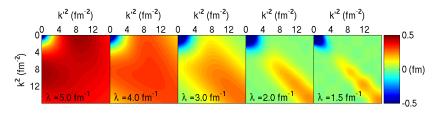
# Similarity RG and Many-Body Operators

**Dick Furnstahl** 

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Collaborators: E. Anderson, S. Bogner, S. Glazek, E. Jurgenson, P. Navratil, R. Perry, L. Platter, A. Schwenk, K. Wendt

### Outline

#### Prelude: Many-body operators from SRG

#### Context: Nuclear physics and three-body forces

Explicit running of three-body (and higher) interactions

**Open questions and issues** 

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## Recap: SRG flow equations [arXiv:0912.3688]

• Transform an initial hamiltonian, H = T + V:

$$H_s = U_s H U_s^\dagger \equiv T + V_s \; ,$$

where *s* is the *flow parameter*. Differentiating wrt *s*:

$$rac{dH_s}{ds} = [\eta_s, H_s] \qquad ext{with} \qquad \eta_s \equiv rac{dU_s}{ds} U_s^\dagger = -\eta_s^\dagger \; .$$

•  $\eta_s$  is specified by the commutator with "generator"  $G_s$ :

$$\eta_{s} = [G_{s}, H_{s}] ,$$

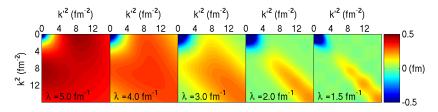
which yields the flow equation (*T* held fixed),

$$\frac{dH_s}{ds} = \frac{dV_s}{ds} = [[G_s, H_s], H_s] \; .$$

•  $G_s$  determines flow  $\implies$  many choices  $(T, H_D, H_{BD} \dots)$ 

## Recap: SRG flow equations [arXiv:0912.3688]

- Implementation issues
  - choosing G<sub>s</sub>
  - choosing a basis
- Features evident from two-body system
  - decoupling of low-energy from high-energy
  - evolves toward universal low-k interactions in free space
  - consistent evolution of operators

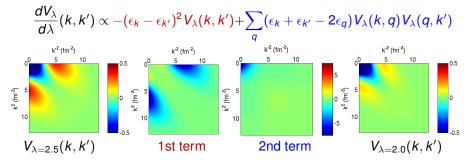


• What about applications to few- or many-body systems?

## Flow in momentum basis with $\eta(s) = [T, H_s]$

• For NN only, project onto relative momentum states  $|k\rangle$ 

$$rac{dV_s}{ds} = [[T_{
m rel}, V_s], H_s]$$
 with  $T_{
m rel} |k\rangle = |\epsilon_k\rangle$  and  $\lambda^2 = 1/\sqrt{s}$ 

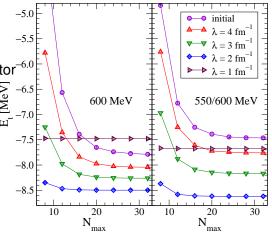


• First term drives  $V_{\lambda}$  toward diagonal:

$$V_{\lambda}(k,k') = V_{\lambda=\infty}(k,k') e^{-\left[\left(\epsilon_k - \epsilon_{k'}\right)/\lambda^2\right]^2} + \cdots$$

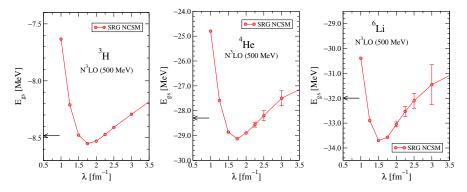
## Variational Calculations in Three-Nucleon Systems

- Triton ground-state energy vs. size of harmonic oscillator<sup>-6.0</sup> basis (N<sub>max</sub>ħω excitations) ₅ -6.5
- Rapid convergence as  $\lambda$  decreases
- Different binding energies
   ⇒ 3-body contribution



# Running of $E_{gs}$ with two-body interaction (NN) only

Not unitary for A ≥ 3 ⇒ ground-state energy depends on λ



- Same qualitative behavior (from NN repulsion/attraction)
- Gives running of net three-body contribution
- Error bars are from extrapolated results (not converged)

