Momentum-space SRG Evolution of Chiral NN+3N forces

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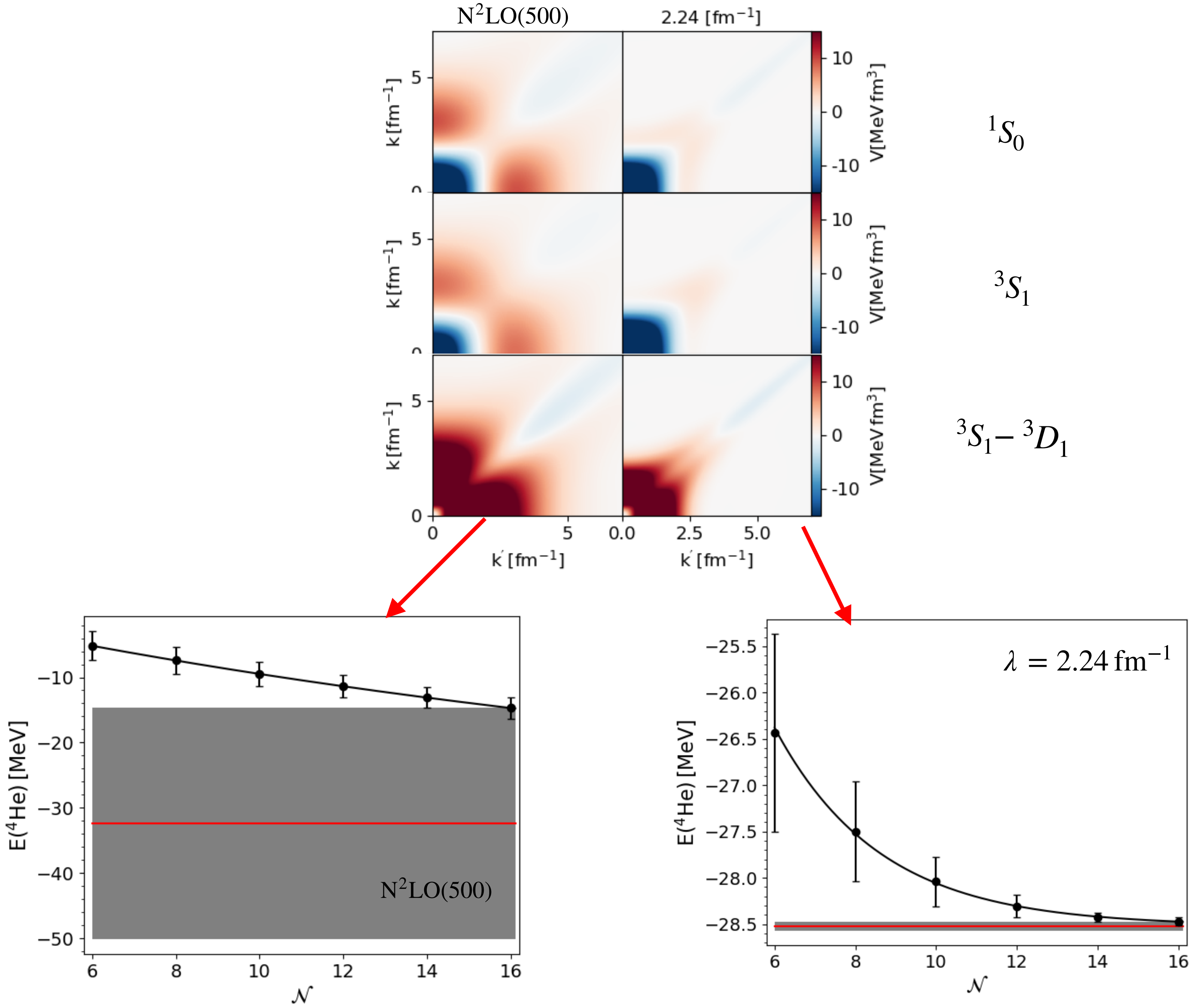
Motivation: convergence of $E(^4\mathrm{He})$ within NCSM



Similarity Renormalization Group (SRG)

Idea: continuously apply **unitary transformation** to the Hamiltonian to decouple **low- and high-momentum states (soften the interactions)**

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

$$\frac{dH(s)}{ds} = [[\underbrace{G}_{G=T_{rel}}, H(s)], H(s)];$$

$$H(s) = T_{rel} + V(s); \quad T_{rel} = T_{12} + t_3 = T_{23} + t_1 = T_{31} + t_2$$

