

Jacobi no-core Shell Model (J-NCSM)

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Ab initio nuclear structure calculations

Goal: solving the non-relativistic A-body Schrödinger Eq. for bound states

$$H|\Psi_n\rangle = E_n |\Psi_n\rangle, \quad H = \sum_{i=1}^A \frac{\mathbf{k}_i^2}{2m} + \sum_{i < j=1}^A V_{ij} + \sum_{i < j < k=1}^A V_{ijk}$$

ab initio:

- protons and neutrons are fundamental degrees of freedom
- realistic (microscopic) nuclear interactions as input
- controlled and improvable truncations

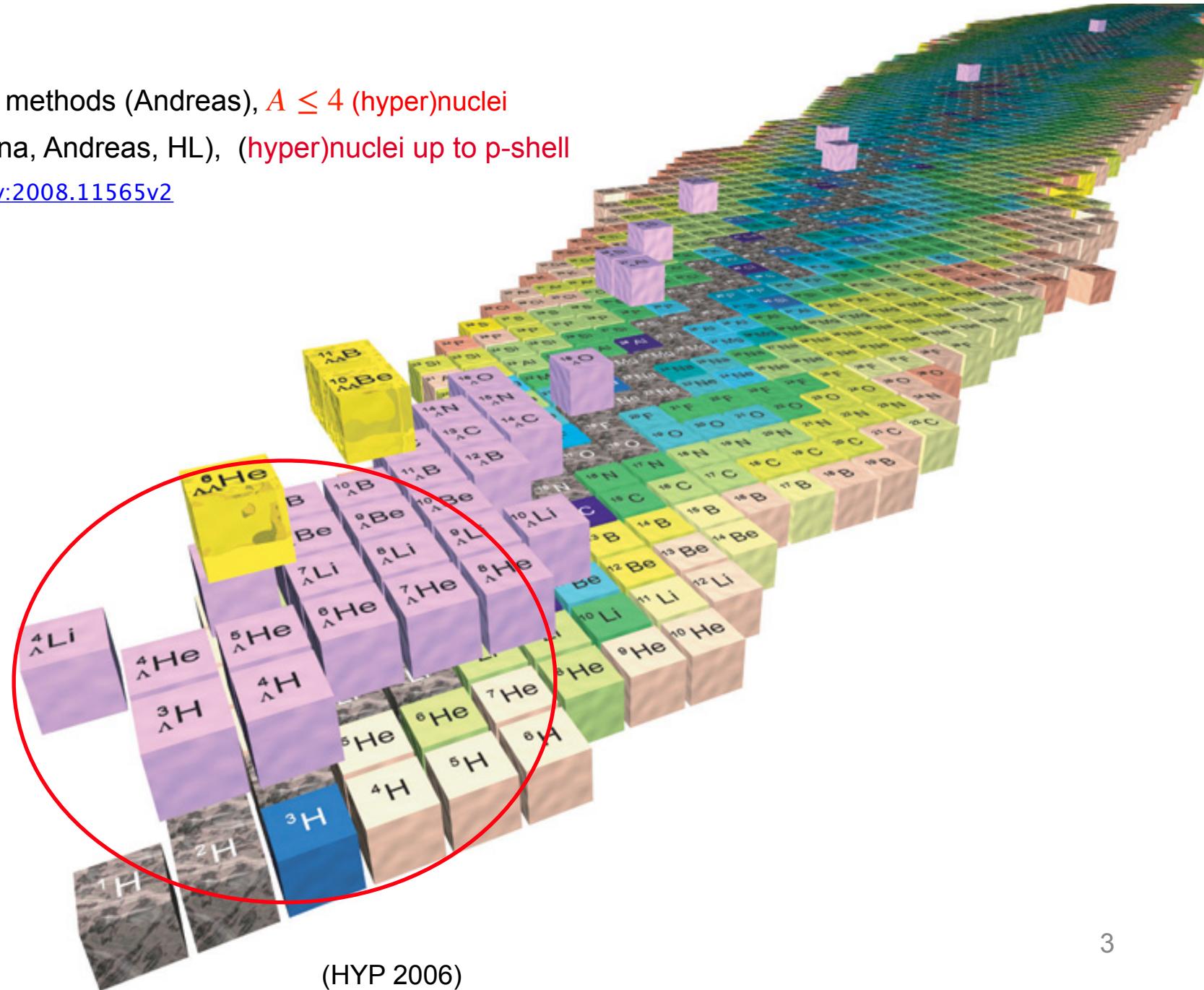
ab initio (few)many-body approaches:

- Faddeev-Yakubovsky integral equation, exact solutions for $A \leq 4$, arXiv:nucl-th/0004023
 - Green's function Monte Carlo, require local interactions, arXiv:0804.3501
 - No-core shell model (NCSM), arXiv:0904.0463
 - Coupled-cluster method, arXiv:1312.7872
 - Lattice Monte Carlo, suitable for states with complex geometries, arXiv:0804.3501
 - ...
- } → need large model space (soft interactions)

Ab initio nuclear structure calculations

at our disposal:

- Faddeev-Yakubovsky methods (Andreas), $A \leq 4$ (hyper)nuclei
- Jacobi NCSM (Susanna, Andreas, HL), (hyper)nuclei up to p-shell
[arXiv:1510.06070v1](https://arxiv.org/abs/1510.06070v1), [arXiv:2008.11565v2](https://arxiv.org/abs/2008.11565v2)



No-core shell model (NCSM)

- Idea: represent the A-body translationally invariant Hamiltonian

$$\begin{aligned} H_{int} &= \sum_{i=1}^A \frac{\mathbf{k}_i^2}{2m} + \sum_{i < j = 1}^A V_{ij} + \sum_{i < j < k = 1}^A V_{ijk} - \frac{\mathbf{P}^2}{2M} \\ &= \sum_{i < j = 1}^A \frac{2}{A} \frac{\mathbf{p}_{ij}^2}{m} + \sum_{i < j = 1}^A V_{ij} + \sum_{i < j < k = 1}^A V_{ijk}, \quad \mathbf{p}_{ij} = \frac{1}{2}(\mathbf{k}_i - \mathbf{k}_j) \end{aligned}$$

in a basis constructed from HO functions, $\phi_{nlm}(\mathbf{p}) = \langle \mathbf{p} | nlm \rangle = R_{nl}(p)Y_{lm}(\hat{p})$

$$R_{nl}(p) = (-1)^n \sqrt{\frac{2(n!)b^3}{\Gamma(n+l+2/3)}} (pb)^l e^{-(pb)^2/2} L_n^{l+1/2}((pb)^2), \quad b = 1/\sqrt{\mu\omega}$$

HO basis →

- essential for evaluating Hamiltonian matrix elements 
- facilitate transformations between different bases
- wrong asymptotic behavior, NCSM results converge slowly \Rightarrow require soft interactions 

- two approaches to construct basis states:

- Slater determinant basis depending on single-particle coordinates (m-scheme importance truncated NCSM)
 - antisymmetric, but contain CM motion \Rightarrow large dimension
 - importance truncated basis (IT-NCSM) for p-shell
- Jacobi basis expressed in relative Jacobi coordinates (Jacobi NCSM)
 - preserve translational symmetry of H, no CM motion, \Rightarrow small dimension
 - antisymmetrization of basis states is demanding $A \leq 8$
- All particles are active (no inert core) \Rightarrow directly employ realistic BB interactions
- H is diagonalised via Lanczos iterations. Converge to exact solutions from above. 