# Flow equations lead to many-body forces

• Schematically:

$$\frac{dV_s}{ds} = \left[ \left[ \sum a^{\dagger} a, \sum \underline{a^{\dagger} a^{\dagger} a a}_{2\text{-body}} \right], \sum \underline{a^{\dagger} a^{\dagger} a a}_{2\text{-body}} \right] = \dots + \sum \underline{a^{\dagger} a^{\dagger} a^{\dagger} a a a}_{3\text{-body}!} + \dots$$

so there will be A-body forces generated

- Is this a problem?
  - Normal ordering and truncation at NN may be sufficient [Achim]
  - Ok if "induced" many-body forces are same size as natural ones
- Nuclear 3-body forces already needed in unevolved potential
  - In fact, there are A-body forces initially
  - Natural hierarchy from chiral EFT
    - $\Longrightarrow$  stop flow equations before unnatural 3-body size
  - Many-body methods must deal with them!

• SRG is a tractable method to evolve many-body operators

#### Outline

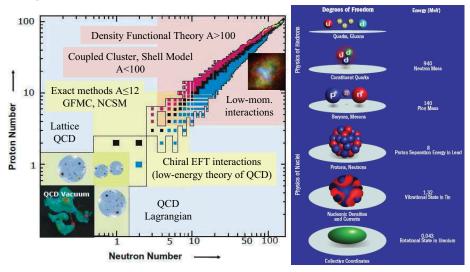
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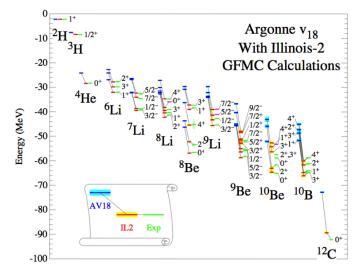
**Open questions and issues** 

### Degrees of Freedom: From QCD to Nuclei



• RG  $\implies$  make nuclear structure look more like quantum chemistry

## Light nuclei: Pieper/Wiringa (Bonner Prize!)



• Three-body forces needed for energies, splittings, ...

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## Atomic 3-body forces: Axilrod-Teller term (1943)

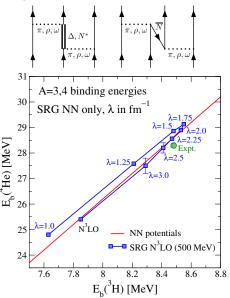
 Three-body potential for atoms/molecules from triple-dipole mutual polarization (3rd-order perturbation correction)

$$V(i,j,k) = \frac{\nu(1+3\cos\theta_i\cos\theta_j\cos\theta_k)}{(r_{ij}r_{ik}r_{jk})^3}$$

- Usually negligible in metals and semiconductors
- Can be important for ground-state energy of solids bound by van der Waals potentials
- Bell and Zuker (1976): 10% of energy in solid xenon

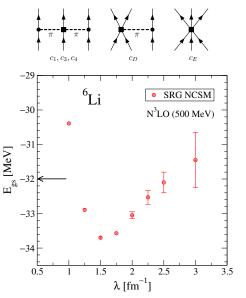
## **Observations on three-body forces**

- Three-body forces arise from eliminating dof's
  - excited states of nucleon
  - relativistic effects
  - high-momentum intermediate states
- Omitting 3-body forces leads to model dependence
  - observables depend on  $\Lambda/\lambda$
  - e.g., Tjon line



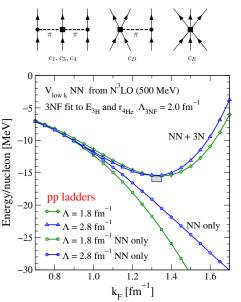
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- NNN at different Λ/λ can be fit to χEFT or evolved
  - how large is 4-body?