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

$$\frac{dV(s)}{ds} = [[T_{rel}, V(s)], H(s)]$$

→ universal operator equations, independent of any basis

- two different approaches:
  - evolve $H(s)$ in a discrete three-body HO basis (R. Roth, D. Jurgenson) or hyperspherical momentum basis (K.A. Wendt), $V_{3N}(s) = V(s) - V_{NN}(s)$
  - evolve $V(s)$ in a continuous Jacobi-momentum basis (K. Hebeler)

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

$$\frac{dV(s)}{ds} = [[T_{rel}, V(s)], H(s)]$$

→ universal operator equations, independent of any basis

- **explicitly** separate the flow equations for 2N and 3N interactions:

S.K. Bogner et al PRC75 (2007)
K. Hebeler PRC85 (2012)

$$\frac{dV_{12}(s)}{ds} = [[T_{12}, V_{12}], T_{12} + V_{12}]$$

$$\frac{dV_{123}}{ds} = [C_{12}, V_{31} + V_{23} + V_{123}] + [C_{31}, V_{12} + V_{23} + V_{123}] + [C_{23}, V_{12} + V_{31} + V_{123}] + [C_{123}, H_s]$$

$$C_{12} = [T_{12}, V_{12}]; \qquad C_{123} = [T_{rel}, V_{123}]$$

Eq.(1)

→ **2NF spectator delta function** on the RHS of equation for $\frac{dV_{123}}{ds}$ can be integrated out analytically

Projection on Jacobi momentum-basis

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$$\frac{dV_{12}(s)}{ds} = [[T_{12}, V_{12}], T_{12} + V_{12}]$$

$$\frac{dV_{123}}{ds} = [C_{12}, V_{31} + V_{23} + V_{123}] \quad + [C_{31}, V_{12} + V_{23} + V_{123}]$$

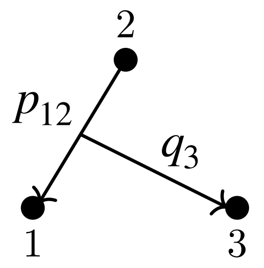
$$+ [C_{23}, V_{12} + V_{31} + V_{123}] \; + \; [C_{123}, H_s]$$

$$C_{12} = [T_{12}, V_{12}]; \qquad C_{123} = [T_{rel}, V_{123}]$$

Eq.(1)

$$|p_{12}\, \alpha_{12}\rangle \equiv |p_{12}, (l_{12}s_{12})J_{12}\, (t_1 t_2)t_{12}\, m_{t12}\rangle; \quad ((-1)^{l_{12}+S_{12}+t_{12}} = -1)$$

$$|p_{12}\, q_3\, \alpha\, J\, T; \alpha_{12}\, I_3 t_3\rangle \equiv |p_{12}\, q_3, ((l_{12}s_{12})J_{12}\; (l_3 s_3)I_3)J\; ((t_1 t_2)T_{12}\, t_3)T\rangle$$



- Evolve antisymmetrized interaction V_{123} **(K. Hebeler PRC85 (2012))**

$$< p_{12}\, q_3 \alpha\, |\, V_{123}\, |\, p_{12}\, q_3 \alpha > \, = \, < pq\alpha\, |\, (1+P) V_{123}^{3} (1+P)\, |\, pq\alpha >$$

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

- Use permutation operators to express V_{23}, V_{31} via V_{12} :

$$V_{23} = P_{12}P_{23}\, V_{12}\, P_{23}P_{12}, \qquad V_{31} = P_{13}P_{23}\, V_{12} P_{23} P_{13}$$

Projection on 2N momentum-basis

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

$$\frac{dV_{12}(s)}{ds} = [[T_{12}, V_{12}], T_{12} + V_{12}]$$

$$\Rightarrow \quad \frac{dV^{12}_{\alpha_{12}\alpha'_{12}}(pp')}{ds} = \sum_{\tilde{\alpha}_{12}} \int_0^\infty dk k^2 \left\{ \frac{p^2}{2\mu^{\alpha_{12}}} + \frac{p'^2}{2\mu^{\alpha'_{12}}} - \frac{k^2}{\mu^{\tilde{\alpha}_{12}}} \right\} V_{12}^{\alpha_{12}\tilde{\alpha}_{12}}(pk) V^{12}_{\tilde{\alpha}_{12}\alpha'_{12}}(kp')$$

$$- \left\{ T^{12}_{\alpha_{12}}(p) \frac{p^2}{2\mu^{\alpha_{12}}} + T^{12}_{\alpha'}(p') \frac{p'^2}{2\mu^{\alpha'_{12}}} - T^{12}_{\alpha_{12}}(p) \frac{p'^2}{2\mu^{\alpha'_{12}}} - T^{12}_{\alpha'_{12}}(p') \frac{p^2}{2\mu^{\alpha_{12}}} \right\} V^{12}_{\alpha_{12}\alpha'_{12}}(pp')$$