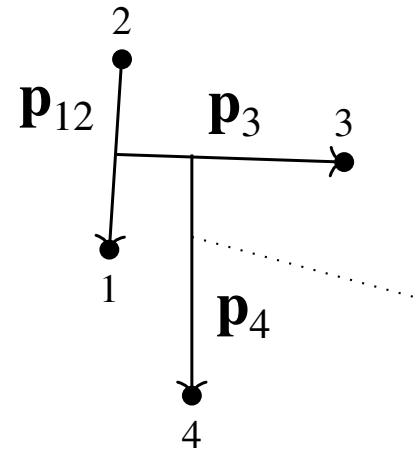
Jacobi NCSM basis

- Jacobi coordinates:

$$\mathbf{p}_{12} = \frac{m_2}{m_1 + m_2} \mathbf{k}_1 - \frac{m_1}{m_1 + m_2} \mathbf{k}_2,$$

$$\mathbf{p}_3 = \frac{m_1 + m_2}{m_1 + m_2 + m_3} \mathbf{k}_3 - \frac{m_3}{m_1 + m_2 + m_3} (\mathbf{k}_1 + \mathbf{k}_2)$$

...



- Two-body Jacobi HO basis: $|\alpha_{12}\rangle$

$$|\alpha_{12}\rangle \equiv |\underbrace{N_{12}(l_{12}S_{12})J_{12}, (t_1 t_2)t_{12}}_{JJ\text{-coupling}}\rangle$$

antisymmetric

$$(-1)^{l_{12}+s_{12}+t_{12}} = -1$$

total HO energy quantum number (model space size): $N_{12} = 2n_{12} + l_{12}$

→ in partial-wave decomposed Jacobi-momentum basis (NN interactions are defined): $|p_{12}(l_{12}S_{12})J_{12}t_{12}\rangle$

$$|\alpha_{12}\rangle = \int dp_{12} p_{12}^2 R_{n_{12}l_{12}}(p_{12}) |p_{12}(l_{12}S_{12})J_{12}t_{12}\rangle$$

$$\Rightarrow \langle \alpha_{12} | V_{NN} | \alpha'_{12} \rangle = \int dp_{12} dp'_{12} p_{12}^2 p'^2_{12} R_{n_{12}l_{12}}(p_{12}) R^*_{n'_{12}l'_{12}}(p'_{12}) \langle p_{12}(l_{12}S_{12})J_{12}t_{12} | V_{NN} | p'_{12}(l'S_{12})J_{12}t'_{12} \rangle$$

dependence on HO ω

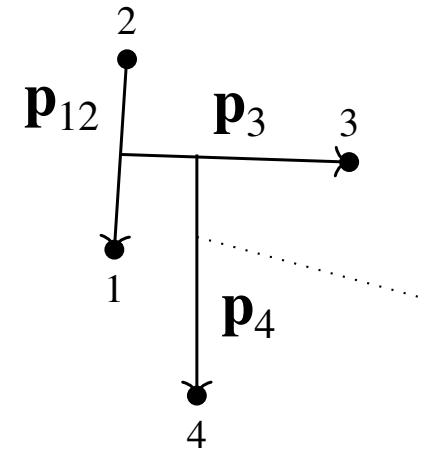
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$$(-1)^{l_{12}+s_{12}+t_{12}} = -1$$

- Three-body Jacobi HO basis: $|\alpha_3(N_3 J_3 T_3)\rangle$

$$|\alpha_3^{*(1)}\rangle \equiv |N_3 J_3 T_3 \alpha_{12} n_3(l_3 s_3) I_3, t_3; (J_{12} I_3) J_3, (t_{12} t_3) T_3\rangle \xrightarrow{\quad} \text{complete, only antisymmetric w.t. r. (1) } \leftrightarrow (2)$$

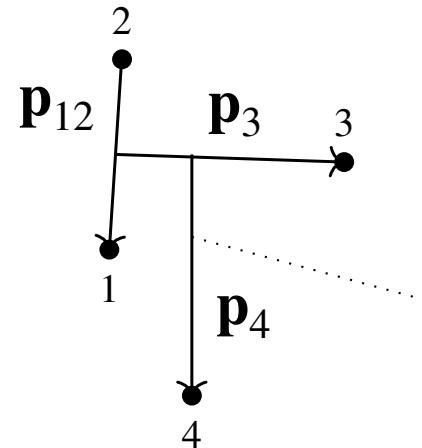
$$\boxed{N_3 = N_{12} + n_3 + 2l_3}$$

- Jacobi coordinates:

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...



- Two-body Jacobi HO basis: $|\alpha_{12}\rangle$

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→ idea: use antisymmetrizer to project out the (non)antisymmetric states

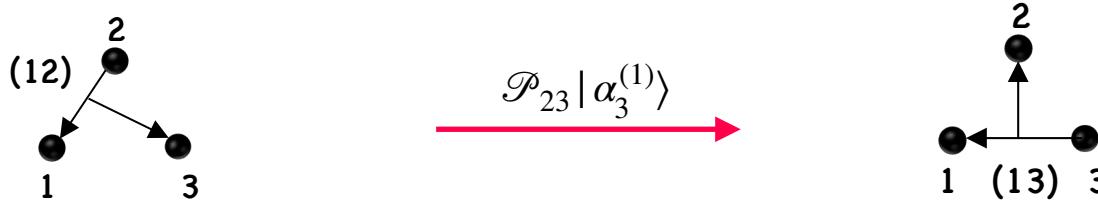
$$\langle \alpha_3^{*(1)} | \frac{1}{3}(1 - 2\mathcal{P}_{23}) | \alpha_3^{*(1)} \rangle \langle \alpha_3^{*(1)} | \alpha_3 \rangle = \lambda \langle \alpha_3^{*(1)} | \alpha_3 \rangle \quad \lambda = (0)1$$

$$\Rightarrow \text{totally antisymmetrized 3-body basis} \quad |\alpha_3\rangle \equiv |iN_3 J_3 T_3\rangle = \sum_{\alpha_3^{*(1)}} \langle \alpha_3^{*(1)} | \alpha_3 \rangle | \alpha_3^{*(1)} \rangle, \quad \lambda = 1$$

coeff. of fractional parentage (cfp)
 ω -independent

Jacobi NCSM basis

- Apply permutation operator \mathcal{P}_{23} to $|\alpha_3^{*(1)}\rangle$



$$|\alpha_3^{*(1)}\rangle \equiv |\alpha_{12} n_3(l_3 s_3) I_3, t_3; (J_{12} I_3) J, (t_{12} t_3) T\rangle$$

$$|\beta_3^{*(1)}\rangle \equiv |\alpha_{13} n_2(l_2 s_2) I_2, t_2; (J_{13} I_2) J, (t_{13} t_2) T\rangle$$



$$\langle \alpha_3^{*(1)} | P_{23}) | \alpha_3^{*(1)} \rangle = \langle \alpha_3^{*(1)} | \beta_3^{*(1)} \rangle \quad \text{← orthogonal basis transformation}$$