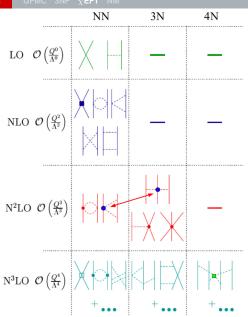
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  - e.g., Tjon line
- NNN at different Λ/λ can be fit to χEFT or evolved
  - how large is 4-body?
  - saturation of nuclear matter
  - cutoff dependence as tool

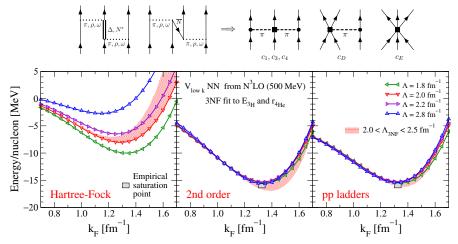


# Chiral EFT hierarchy

- Power counting still unsettled
- But many-body hierarchy consistent with calculations in few-body systems
- 3-body at N<sup>2</sup>LO without  $\Delta$ and NLO with  $\Delta$
- 4-body at N<sup>3</sup>LO



## Nuclear matter with RG-evolved NN plus fit NNN



- At low resolution, nuclear saturation driven by NNN
- Can we validate use of the chiral EFT operator basis?

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### Explicit running of three-body (and higher) interactions

**Open questions and issues** 

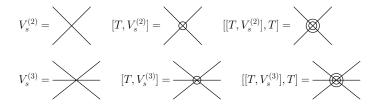
## SRG with normal-ordering in the vacuum

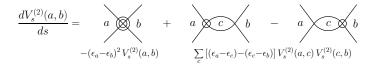
- SRG flow equation  $\frac{dH_s}{ds} = [[G_s, H_s], H_s]$ , e.g.,  $G_s = T_{rel}$ 
  - Right side evaluated w/o solving bound-state or scattering eqs.
  - Can be applied directly in three-particle space
- A-body operators completely fixed in A-particle subspace
- What about spectator nucleons?
  - Decoupling of 3N part in momentum space

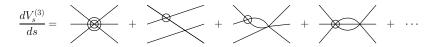
$$\frac{dV_s}{ds} = \frac{dV_{12}}{ds} + \frac{dV_{13}}{ds} + \frac{dV_{23}}{ds} + \frac{dV_{123}}{ds} = [[T_{rel}, V_s], H_s],$$
  
$$\implies \frac{dV_{123}}{ds} = [[T_{12}, V_{12}], (T_3 + V_{13} + V_{23} + V_{123})] + \{123 \rightarrow 132\}$$
$$+ \{123 \rightarrow 231\} + [[T_{rel}, V_{123}], H_s]$$

- No "multi-valued" two-body interactions (dependence on excitation energy of unlinked spectators)
- Or, direct solution in discrete harmonic oscillator basis

## **Diagrams for SRG** $\implies$ **Disconnected cancels**

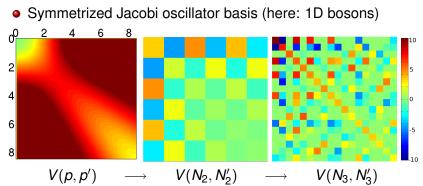






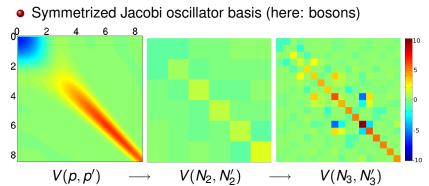
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# **Embedding: Initial potential**



- Diagonalize symmetrizer  $\Rightarrow \langle N_A || N_{A-1}; n_{A-1} \rangle$ ; use recursively
- Embedding is everything, SRG coding is trivial
- 3D: Use Navratil et al. technology for NCSM

# Embedding: SRG evolved potential at $\lambda = 2$



- Diagonalize symmetrizer  $\Rightarrow \langle N_A || N_{A-1}; n_{A-1} \rangle$ ; use recursively
- Embedding is everything, SRG coding is trivial
- 3D: Use Navratil et al. technology for NCSM