- using non-equidistant momentum grid with: $p_n, w_{p_n}\ (n = 1, \cdots \mathrm{N}_{mesh})$

$$\Rightarrow \quad \frac{dV^{12}_{mm'}}{ds} = C^{const}_{mn} V^{12}_{mn} V^{12}_{nm'} + V^{12}_{mn} \bar{C}^{const}_{nm'} V^{12}_{nm'} - \left(T^{12}_m - T^{12}_{m'}\right)^2 V^{12}_{mm'}$$

$$C^{const}_{mn} = p_n^2 w_n (T^{12}_m - T^{12}_n); \qquad \bar{C}^{const}_{nm'} = p_n^2 w_n (T^{12}_{m'} - T^{12}_n)$$

→ element-wise matrix multiplication

Projection on 3N momentum-basis

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

$$\frac{dV_{123}}{ds} = [C_{12}, V_{31} + V_{23} + V_{123}] + [C_{31}, V_{12} + V_{23} + V_{123}] + [C_{23}, V_{12} + V_{31} + V_{123}] + [C_{123}, H_s]$$

$$\Rightarrow \quad 9\,\langle p'q'\alpha'|\frac{dV_{123}}{ds}|pq\alpha\rangle = 6\,\langle p'q'\alpha'|(1+P)C_{12}P_{12}P_{23}V_{12} - V_{12}P_{12}P_{23}C_{12}(1+P)|pq\alpha\rangle$$
$$+3\,\langle p'q'\alpha'|(1+P)C_{12}V_{123} - V_{123}C_{12}(1+P)|pq\alpha\rangle$$
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$$+\langle p'q'\alpha'|(1+P)C_{123}V_{123} - V_{123}C_{123}(1+P)|pq\alpha\rangle$$
$$+\langle p'q'\alpha'|(1+P)C_{123}T_{123} - T_{123}C_{123}(1+P)|pq\alpha\rangle$$
$$= \langle p'q'\alpha'|\frac{dV^{+}_{123}}{ds}|pq\alpha\rangle + \langle p'q'\alpha'|\frac{dV^{-}_{123}}{ds}|pq\alpha\rangle$$
$$= \langle p'q'\alpha'|\frac{dV^{+}_{123}}{ds}|pq\alpha\rangle + TRANSPOSE\left(\langle p'q'\alpha'|\frac{dV^{-}_{123}}{ds}|pq\alpha\rangle\right)$$

- using non-equidistant momentum grid with: $p_n, w_{p_n};\ q_n, w_{q_n}\ \ (n = 1,\cdots \mathrm{N}_{mesh})$

$$\Rightarrow \quad \frac{dV^{+}_{123}}{ds} = M\left(6C_{12}\tilde{M}V_{12} + 3\,C^{const,3N}\,V_{123}\,\bar{V}_{12} + (3\bar{C}_{12} + C^{const,3N}V_{123})V_{123}\right)\bar{M} + 9\,\bar{C}^{const,3N}\,V_{123}$$

$$M_{mn} = \int_{-1}^{1} dx\, 2G_{\alpha\alpha'}(pqx)\, S(\chi pqx)\, S(\pi'(p'q'x)); \qquad \bar{C}^{const,3N}_{mn} = -\,(T^{123}_{m} - T^{123}_{n})^2$$

System of differential equations for 2N & 3N

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$$\frac{dV^{12}_{mm'}}{ds} = C^{const}_{mn}\, V^{12}_{mn}\, V^{12}_{nm'} \;+\; V^{12}_{mn}\, \bar{C}^{const}_{nm'}\, V^{12}_{nm'} \;-\; \left(T^{12}_{m} - T^{12}_{m'}\right)^2 V^{12}_{mm'} \qquad \text{Eq.(3)}$$

→ **linear in V^{12}**
(element-wise matrix multiplication)

$$\frac{dV^{+}_{123,mm'}}{ds} = M_{mn}\left(6C^{12}_{nn'}\tilde{M}_{n'n''}V^{12}_{n''\tilde{n}} + 3\,C^{const,3N}_{nn'}\,V^{123}_{nn'}\,\bar{V}^{12}_{n''} + (3\bar{C}^{12}_{nn'} + C^{const,3N}_{nn'}\,V^{123}_{nn'})\,V^{123}_{n'\tilde{n}}\right)\bar{M}_{\tilde{n}m'}$$

$$- (T^{123}_{m} - T^{123}_{m'})^2\, V^{123}_{mm'} \qquad \text{Eq.(4)}$$

→ **linear in V^{123}**
(element-wise matrix multiplication)

