|a'b'\right\rangle = \sum_c \left\langle abc|V_{3N}|a'b'c\right\rangle$$



- Matrix elements are stored in Jacobi basis.



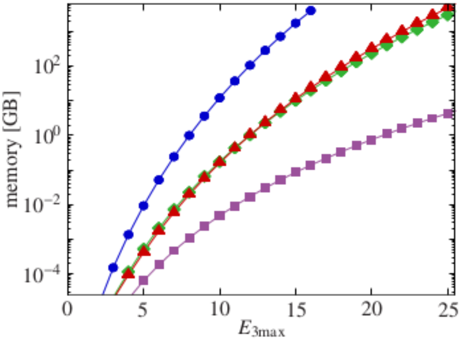
$$\langle V_{3N}\rangle_{\text{stored}} = \left\langle \mathbf{pq}|V_{3N}|\mathbf{p}'\mathbf{q}'\right\rangle$$

- Regular strategy:

Normal ordered matrix elements

Challenges:

- Transformation to m-scheme basis is slow.
- Storage of matrix elements is challenging memory-wise.
- Expansion of the model space following the regular strategy is difficult!



Roth et al., Phys. Rev. C 90 (2013)

Normal ordered matrix elements

Our goal: perform 2BNO in Jacobi basis.

Key points of the derivation:

- Start with 3rd particle in single particle basis
- Expression involving $\left\langle \mathbf{k}_a \mathbf{k}_b \mathbf{k}_c | V_{3N} | \mathbf{k}'_a \mathbf{k}'_b \mathbf{k}'_c \right\rangle$
- Transformation to Jacobi basis
- Only approximation: $\mathbf{P} = \mathbf{k}_a + \mathbf{k}_b = 0$
- Partial wave decomposition.

$$\left\langle \mathbf{k}_a \mathbf{k}_b | V_{\text{eff}} | \mathbf{k}'_a \mathbf{k}'_b \right\rangle = \sum_{\text{c}} \left\langle \mathbf{k}_a \mathbf{k}_b c | V_{3N} | \mathbf{k}'_a \mathbf{k}'_b c \right\rangle$$

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$$\left\langle \mathbf{k}_a \mathbf{k}_b | V_{\text{eff}} | \mathbf{k}'_a \mathbf{k}'_b \right\rangle = \int d\mathbf{k}_3 d\mathbf{k}'_3 \sum_{\text{c}} \langle c | \mathbf{k}_3 \rangle \left\langle \mathbf{k}'_3 | c \right\rangle \left\langle \mathbf{k}_a \mathbf{k}_b \mathbf{k}_c | V_{3N} | \mathbf{k}'_a \mathbf{k}'_b \mathbf{k}'_c \right\rangle$$

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$$\left\langle \mathbf{pP} | V_{\text{eff}} | \mathbf{p}'\mathbf{P}' \right\rangle = \int d\mathbf{k}_3 d\mathbf{k}'_3 \sum_{\text{c}} \langle c | \mathbf{k}_3 \rangle \left\langle \mathbf{k}'_3 | c \right\rangle \left\langle \mathbf{pq} | V_{3N} | \mathbf{p}'\mathbf{q}' \right\rangle \delta^3(\mathbf{P} + \mathbf{k}_3 - \mathbf{P}' - \mathbf{k}'_3)$$

Normal ordered matrix elements

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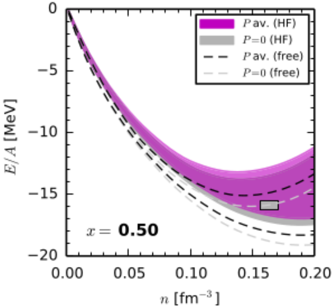

Drischler et al., Phys. Rev. C 93 (2016)