## Few-Body Embedding

Legend: Embedding, Evolving, BE calculation, Initial 3NF

• A=3 (2N only):

$$V_{osc}^{(2)} \stackrel{SRG}{\Longrightarrow} V_{\lambda,osc}^{(2)} \stackrel{embed}{\Longrightarrow} V_{\lambda,3Nosc}^{(2)} \stackrel{diag}{\Longrightarrow} BE_3^{(2Nonly)}$$

• A=4 (2N only):

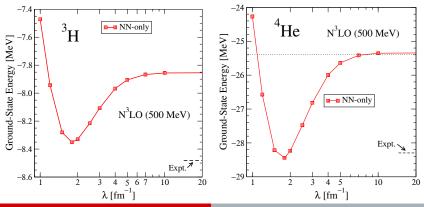
 $V_{osc}^{(2)} \stackrel{SRG}{\Longrightarrow} V_{\lambda,osc}^{(2)} \stackrel{embed}{\Longrightarrow} V_{\lambda,3Nosc}^{(2)} \stackrel{embed}{\Longrightarrow} V_{\lambda,4Nosc}^{(2)} \stackrel{diag}{\Longrightarrow} BE_4^{(2Nonly)}$ 

• A=4 (2N+3N only):

$$V_{osc}^{(2)} \stackrel{embed}{\Longrightarrow} V_{3Nosc}^{(2)} \stackrel{SRG}{\Longrightarrow} V_{\lambda,3Nosc}^{(2+3)} \stackrel{embed}{\Longrightarrow} V_{\lambda,4Nosc}^{(2+3)} \stackrel{diag}{\Longrightarrow} BE_{4}^{(2N+3Nonly)}$$

$$\stackrel{3NF}{\Longrightarrow} + V_{3Nosc}^{(3init)} \dots$$

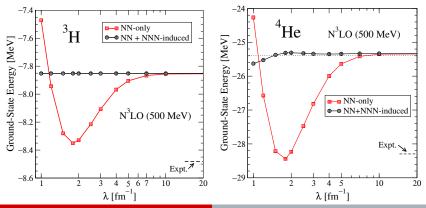
- Evolve in any basis [momentum space in progress by L. Platter]
  - Here: use anti-symmetric Jacobi HO basis from NCSM
  - directly obtain SRG matrix elements in HO basis
  - separate 3-body evolution not needed
- Compare 2-body only to full 2 + 3-body evolution:



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SRG and Many-Body Operators

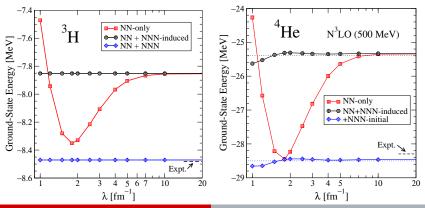
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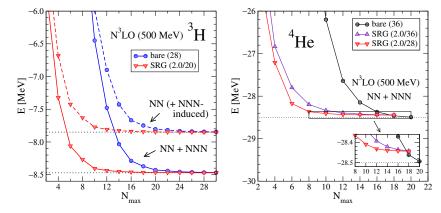
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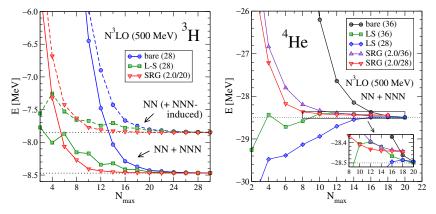
SRG and Many-Body Operators

• Good convergence properties independent of 3-body:



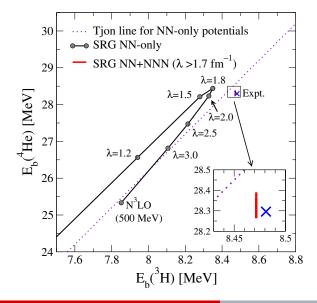
- HO matrix elements (to be) available for NCFC, CC, ...
- Challenge: efficient (on-the-fly) conversion to m-scheme