- total number of ODEs $\sim 10^8 - 10^9$ → using distributed memory
- linear terms in Eqs.(3-4) can be computed locally and very fast
- evaluations of non-linear terms are expensive (employ ScaLAPACK subroutines)

→ using ARKode solver from SUNDIALS to solve the system of ODEs for 2N+3N interactions (based on adaptive-step additive Runge Kutta Methods)

ARKode Solver

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$$M\dot{y} = f^E(t,y) + f^I(t,y), \qquad y(t_0) = y_0 \quad (M \equiv I)$$

- $f^E(t,y)$ contains the "nonstiff " time scale components, integrated explicitly
- $f^I(t,y) = \tilde{f}^I(t)\,y$ contains the "stiff" time scale components, integrated implicitly
- using one-step multirate method to update solution at each time step

$$y_n = y_{n-1} + h_n \sum_{i=1}^{s} \left(b_i^E f^E(t_{n,i}^E, z_i), + b_i^I f^I(t_{n,i}^I, z_i) \right)$$

$$z_i = y_{n-1} + h_n \sum_{j=1}^{i-1} \left(A_{i,j}^E f^E(t_{n,j}^E, z_j) + h_n A_{i,j}^I f^I(t_{n,j}^I, z_j) \right) + h_n A_{i,i}^I f^I(t_{n,i}^I, z_i), \qquad i = 1, \cdots, s$$

- stage solutions $z_i, \; i = 1, \cdots, s$ are obtained by solving

$$G(z_i) \equiv z_i - y_{n-1} - h_n \sum_{j=1}^{i-1} \left(A_{i,j}^E f^E(t_{n,j}^E, z_j) + h_n A_{i,j}^I f^I(t_{n,j}^I, z_j) \right) - \underbrace{h_n A_{i,i}^I f^I(t_{n,i}^I, z_i)}_{h_n A_{i,i}^I \tilde{f}^I(t_{n,i}^I)\, z_i} = 0$$

- $N(f^I) = s \times N(f^E)$

Solving the evolution equations

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$$\frac{dV^{12}_{mm'}}{ds} = \underbrace{C^{const}_{mn} V^{12}_{mn} V^{12}_{nm'} + V^{12}_{mn} \bar{C}^{const}_{nm'} V^{12}_{nm'}}_{f^E_1} - \underbrace{\left(T^{12}_{m} - T^{12}_{m'}\right)^2 V^{12}_{mm'}}_{f^I_1} \quad \text{Eq.(3)}$$

$$\frac{dV^{+}_{123,mm'}}{ds} = \underbrace{M_{mn}\left(6C^{12}_{nn'}\tilde{M}_{n'n''}V^{12}_{n''\tilde{n}} + 3\,C^{const,3N}_{nn'} V^{123}_{nn'} \bar{V}^{12}_{n''} + (3\bar{C}^{12}_{nn'} + C^{const,3N}_{nn'} V^{123}_{nn'})\, V^{123}_{n'\tilde{n}}\right)\bar{M}_{\tilde{n}m'}}_{f^E_2} \quad \text{Eq.(4)}$$

$$- \underbrace{(T^{123}_{m} - T^{123}_{m'})^2\, V^{123}_{mm'}}_{f^I_2}; \qquad s = 0 \to \infty$$

- use rather sparse momentum grid: $N^{3N}_{mesh} = 32\,(24),\ (N^{NN}_{mesh} = 150 - 200$ for NN-evolution)