Normal ordered matrix elements

- Final result

$$\langle p(LS)JT|\, V_{\text{eff}} \left|p'(L'S')JT\right\rangle =$$

$$\frac{(-i)^{L-L'}}{(4\pi)^2(2\pi)^3} \sum_{\substack{n_c,l_c \\ occupied}} \sum_{\mathcal{J},j_c,\mathcal{T}} \frac{2\mathcal{J}+1}{2J+1}\frac{2\mathcal{T}+1}{2T+1} \int k_3^2 dk_3 \int {k_3'}^2 dk_3' \int dcos(\theta_{k_3'})$$

$$\times \frac{2l_c+1}{4\pi} P_{l_c}\left(cos(\theta_{k_3'})\right) R_{n_c l_c}(k_3) R_{n_c l_c}(k_3') \left\langle p, \frac{2}{3}k_3, \alpha \right| V^{3N} \left| p', \frac{1}{3}|(\mathbf{k}_3+\mathbf{k}_3')|, \alpha' \right\rangle$$

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$\rightarrow$ effective two-body matrix elements (relative quantum numbers).

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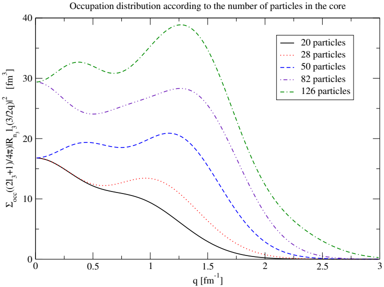
→ effective two-body matrix elements (relative quantum numbers).

→ occupation number regulated by harmonic oscillator wave function.



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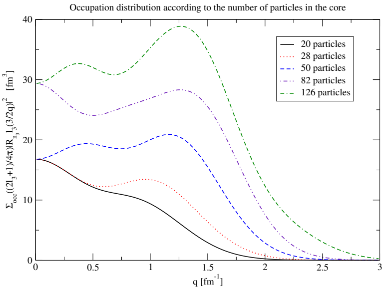


Normal ordered matrix elements

Extra steps towards single-particle basis:

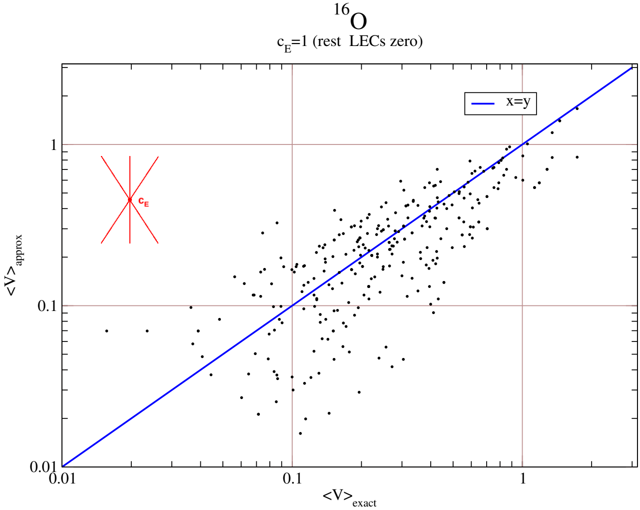
- Transformation to harmonic oscillator basis

$$\left\langle n(LS)JT|V_{\text{eff}}|n'(L'S')JT\right\rangle = \int dpp^2 R_{nL}(p)dp'p'^2 R_{n'L'}(p') \left\langle p|V|p'\right\rangle$$

- Talmi-Moshinsky transformation.

$$\left\langle n(LS)JT|V_{\text{eff}}|n'(L'S')JT\right\rangle \to$$
$$\left\langle n_1 n_2 \left[(l_1\frac{1}{2})j_1(l_2\frac{1}{2})j_2\right] J|V_{\text{eff}}|n'_1 n'_2 \left[(l'_1\frac{1}{2})j'_1(l'_2\frac{1}{2})j'_2\right] J\right\rangle$$