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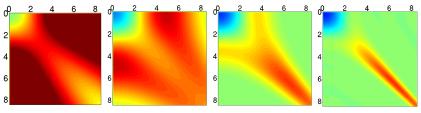
## Tjon line revisited



### **Explore Using a One-Dimensional Model**

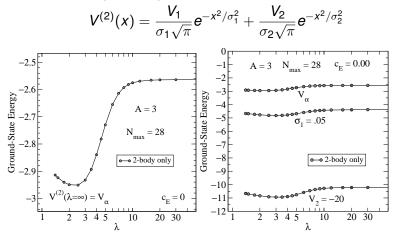
• 1-D model [Negele et al.: Phys.Rev.C 39 1076 (1989)]:

$$V^{(2)}(x) = \frac{V_1}{\sigma_1 \sqrt{\pi}} e^{-x^2/\sigma_1^2} + \frac{V_2}{\sigma_2 \sqrt{\pi}} e^{-x^2/\sigma_2^2}$$

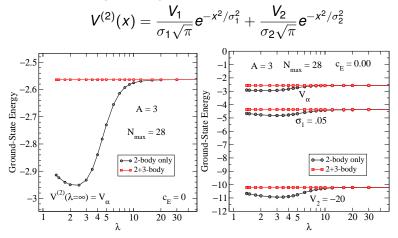


 $\lambda = \infty$   $\lambda = 5$   $\lambda = 3$   $\lambda = 2$ 

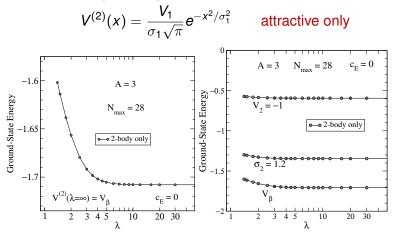
- Same features as in 3D, but much easier!
- See E. Jurgenson, rjf, arXiv:0809.4199 for details



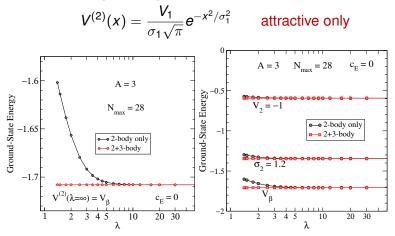
- Basis independent: same evolution in k or HO basis
- Black: Same evolution pattern for 2-body-only as 3D NN-only



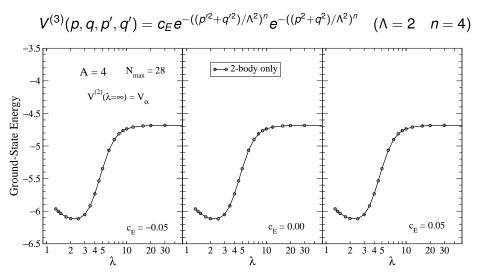
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- Red: Includes induced 3NF Unitary!



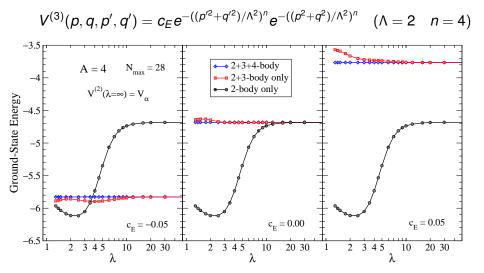
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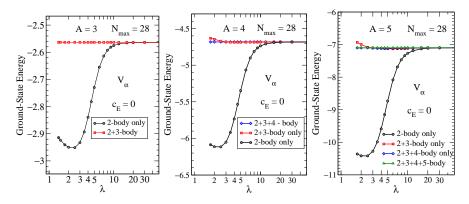
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#### **Induced Many-Body Forces:** *A* = 4



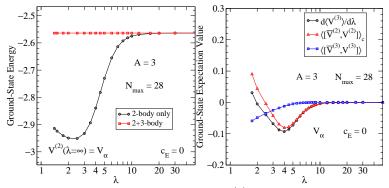
## **Induced Many-Body Forces:** *A* = 5