$$= \hat{J}_{13} \hat{I}_2 \hat{J}_{12} \hat{I}_3 \sum_{LS} \hat{L}^2 \hat{S}^2 \left\{ \begin{array}{c} l_{13} \\ l_2 \\ L \end{array} \begin{array}{c} S_{13} \\ s_2 \\ S \end{array} \begin{array}{c} J_{13} \\ I_2 \\ J \end{array} \right\} \left\{ \begin{array}{c} l_{12} \\ l_3 \\ L \end{array} \begin{array}{c} S_{12} \\ s_3 \\ S \end{array} \begin{array}{c} J_{12} \\ I_3 \\ J \end{array} \right\}$$

$$(-1)^{l_2 + l_3} \langle n_{13} l_{13}, n_2 l_2 : L | n_{12} l_{12}, n_3 l_3 : L \rangle_d \quad \text{← HO (Tamil-Moschinsky) bracket}$$

$$(-1)^{S_{13} + s_2 + S_{12} + s_3} \hat{S}_{13} \hat{S}_{12} \left\{ \begin{array}{c} s_2 \\ s_3 \\ S \end{array} \begin{array}{c} s_1 \\ S \\ S_{13} \end{array} \right\} (-1)^{T_{13} + t_2 + T_{12} + t_3} \hat{T}_{13} \hat{T}_{12} \left\{ \begin{array}{c} t_2 \\ t_3 \\ T \end{array} \begin{array}{c} t_1 \\ T \\ T_{13} \end{array} \right\}$$

$$\hat{J}_{13} = \sqrt{2J_{13} + 1}$$

S. Liebig et al. EPJA (2017) [arXiv:1510.06070v1](https://arxiv.org/abs/1510.06070v1)

- Evaluation of 3N matrix elements:

$$\langle \alpha'_3 | V_{3N} | \alpha_3 \rangle = \langle \alpha'_3 | \alpha_3^{*(1)} \rangle \underbrace{\langle \alpha_3^{*(1)} | V_{3N} | \alpha_3^{*(1)} \rangle}_{\text{similar to } \langle \alpha_{12} | V_{NN} | \alpha'_{12} \rangle} \langle \alpha_3^{*(1)} | \alpha_3 \rangle$$

Jacobi NCSM basis

- A-body Jacobi HO basis: $|\alpha_A(NJT)\rangle \equiv |\bullet\circlearrowleft\rangle_A$ constructed from (A-1) basis states

$$|\alpha_A^{*(1)}\rangle = |NJT \alpha_{A-1} n_A(l_A, s_A) I_A, t_A; (J_{A-1} I_A) J, (T_{A-1} t_A) T\rangle \equiv |\bullet\circlearrowleft\rangle$$

↑
antisym. state of (A-1) $\equiv |\bullet\circlearrowleft\rangle_{A-1}$

- diagonalize A-body antisymmetrizer to obtain antisymmetric states:

$$\langle \bullet\circlearrowleft | \frac{1}{A} (1 - (A-1) \mathcal{P}_{A-1,A}) |\bullet\circlearrowleft\rangle \langle \bullet\circlearrowleft | \bullet\circlearrowleft\rangle_A = \lambda \langle \bullet\circlearrowleft | \bullet\circlearrowleft\rangle_A \quad \lambda = 1 \quad (\text{for certain (NJT) block})$$

► expand $|\bullet\circlearrowleft\rangle$ in a complete basis set : $|(\alpha^{*(1)})^{*(1)}\rangle \equiv |\bullet\circlearrowleft\bullet\circlearrowright\rangle$

$$|\bullet\circlearrowleft\rangle = \sum_{|\bullet\circlearrowleft\rangle} \langle \bullet\circlearrowleft | \bullet\circlearrowleft\rangle |\bullet\circlearrowleft\rangle = \sum_{|\bullet\circlearrowleft\rangle} \delta_{\text{spectator}} \langle \bullet\circlearrowleft | \bullet\circlearrowleft\rangle_{A-1} |\bullet\circlearrowleft\rangle$$

↑
cfp(A-1), HO- ω independent

$$\rightarrow \langle \bullet\circlearrowleft | \mathcal{P}_{A-1,A} |\bullet\circlearrowleft\rangle = \langle \bullet\circlearrowleft | \bullet\circlearrowleft\bullet\circlearrowright \underbrace{\langle \bullet\circlearrowleft | \mathcal{P}_{A-1,A} | \bullet\circlearrowleft\rangle}_{\text{orth. transformation}} \langle \bullet\circlearrowleft | \bullet\circlearrowleft\bullet\circlearrowright \rangle$$

⇒ totally antisymmetrized A-body basis state

$$|\bullet\circlearrowleft\rangle = |\alpha_A\rangle \equiv |iNJT\rangle = \sum_{\alpha_A^{*(1)}} \langle \alpha_A^{*(1)} | \alpha_A \rangle_{\text{cfp}} |\alpha_A^{*(1)}\rangle$$

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HO- ω independent

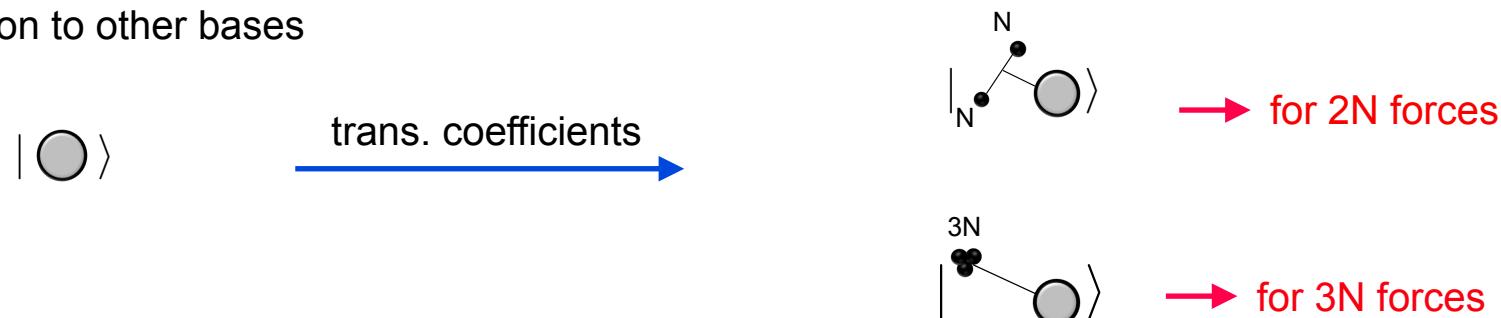
- basis truncation: $N = \mathcal{N}_{A-1} + 2n_A + l_A \leq N_{max} \Rightarrow E_b = E_b(\omega, N_{max})$

→ require $N_{max} \rightarrow \infty$ extrapolation 

Hamiltonian matrix elements in Jacobi basis

$$H_{rel} = \sum_{i < j=1}^A \left(\frac{2}{A} \frac{\mathbf{p}_{ij}^2}{m} + V_{ij} \right) + \sum_{i < j < k=1}^A V_{ijk} = \sum_{i < j=1}^A h_{ij}^{NN} + \sum_{i < j < k=1}^A V_{ijk}, \quad \langle \bigcirc | H_{rel} | \bigcirc \rangle$$