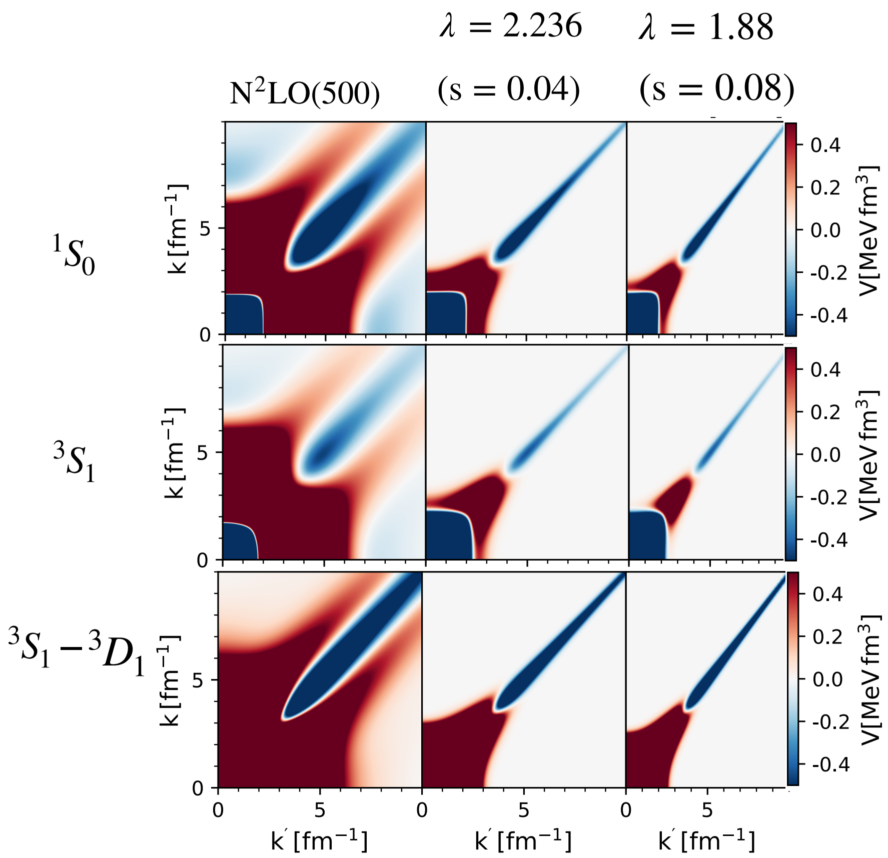
→ **perform evolution of Eqs.(3-4) in two steps:**

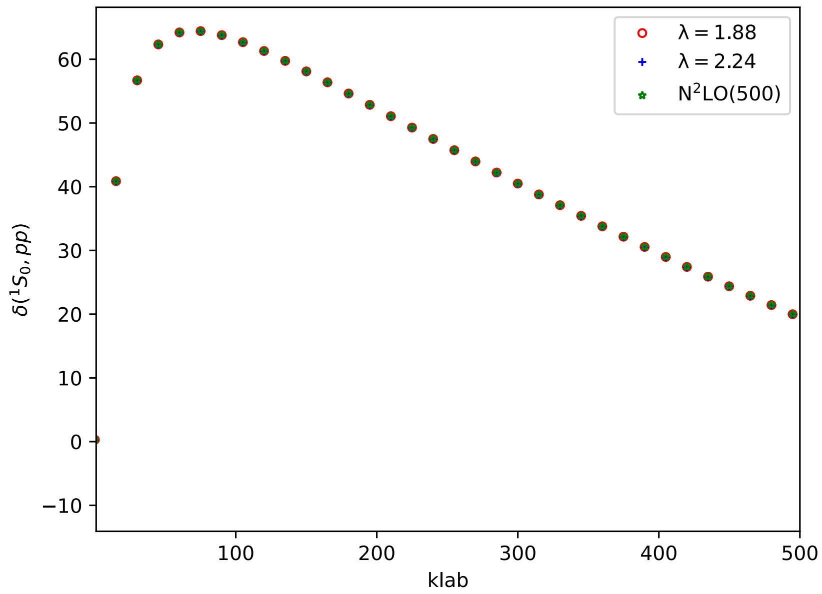
1. evolve Eqs.(3-4) from $s = 0$ to $s_{int} = 0.001\ \mathrm{fm}^4$, save the intermediate result for $V^{123}(s_{int})$
   evolve Eq.(3) in two-body space on much denser momentum grid.
2. read V^{12} (from a denser grid) + V^{123} at $s_{int} = 0.001\ \mathrm{fm}^4$ and evolve further.

SRG evolution of NN $\chi N^2LO(500)$

- use $\lambda = (4\mu^2/s)^{1/4}$ $[\lambda] = [p]$ to characterise the SRG-evolved potentials

  (provide a measure of the width of V in momentum space) **S.K. Bogner et al. PRC (2007))**