- Five-body force is negligible
- Hierarchy of induced many-body forces

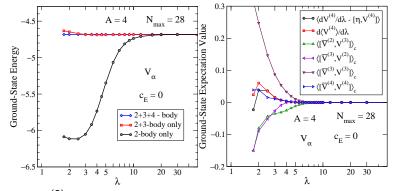
## $V^{(3)}$ analysis

$$\frac{d}{d\lambda}\langle\psi_{\lambda}^{(3)}|V_{\lambda}^{(3)}|\psi_{\lambda}^{(3)}\rangle = \langle\psi_{\lambda}^{(3)}|[\overline{V}_{\lambda}^{(2)},V_{\lambda}^{(2)}]_{\mathcal{C}} - [\overline{V}_{\lambda}^{(3)},V_{\lambda}^{(3)}]|\psi_{\lambda}^{(3)}\rangle$$



- Majority evolution dominated by  $[\overline{V}^{(2)}, V^{(2)}], (\overline{V} \equiv [T, V])$
- Hierarchy of contributions





• No  $[\overline{\mathcal{V}}^{(2)}, \mathcal{V}^{(2)}] \Longrightarrow$  Induced 4-body is small!

• Initial hierarchy of few-body forces is maintained

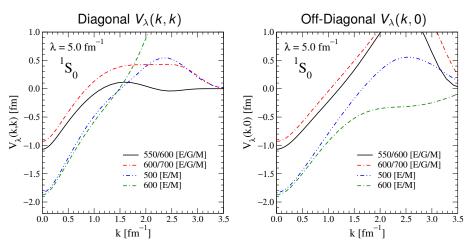
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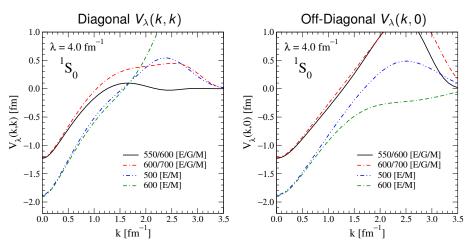
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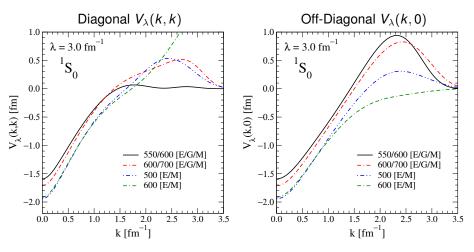
Open questions and issues



Will evolved NNN interactions be universal?

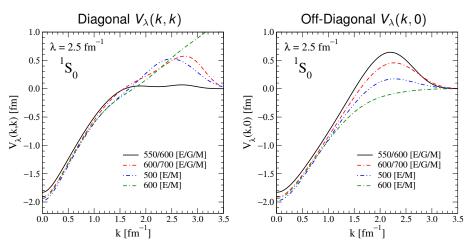


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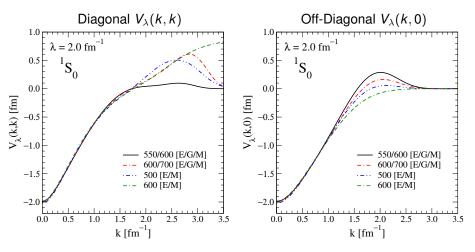
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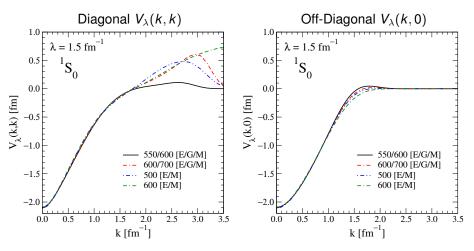


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Will evolved NNN interactions be universal?



Will evolved NNN interactions be universal?