- transformation to other bases



$$\Rightarrow \langle \bigcirc | \sum_{i < j=1}^A h_{ij}^{NN} | \bigcirc \rangle = \langle \bigcirc | \cdot \cdot \bigcirc \rangle \langle \cdot \cdot \bigcirc | \sum_{i < j=1}^A h_{ij}^{NN} | \cdot \cdot \bigcirc \rangle \langle \cdot \cdot \bigcirc | \bigcirc \rangle$$

$$= \langle \bigcirc | \cdot \cdot \bigcirc \rangle \underbrace{\delta_{core(A-2)} \binom{A}{2}}_{2\text{-body matrix element}} \underbrace{\langle \alpha_{12} | h_{ij}^{NN} | \alpha'_{12} \rangle}_{\text{2-body matrix element}} \langle \cdot \cdot \bigcirc | \bigcirc \rangle \quad \text{arXiv:1510.06070v1}$$

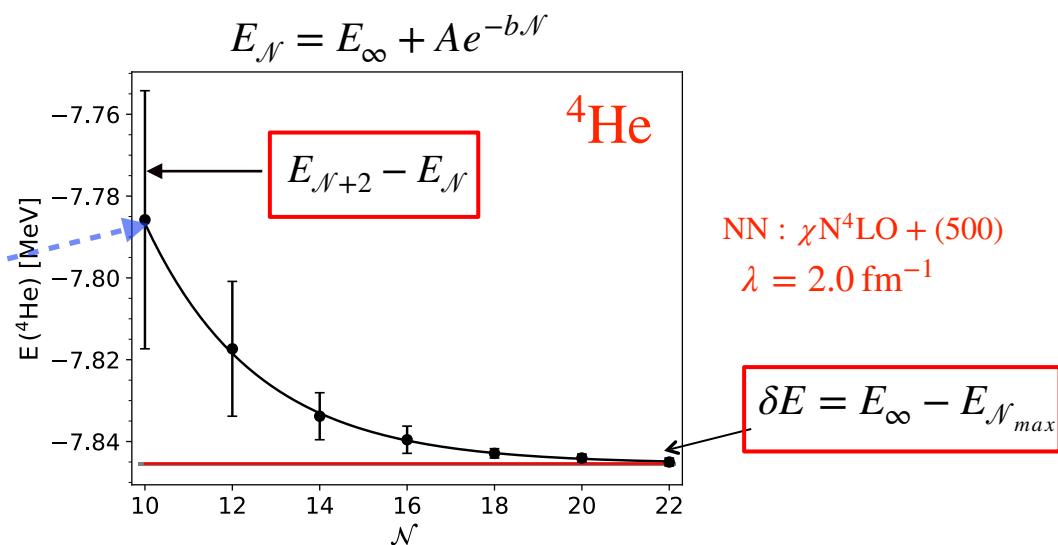
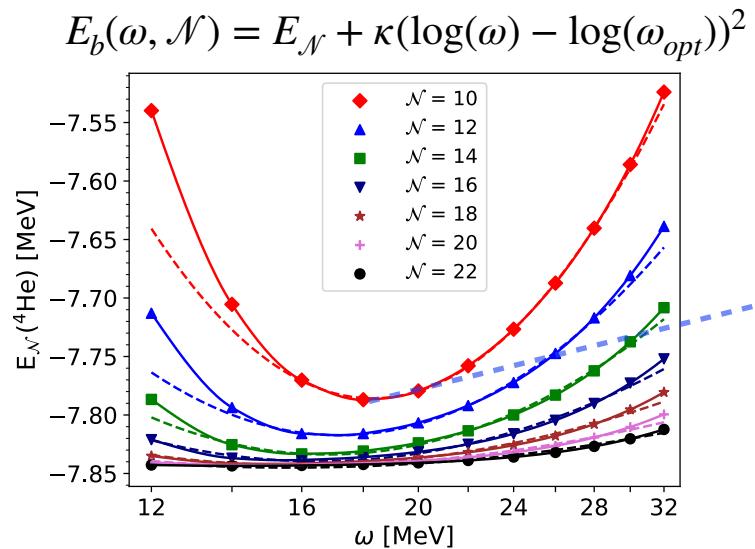
- transition coefficients:

$$\langle \bigcirc | \cdot \cdot \bigcirc \rangle = \underbrace{\langle \bigcirc | \bigcirc \cdot \cdot \rangle}_{\text{cfp}(A)} \underbrace{\langle \bigcirc \cdot \cdot | \cdot \cdot \bigcirc \rangle}_{\delta_{spec} \text{ cfp}(A-1)} \underbrace{\langle \cdot \cdot \bigcirc | \cdot \cdot \bigcirc \rangle}_{\text{orth. trans.}} \quad \rightarrow \text{HO-}\omega\text{ independent}$$

→ transition coefficients + cfp are prepared for each NJT block separately and stored in HDF5 format that allows an efficient parallel input/output

Extrapolation of binding energies

- Two parameters in NCSM: HO- ω , and $\mathcal{N} \Rightarrow E_b = E_b(\omega, \mathcal{N})$

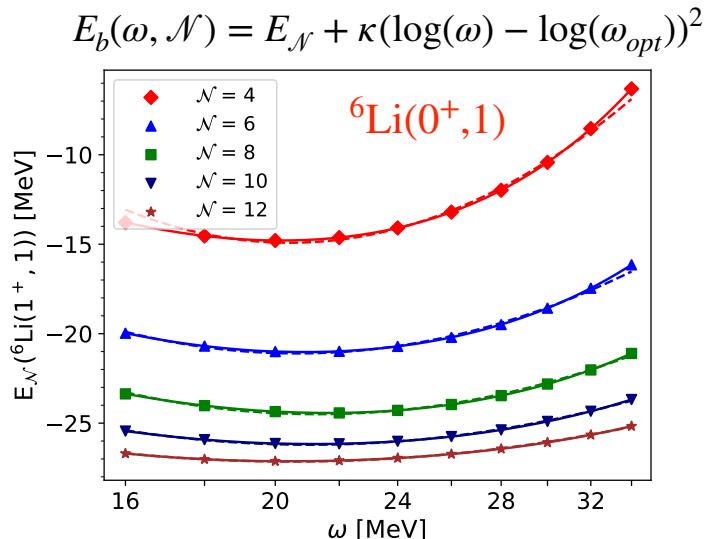
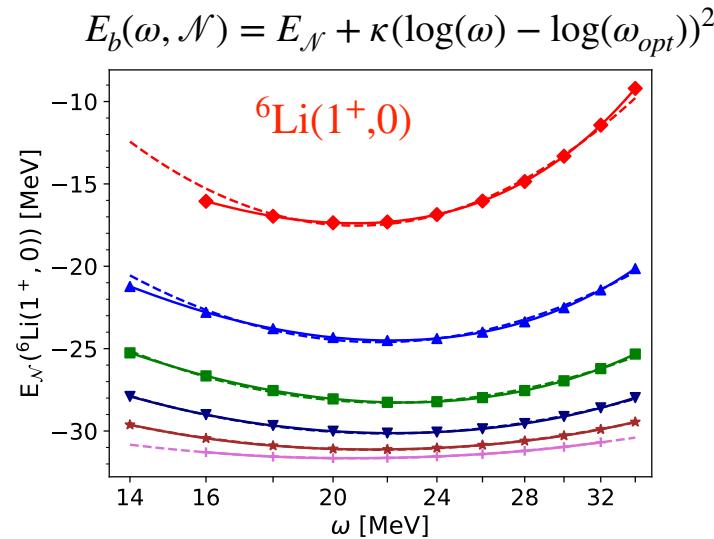