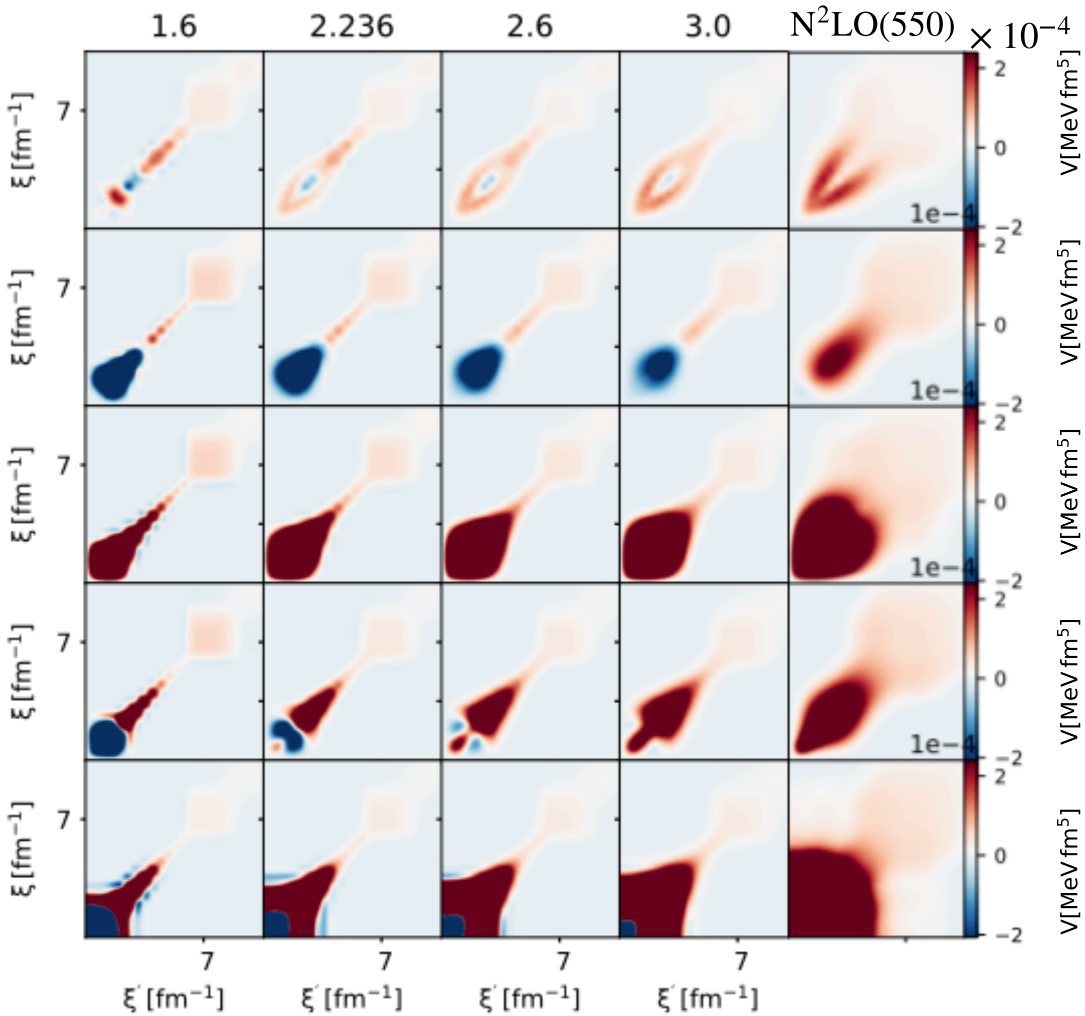




SRG evolution of $V^{NNN}(pq\alpha, p'q'\alpha')$

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

(K. Hebeler PRC85 (2012))



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

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

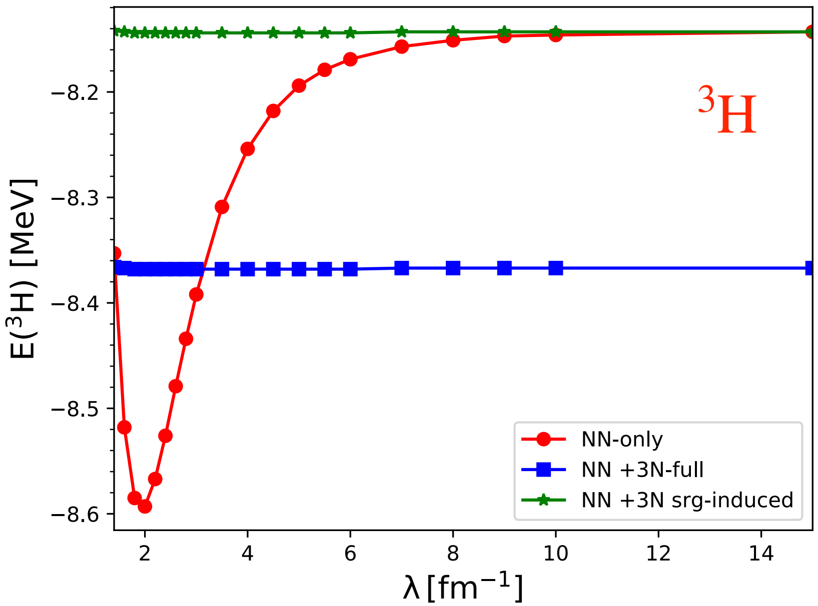
$(J^\pi, T) = (5/2^+, 1/2)$

$(J^\pi, T) = (3/2^+, 1/2)$

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

→ study nucleon-deutron (Nd) scattering phase shifts for bare + SRG-evolved 3N forces (need help from R. Skibinski, H. Witala…)