## Every operator flows

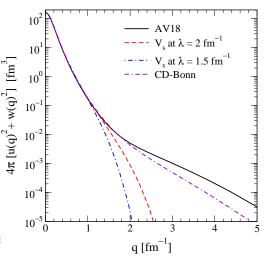
Evolution with s of any operator O is given by:

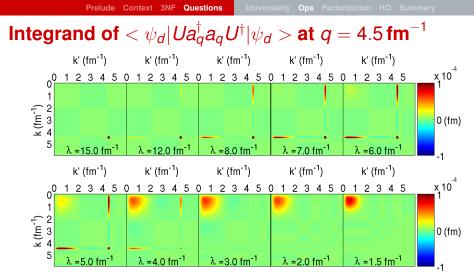
$$O_{s} = U_{s}OU_{s}^{\dagger}$$

so  $O_s$  evolves via

$$\frac{dO_s}{ds} = [[G_s, H_s], O_s]$$

- $U_s = \sum_i |\psi(\mathbf{0})_i\rangle \langle \psi(s)_i|$
- Matrix elements of evolved operators are unchanged
- Consider momentum distribution  $\langle \psi_d | a_q^{\dagger} a_q | \psi_d \rangle$ at  $q = 4.5 \, \text{fm}^{-1}$

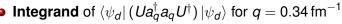


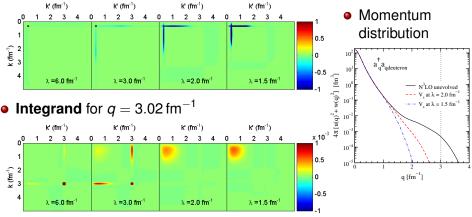


- Flow of deuteron matrix element integrand is toward low k
- Simple variational ansatz works well  $\Longrightarrow$  No fine-tuning
- Factorization:  $U(k,q) \longrightarrow K(k)Q(q)$  for  $k \le \lambda, q \gg \lambda$

Factorization HO Summary

# High and low momentum operators in deuteron

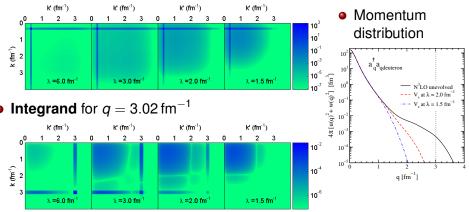




- Decoupling => High momentum components suppressed
- Integrated value does not change, but nature of operator does
- Similar for other operators:  $\langle r^2 \rangle$ ,  $\langle Q_d \rangle$ ,  $\langle 1/r \rangle$

## High and low momentum operators in deuteron

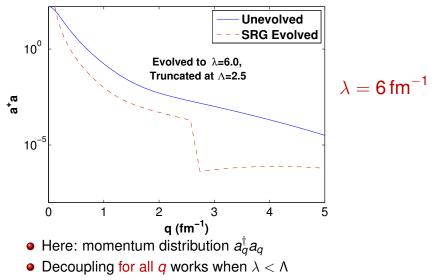
• Integrand of  $raket{\psi_d}(Ua_q^\dagger a_q U^\dagger)\ket{\psi_d}$  for q= 0.34 fm $^{-1}$ 



- Integrated value does not change, but nature of operator does
- Similar for other operators:  $\langle r^2 \rangle$ ,  $\langle Q_d \rangle$ ,  $\langle 1/r \rangle$

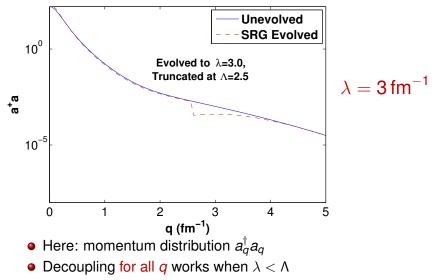
## Decoupling in operator expectation values

• Evolve to  $\lambda$  in full space  $\rightarrow$  **TRUNCATE at**  $\Lambda = 2.5 \text{ fm}^{-1}$ :