- ▶ ω_{opt} shifts to smaller values as \mathcal{N} increases
 ▶ ω -dependence energy curves flatten with increasing \mathcal{N}

- ▶ $E_{\mathcal{N}}$ converges to E_{∞} strictly from above

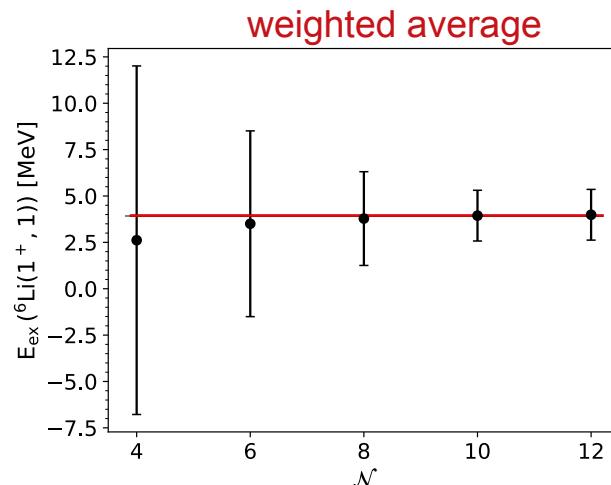
Extrapolation of excitation energies

- Two parameters in NCSM: HO- ω , and $\mathcal{N} \Rightarrow E_b = E_b(\omega, \mathcal{N})$
 - ▶ ω_{opt} for ground and excited states are not necessarily the same



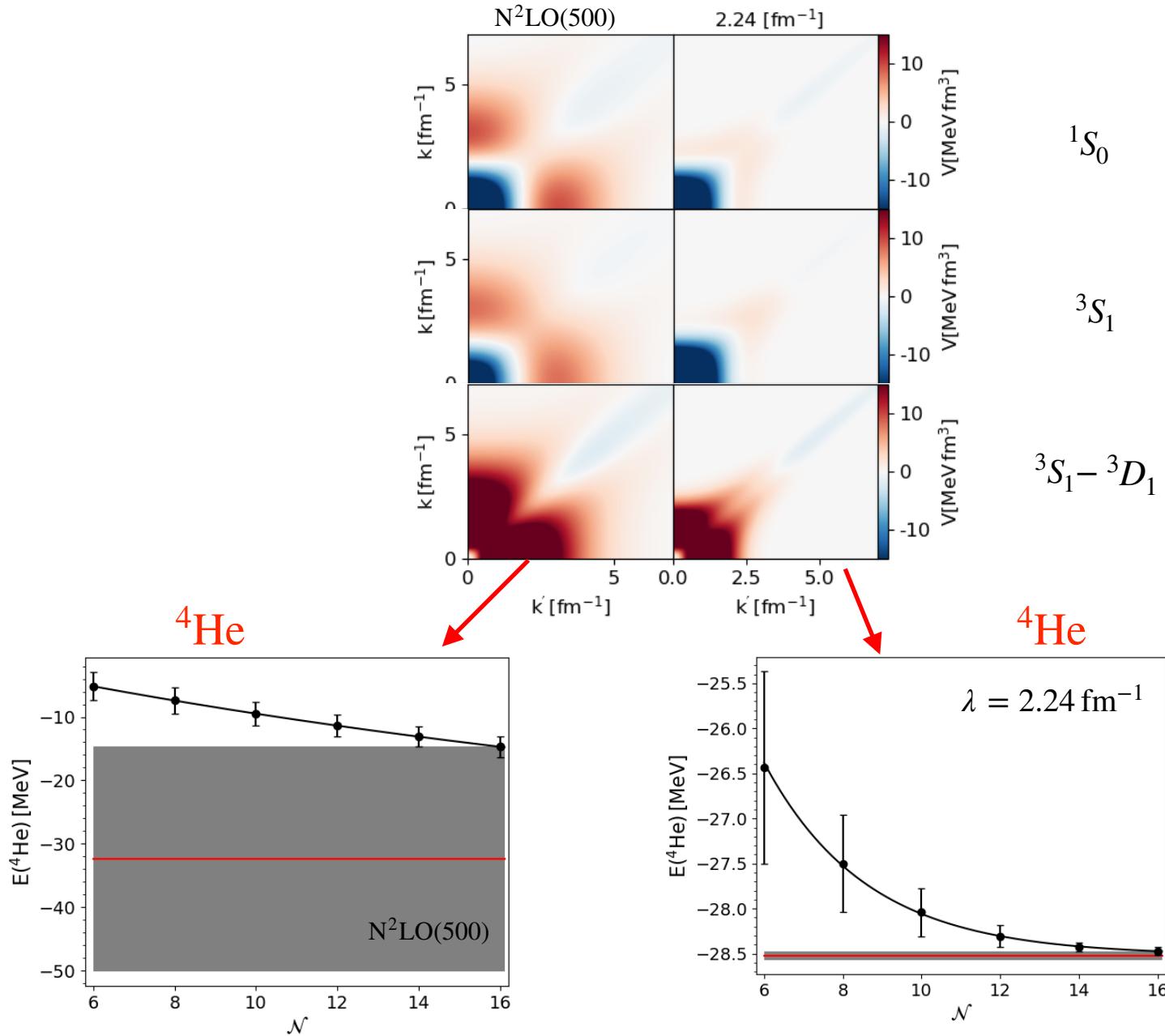
→ perform \mathcal{N} -space extrapolation on $E_{ex,\mathcal{N}}$

$$E_{ex,\mathcal{N}}(1^+,1) = E_{\mathcal{N}}(1^+,1) - E_{\mathcal{N}}(1^+,0)$$



Convergence of E with respect to \mathcal{N}

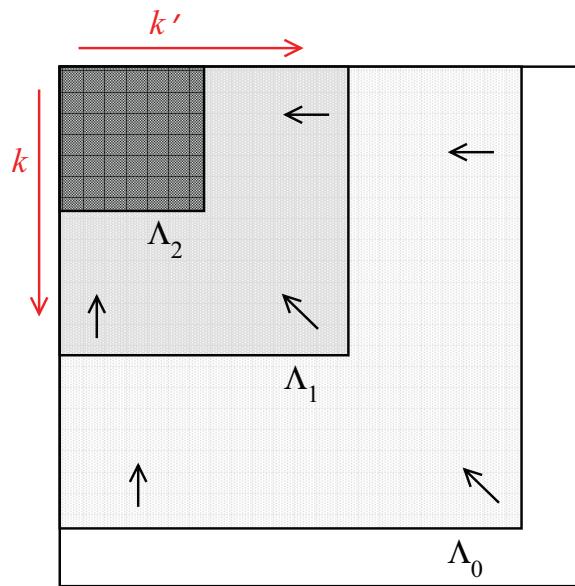
low-energy observables (long-wavelength information) converge slowly due strong couplings of low- and high-momentum states