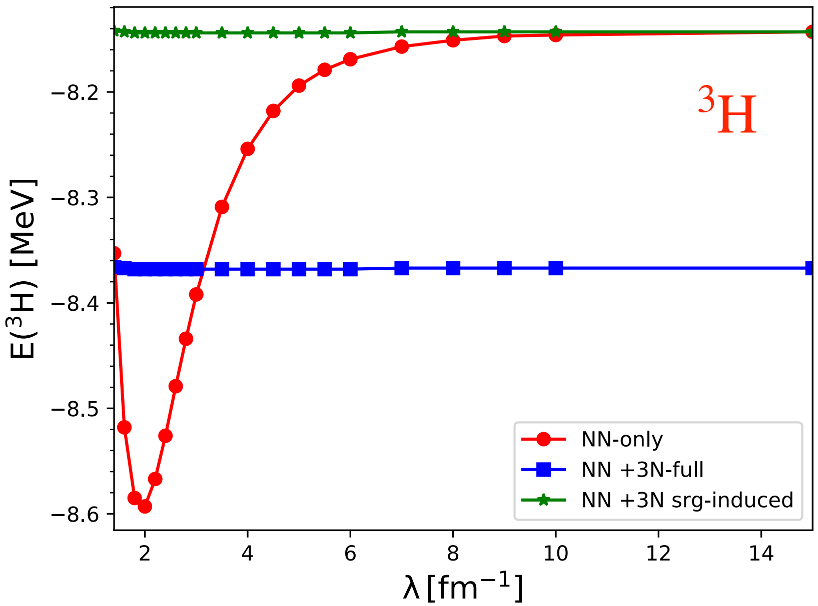
$E(^3H)$ with $N^2LO(500)$



NN: $N^2LO(500)$

3N: $N^2LO(500)$

$E(^3H)$ with $N^2LO(500)$



NN: $N^2LO(500)$

3N: $N^2LO(500)$

Project $V^{3N}(pq\alpha, p'q'\alpha')$ to a HO basis: $|\Gamma_{3N}\rangle = |\mathrm{N}\, J\, T, i\rangle$

- Jacobi HO basis: $|\beta_{3N}\rangle = |\mathrm{N}\, J\, T, n_{12}n_3; ((l_{12}s_{12})J_{12}, (l_3, s_3)I_3)J, (t_{12}t_3)T\rangle \equiv |\mathrm{N}\, J\, T, n_{12}n_3; \alpha\rangle$

$$\langle \beta_{3N} | V^{3N} | \beta'_{3N} \rangle = \int dp dp' p^2 p'^2 \int dq dq' q^2 q'^2 R^{b_{12}}_{n_{12}l_{12}}(p)\, R^{b_3}_{n_3 l_3}(q)\, \langle pq\alpha | V^{3N} | p'q'\alpha' \rangle\, R^{b_{12}}_{n'_{12}l'_{12}}(p')\, R^{b_3}_{n'_3 l'_3}(q')$$

$$\rightarrow \quad \langle \Gamma_{3N} | V^{3N} | \Gamma'_{3N} \rangle = \sum_{\beta_{3N}, \beta'_{3N}} \langle \Gamma_{3N} | \beta_{3N} \rangle \langle \beta_{3N} | V^{3N} | \beta'_{3N} \rangle \underbrace{\langle \beta'_{3N} | \Gamma'_{3N} \rangle}_{\text{cfp}}$$