Comparison with exact matrix elements



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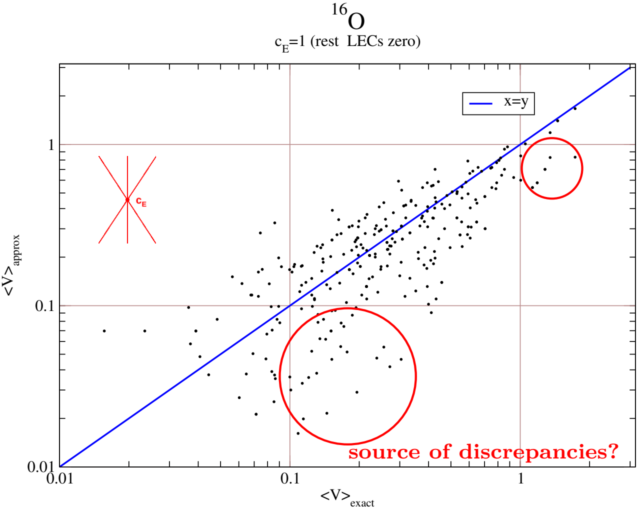


Inclusion of center-of-mass degrees of freedom

- Get rid of the approximation $\mathbf{P} = 0$.
- Simplified expression feasible for an S-wave interaction (c_E term of the Hamiltonian)

$$\langle pP[(LS)j_{\rm rel}L_{\rm cm}]JT\,|V_{\rm eff}|\,p'P'[(L'S')j'_{\rm rel}L'{\rm cm}]JT\rangle_{c_E} \propto$$

$$\sum_c \sum_{\mathcal{J}} \sum_{\mathcal{T}} \sum_{s_3 s'_3} \frac{2\mathcal{J}+1}{2S+1}\frac{2\mathcal{T}+1}{2T+1} \int d(\cos\theta_{P'}) P_{L_{cm}}(\cos\theta_{P'})$$

$$\times \int d^3k_3 R_{n_c l_c}(k_3) R_{n_c l_c}(k'_3) \frac{2l_c+1}{4\pi} P_{l_c}(\cos(\hat{\mathbf{k}}_3 \cdot \hat{\mathbf{k}}'_3))$$

$$\times \left\langle p, \left|\frac{2}{3}\mathbf{k}_3 - \frac{\mathbf{P}}{3}\right|, \alpha \left| V^{3N} \right| p', \left|\frac{2}{3}\mathbf{k}_3 + \frac{2}{3}\mathbf{P} - \mathbf{P}'\right|, \alpha' \right\rangle$$

→ effective two-body matrix elements (relative and center-of-mass quantum numbers).
→ center-of-mass angular contribution.
→ occupation number regulated by harmonic oscillator wave function.
→ three-body matrix elements in Jacobi basis as a function of $\mathbf{k}_c$, $\mathbf{P}$ and $\mathbf{P}'$.

Normal ordered matrix elements

Extra steps towards single-particle basis:

- Transformation to harmonic oscillator basis

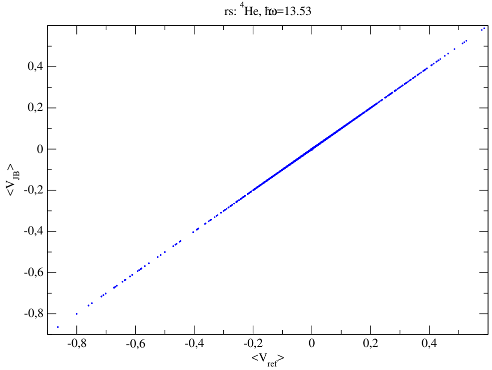
$$\left\langle Nn[(LS)j_{\rm rel}L_{\rm cm}]J|V_{\rm eff}|N'n'[(L'S')j'_{\rm rel}L'_{\rm cm}]J\right\rangle =$$
$$\int dPP^2 R_{NL_{\rm cm}}(P)\int dP'P'^2 R_{N'L'_{\rm cm}}(P')\int dpp^2 R_{nL}(p)\int dp'p'^2 R_{nL'}(p')$$
$$\left\langle Pp[(LS)j_{\rm rel}L_{cm}]J|V_{\rm eff}|P'p'[(L'S')j'_{\rm rel}L'_{\rm cm}]J\right\rangle .$$

- (Modified) Talmi-Moshinsky transformation including center-of-mass degrees of freedom as input.