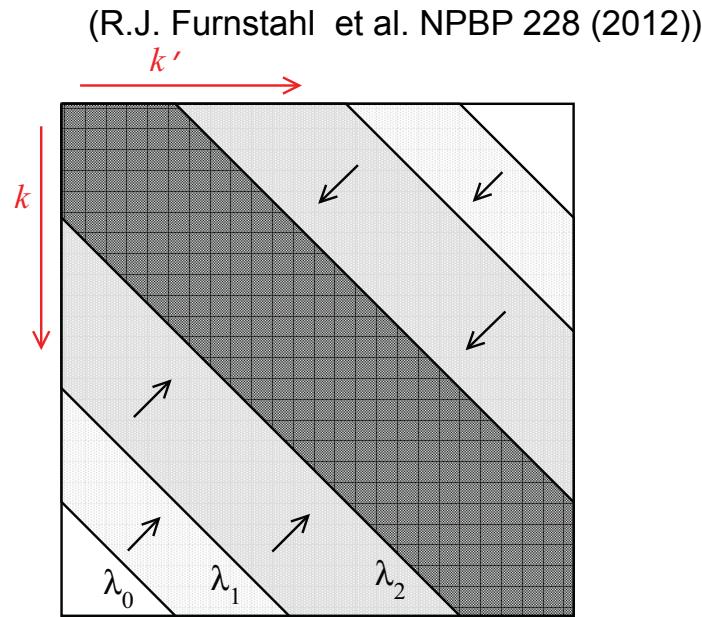
Renormalization Group (RG) methods

Idea: use RG methods to decouple low- and high-energy degrees of freedom

- $V_{low\ k}$ transformation
- Similarity renormalization group (SRG) evolution approach



$V_{low\ k}$ transformation



SRG evolution

- $V_{low\ k}$ is phase equivalent to V_{SRG} at low momentum
- SRG technique is much simpler + inclusion of higher body forces is straightforward

Idea: continuously apply unitary transformation to H to suppress off-diagonal matrix elements

→ observables are conserved due to unitarity of transformation ✓

F.J. Wegner NPB 90 (2000). S.K. Bogner, R.J. Furnstahl, R.J. Perry PRC 75 (2007)

$$\frac{dV(s)}{ds} = [[T_{rel}, V(s)], H(s)], \quad H(s) = T_{rel} + V(s); \quad T_{rel} = T_{12} + T_3 = T_{23} + T_1 = T_{31} + T_2$$

$$V(s) = V_{12}(s) + V_{13}(s) + V_{23}(s) + V_{123}(s) + \dots$$

- separate SRG flow equations for 2N and 3N interactions:

$$\begin{aligned} \frac{dV_{ij}}{ds} &= [[T_{ij}, V_{ij}], T_{ij} + V_{ij}], \\ \frac{dV_{123}}{ds} &= [[T_{12}, V_{12}], V_{31} + V_{23} + V_{123}] \\ &\quad + [[T_{31}, V_{31}], V_{12} + V_{23} + V_{123}] \\ &\quad + [[T_{23}, V_{23}], V_{12} + V_{31} + V_{123}] \\ &\quad + [[T_{rel}, V_{123}], H_s]. \end{aligned} \quad \text{Eqs.(1)}$$

→ no disconnected terms in $\frac{dV_{123}}{ds}$: dangerous delta functions are cancelled

- Eqs.(1) are solved by projecting on a partial-wave decomposed Jacobi-momentum basis

SRG flow equations

- SRG flow equation for 2N potential: $|p \alpha_{12}\rangle \equiv |p, (l_{12}s_{12})J_{12}(t_1t_2)t_{12} m_{t12}\rangle$

$$\frac{dV_{12}^{\alpha_{12}\alpha'_{12}}(pp')}{ds} = \underbrace{\left\{ T_{12}^{\alpha_{12}}(p) \frac{p^2}{2\mu^{\alpha_{12}}} + T_{12}^{\alpha'_{12}}(p') \frac{p^2}{2\mu^{\alpha_{12}}} - T_{12}^{\alpha_{12}}(p) \frac{p^2}{2\mu^{\alpha_{12}}} - T_{12}^{\alpha'_{12}}(p') \frac{p^2}{2\mu^{\alpha_{12}}} \right\}}_{\text{drives } V_{12} \text{ towards the }} V_{12}^{\alpha_{12}\alpha'_{12}}(pp')$$

drives V_{12} towards the

$$+ \sum_{\tilde{\alpha}_{12}} \int_0^\infty dk k^2 \underbrace{\left\{ \frac{p^2}{2\mu^{\alpha_{12}}} + \frac{p^2}{2\mu^{\alpha'_{12}}} - \frac{k^2}{\mu^{\tilde{\alpha}_{12}}} \right\}}_{\text{preserves unitarity}} V_{12}^{\alpha_{12}\tilde{\alpha}_{12}}(pk) V_{12}^{\tilde{\alpha}_{12}\alpha'_{12}}(kp')$$

Eq.(2)

- SRG flow equation for 3N interactions: $|pq\alpha\rangle \equiv |pq, ((l_{12}s_{12})J_{12} (l_3s_3)I_3)J ((t_1t_2)T_{12} t_3)T\rangle$

$$\begin{aligned} \langle p'q'\alpha' | \frac{dV_{123}}{ds} | pq\alpha \rangle &= \frac{2}{3} \langle p'q'\alpha' | (1+P)([T_{12}, V_{12}])P_{12}P_{23}V_{12} - V_{12}P_{12}P_{23}[T_{12}, V_{12}](1+P) | pq\alpha \rangle \\ &\quad + \frac{1}{3} \langle p'q'\alpha' | (1+P)([T_{12}, V_{12}])V_{123} - V_{123}[T_{12}, V_{12}](1+P) | pq\alpha \rangle \\ &\quad + \frac{1}{9} \langle p'q'\alpha' | (1+P)([T_{123}, V_{123}]T_{123} - T_{123}[T_{123}, V_{123}](1+P)) | pq\alpha \rangle \\ &\quad + \frac{1}{9} \langle p'q'\alpha' | (1+P)([T_{123}, V_{123}]V_{12} - V_{12}[T_{123}, V_{123}](1+P)) | pq\alpha \rangle \\ &\quad + \frac{2}{9} \langle p'q'\alpha' | (1+P)([T_{123}, V_{123}]P_{12}P_{23}V_{12} - V_{12}P_{12}P_{23}[T_{123}, V_{123}](1+P)) | pq\alpha \rangle \\ &\quad + \frac{1}{9} \langle p'q'\alpha' | (1+P)([T_{123}, V_{123}]V_{123} - V_{123}[T_{123}, V_{123}](1+P)) | pq\alpha \rangle \end{aligned}$$