Results for $A = 3 - 6$ nuclei

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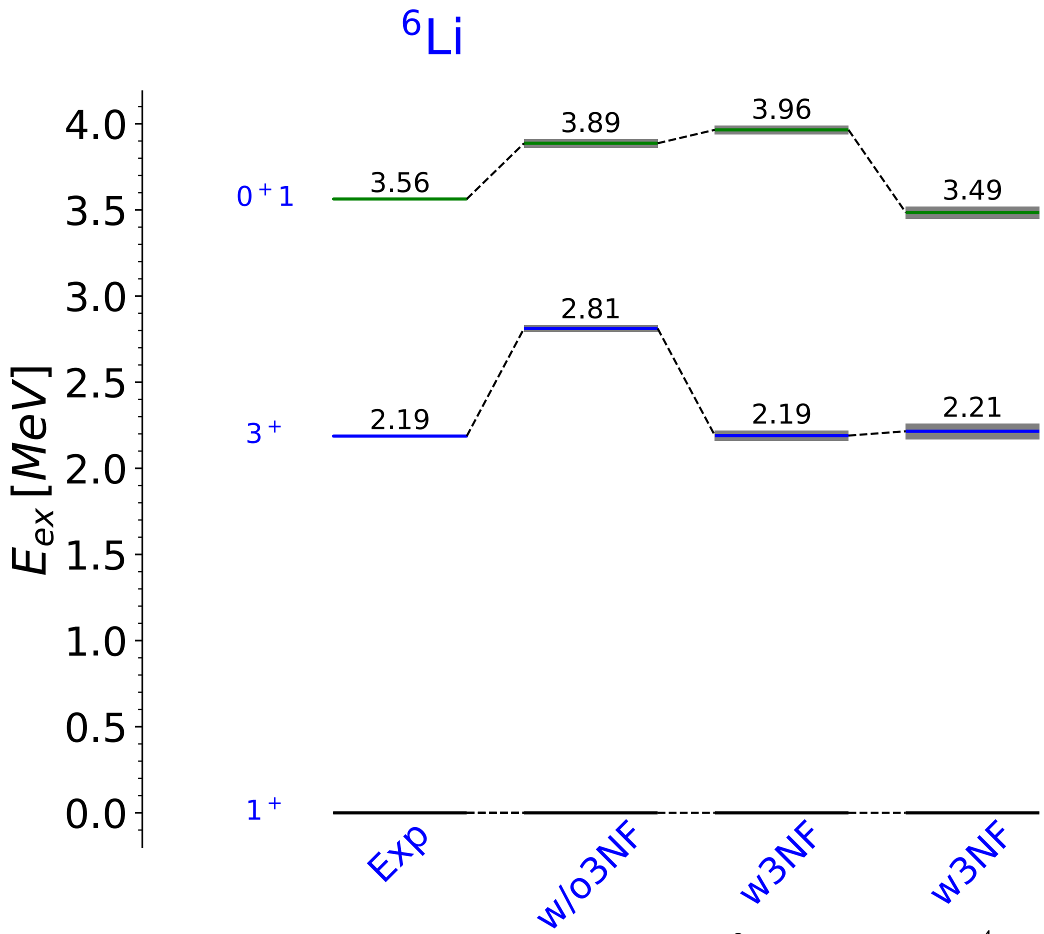
$\mathrm{NN} + 3\mathrm{N}: \ \mathrm{N^2LO(500)}$

	J−NCSM $\lambda = 2.236\,\mathrm{fm}^{-1}$	NCCI* $s = 0.04\,\mathrm{fm}^4$	F−Y*	Exp.
^{3}H	−8.480(3)		−8.482	−8.482
^{4}He	−28.572	−28.585(5)	−28.72	−28.296
	−28.295$^{(1)}$	−28.290(3)$^{(1)}$	−28.31$^{(1)}$	
^{6}Li(1^+,0)	−32.19(1.05)	−32.17(20)		−31.99
^{6}He(0^+,1)	−29.05(1.04)	−29.08(20)		−29.27

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

$^{(1)}$ $\mathrm{NN} + 3\mathrm{N}: \ \mathrm{N^4LO+(450)} + \mathrm{N^2LO(450)}$

Energy spectrum of ^{6}Li



$N^2LO(500)$ $N^4LO+(450)$

Summary

- Evolve NN & 3N interactions in momentum space (use ARKODE solver from SUNDIALS)
    - SRG-evolved 2N & 3N potentials available in both momentum and HO bases
- Good agreement between J-NCSM and NCCI binding energies for A=4-6
- Study Nd scattering phase shifts for SRG-3N forces
- Quantify effect of SRG-induced 4NFs on A=4,6 systems for different combinations of chiral NN & 3N interactions

Thank You!

System of differential equations for 2N & 3N

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$l_{12}^{max} = 6; \; l_3^{max} = 7; \;\; p_{max} = q_{max} = 15\,\text{fm}^{-1}$

J_{3N}	$N_{\alpha_{3N}}$	N_{mesh}	N_{eqs}
$\frac{1}{2}$	42	32	9×10^8
$\frac{3}{2}$	78	28	1.8×10^9
$\frac{5}{2}$	104	24	2.1×10^9
$\frac{7}{2}$	120	24	2.4×10^9