$$\left\langle nN[(LS)j_{\rm rel}L_{\rm cm}]JT|V_{\rm eff}|n'[(L'S')j'_{\rm rel}L'_{\rm cm}]JT\right\rangle \to$$
$$\left\langle n_1n_2\left[(l_1\frac{1}{2})j_1(l_2\frac{1}{2})j_2\right]J|V_{\rm eff}|n'_1n'_2\left[(l'_1\frac{1}{2})j'_1(l'_2\frac{1}{2})j'_2\right]J\right\rangle$$

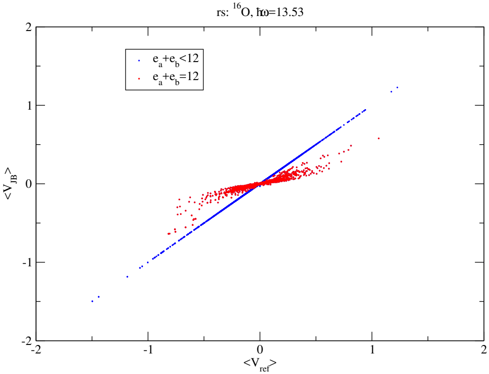
Results for S-wave Hamiltonians

- Reference state: ^{4}He.
- energy of particles in reference state: $e_{rs} = 0$
- e_{Max} =6.
- Perfect agreement with reference matrix elements.



Results for S-wave Hamiltonians

- Reference state: ^{16}O.
- Energy of particles in reference state: $e_{rs} = 0, 1$
- e_{Max} =6.
- For the 2BNO taken as reference, the condition $E_{3N} = e_a + e_b + e_c \leq 12$ is applied.
- Perfect agreement with reference matrix elements with energy up to 12.



Inclusion of center-of-mass degrees of freedom: general

$$\langle pP\,[(LS)j_{rel}L_{cm}]\,J|\,\overline{V}\,\left|p'P'\,\left[(L'S')j'_{rel}L'_{cm}\right]\,J\right\rangle \propto$$

$$\sum_{c}\sum_{\alpha,\alpha'}\sum_{M'_{cm},M'_j,M_J}\sum_{\mathcal{T}}\sum_{\mathcal{J},M_{\mathcal{J}}}\sum_{m_j,m'_j}$$

$$\times\,\mathcal{C}^{JM_J}_{j_{rel}M_j\,L_{cm}M_{cm}}\,\mathcal{C}^{JM_J}_{j'_{rel}M'_j\,L'{}_{cm}M'_{cm}}\,\mathcal{C}^{\mathcal{J}M_{\mathcal{J}}}_{j_{rel}M_j\,jm_j}\,\mathcal{C}^{jm_j}_{lm_l1/2m_{s_c}}\,\mathcal{C}^{\mathcal{J}M_{\mathcal{J}}}_{j'_{rel}M'_j\,j'm'_j}\,\mathcal{C}^{j'm'_j}_{l'm'_l1/2m_{s_c}}$$

$$\times\sqrt{\frac{1+2L_{cm}}{4\pi}}\int d\theta_{P'}\sin\theta_{P'}Y_{L'_{cm}M'_{cm}}(\theta_{P'},0)Y^{*}_{lm_l}(\hat{\mathbf{q}})Y_{l'm'_l}(\hat{\mathbf{q}}')$$

$$\times\int\frac{d\mathbf{k}_3}{(2\pi)^3}\sum_{n_c,l_c}R_{n_cl_c}(k_3)R_{n_cl_c}(k'_3)\frac{2l_c+1}{4\pi}P_{l_c}(\mathbf{k}_3\cdot\mathbf{k}'_3)\left\langle pq\alpha|V_{3N}|p'q'\alpha'\right\rangle$$

→ effective two-body matrix elements (relative and center-of-mass quantum numbers).

→ center-of-mass angular contribution.

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→ three-body matrix elements in Jacobi basis as a function of $\mathbf{k}_c$, $\mathbf{P}$ and $\mathbf{P}'$.

Summary

- Current limitations in treatment of three-body forces will lead to significant truncation effects in calculations for heavy nuclei.
- The approximtion **P**=0 is not applicable to finite nuclei calculations.
- Purely S-wave interaction normal ordered matrix elements including center-of-mass degrees of freedom agree with reference calculations.
- Generalization of the input Hamiltionian in progress...

Thank you for your attention!

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