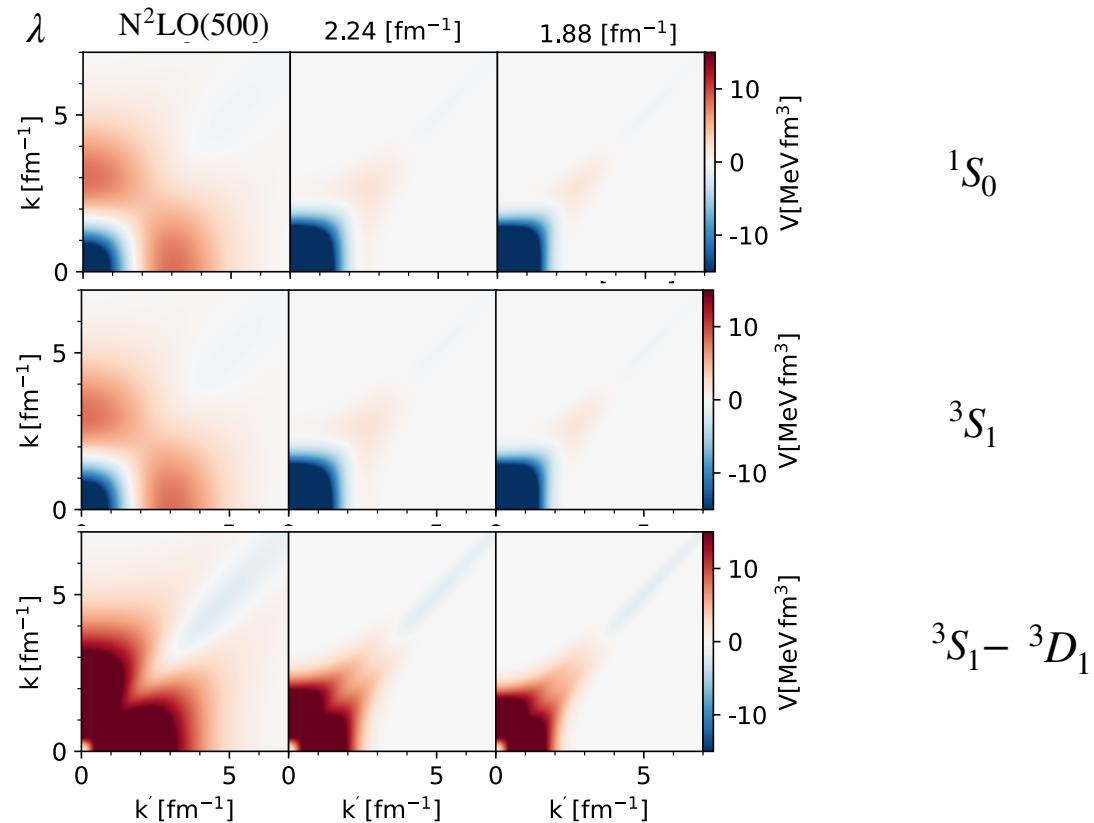
$$P = P_{12}P_{23} + P_{23}P_{13}$$

Eq.(3)

- SRG evolution is only approximately unitary if higher-body forces are omitted 

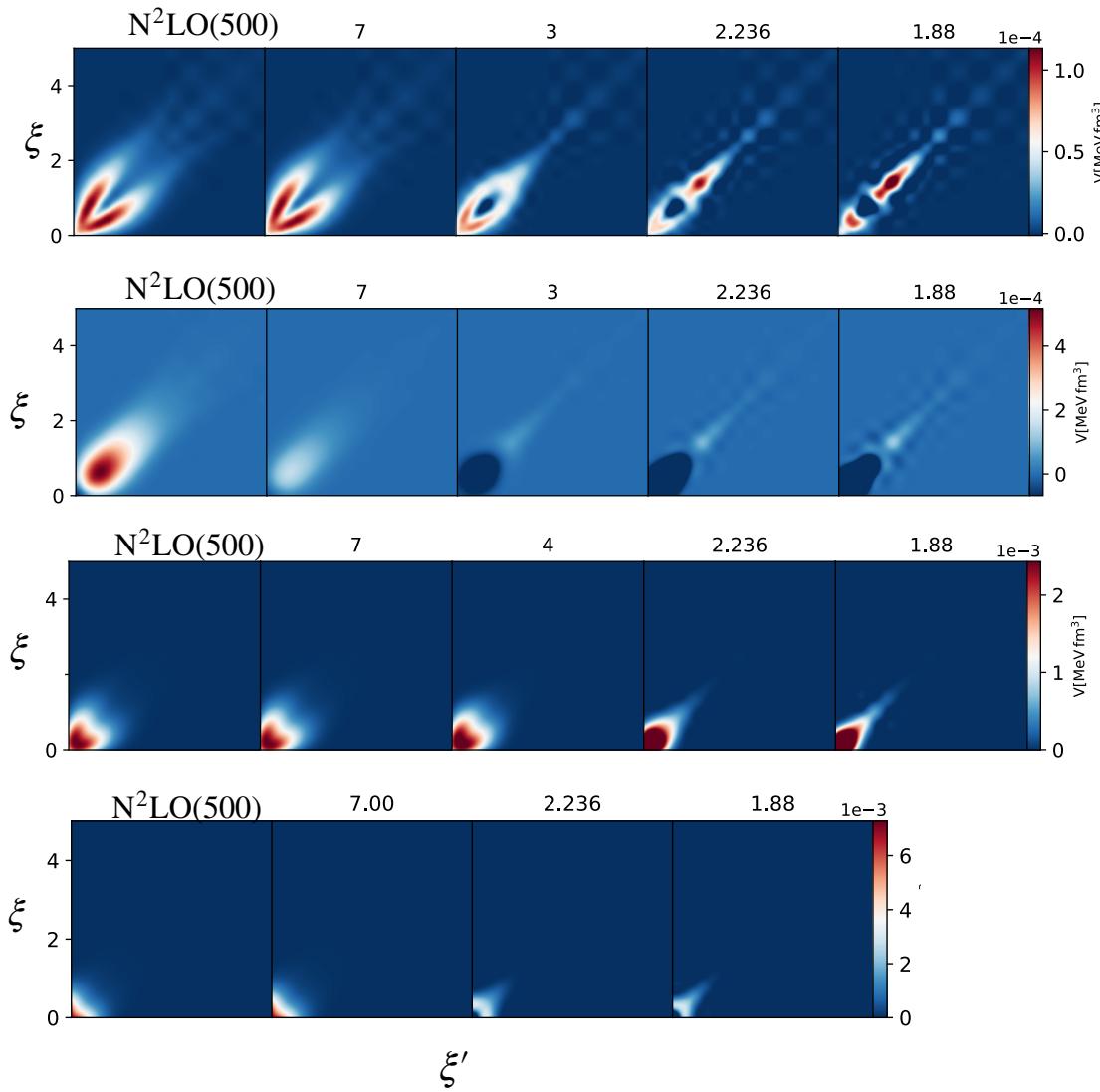
SRG evolution of NN χ N²LO(500)

- $\lambda = (4\mu^2/s)^{1/4}$, $[\lambda] = [p]$: $\lambda \sim$ width of the band-diagonal structure of V_{NN} in p-space
(S.K. Bogner et al. PRC 75 (2007))



SRG evolution of $V_{123}(pq\alpha, p'q'\alpha')$ χ N²LO(500)

- hyperradius $\xi^2 = p^2 + \frac{3}{4}q^2$, $\tan\theta = \frac{2p}{\sqrt{3}q} = \frac{\pi}{12}$, $\alpha = \alpha' = 1 \Rightarrow V_{123} = V_{123}(\xi', \xi)$



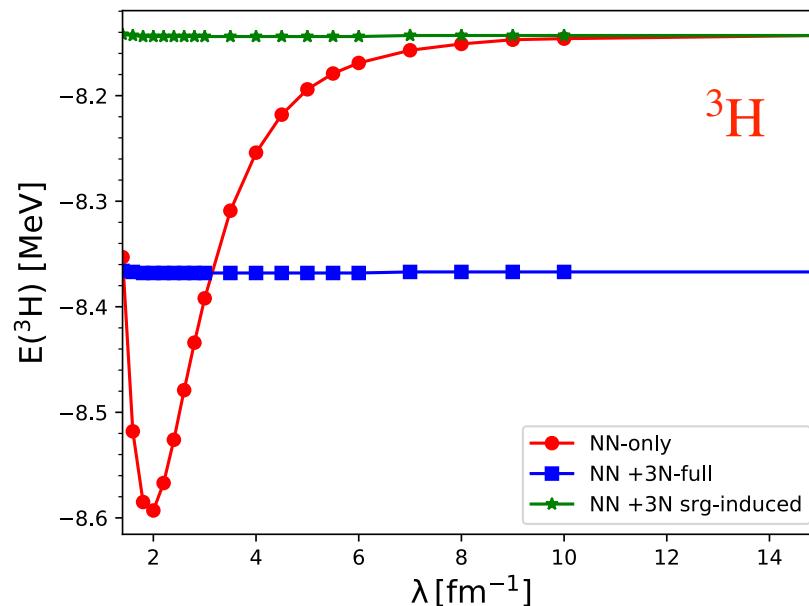
$(J^\pi, T) = (9/2^+, 1)$

$(J^\pi, T) = (7/2^+, 1)$

$(J^\pi, T) = (5/2^+, 1)$

$(J^\pi, T) = (1/2^+, 1)$

E(^3H) with $\chi\text{N}^2\text{LO}(500)$



3N: $\text{N}^2\text{LO}(500)$

$c_D = -1.28, c_E = -0.38$

- SRG is approximately unitary if higher-body forces are omitted
- SRG-induced 3N forces are comparable to the initial (bare) 3N forces

Results for A=3-6

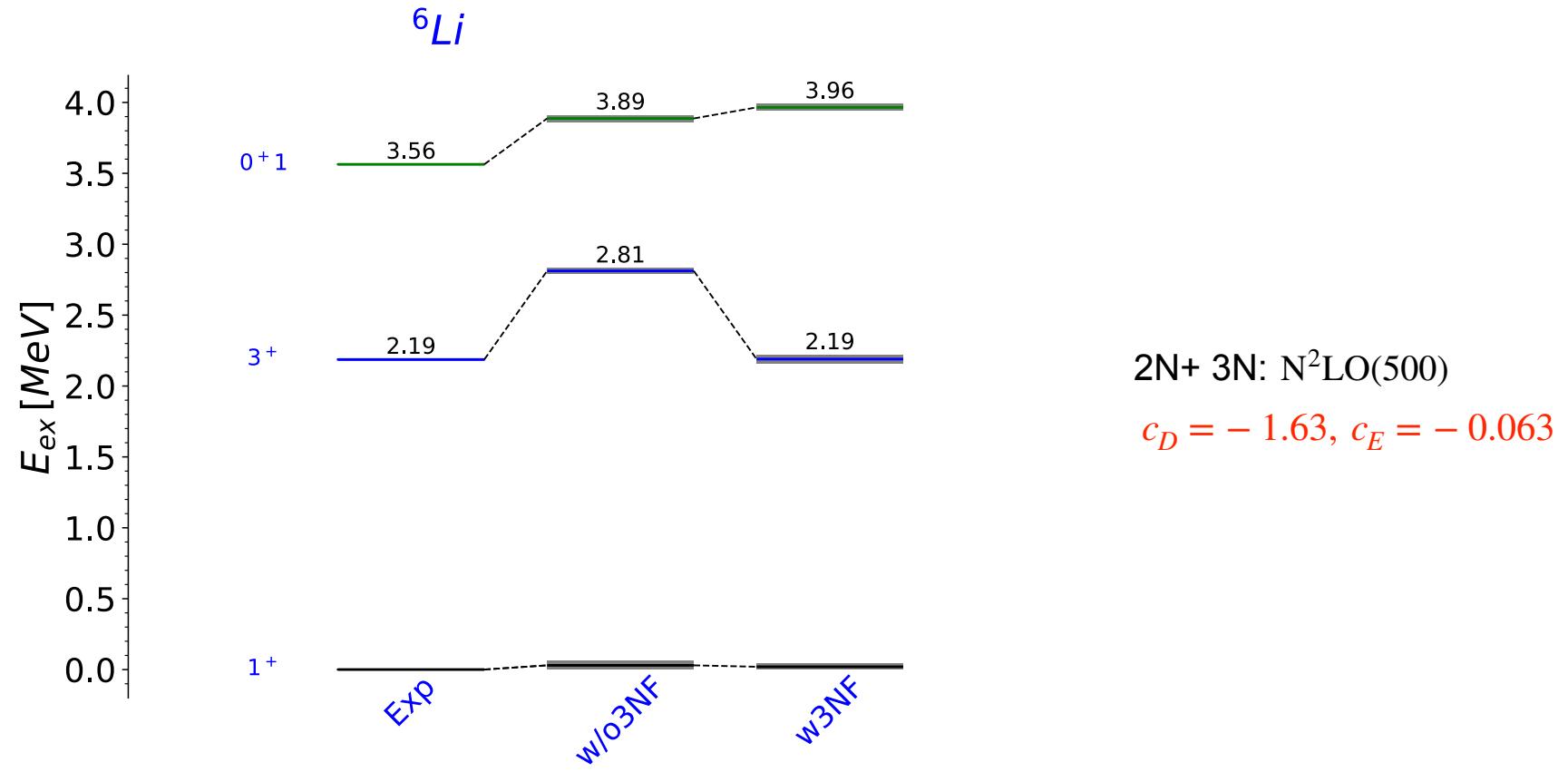
3N: N²LO(500)

$$c_D = -1.63, c_E = -0.063$$

	N ² LO(500) + 3N		N ² LO(500)*	Exp.
	J-NCSM	F-Y		
³ H	-8.477	-8.482	-7.92	-8.482
⁴ He	-28.57	-28.72	-25.85	-28.296
⁶ Li	-32.19		-28.77	-31.99

* P. Maris et. al., PRC 103. 054001

Energy spectrum of ${}^6\text{Li}$



→ $2\text{N} + 3\text{N}$ at N^2LO give a good prediction for $(3^+, 0)$ state.

Summary

- Jacobi NCSM approach:
 - ▶ Construction Jacobi basis state, intermediate bases for $2N + 3N$ forces
 - ▶ Extrapolation of binding and excitation energies
- Similarity Renormalisation Group (SRG):
 - ▶ Construct flow equations for $2N + 3N$ forces
 - ▶ Study SRG evolution of $2N + 3N$ at $N^2LO(500)$
- NCSM results for $A=4-6$ nuclei

Questions?