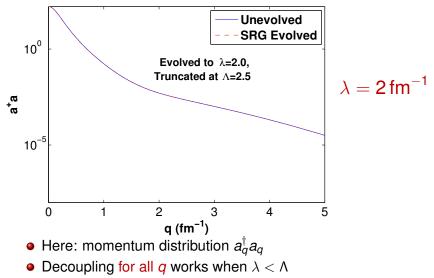
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## Decoupling in operator expectation values

• Evolve to  $\lambda$  in full space  $\rightarrow$  **TRUNCATE at**  $\Lambda = 2.5 \text{ fm}^{-1}$ :



## **Factorization**

- If  $k < \lambda$  and  $q \gg \lambda \Longrightarrow$  factorization:  $U_{\lambda}(k,q) \to K_{\lambda}(k)Q_{\lambda}(q)$ ?
- Operator product expansion for nonrelativistic wf's (Lepage)

$$\Psi_{true}(\mathbf{r}) = \overline{\gamma}(\mathbf{r}) \int d\mathbf{r}' \,\Psi_{eff} \delta_a(\mathbf{r}') + \overline{n}(\mathbf{r}) a^2 \int d\mathbf{r}' \,\Psi_{eff} \nabla^2 \delta_a(\mathbf{r}') + \mathcal{O}(a^4)$$

• Similarly, in momentum space  $\Psi^{\infty}_{\alpha}(q) \approx \gamma^{\lambda}(q) \int_{0}^{\lambda} p^{2} dp \ Z(\lambda) \Psi^{\lambda}_{\alpha}(p) + \eta^{\lambda}(q) \int_{0}^{\lambda} p^{2} dp \ p^{2} \ Z(\lambda) \Psi^{\lambda}_{\alpha}(p) + \cdots$ 

• By projecting potential in momentum subspace, recover OPE via:

$$\begin{split} \gamma^{\lambda}(\boldsymbol{q}) &\equiv -\int_{\lambda}^{\infty} \boldsymbol{q}'^{2} \boldsymbol{d} \boldsymbol{q}' \left\langle \boldsymbol{q} \right| \frac{1}{\widehat{Q}_{\lambda} H^{\infty} \widehat{Q}_{\lambda}} |\boldsymbol{q}' \right\rangle V^{\infty}(\boldsymbol{q}', \boldsymbol{0}) \\ \eta^{\lambda}(\boldsymbol{q}) &\equiv -\int_{\lambda}^{\infty} \boldsymbol{q}'^{2} \boldsymbol{d} \boldsymbol{q}' \left\langle \boldsymbol{q} \right| \frac{1}{\widehat{Q}_{\lambda} H^{\infty} \widehat{Q}_{\lambda}} |\boldsymbol{q}' \right\rangle \frac{\partial^{2}}{\partial p^{2}} V^{\infty}(\boldsymbol{q}', \boldsymbol{p})|_{p^{2} = 0} \end{split}$$

• Construct unitary transformation to get  $U_{\lambda}(k, q) \approx K_{\lambda}(k)Q_{\lambda}(q)$  $U_{\lambda}(k, q) = \sum_{\alpha} \langle k | \psi_{\alpha}^{\lambda} \rangle \langle \psi_{\alpha}^{\infty} | q \rangle \rightarrow \Big[ \sum_{\alpha}^{\alpha_{low}} \langle k | \psi_{\alpha}^{\lambda} \rangle \int_{0}^{\lambda} p^{2} dp \ Z(\lambda) \Psi_{\alpha}^{\lambda}(p) \Big] \gamma^{\lambda}(q) + \cdots$ 

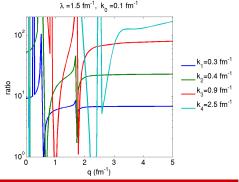
## **Numerical Factorization**

• Test of factorization of *U*:

 $\frac{U_{\lambda}(k_i,q)}{U_{\lambda}(k_0,q)} \rightarrow \frac{K_{\lambda}(k_i)Q_{\lambda}(q)}{K_{\lambda}(k_0)Q_{\lambda}(q)},$ 

so for  $q \gg \lambda \Rightarrow \frac{K_{\lambda}(k_i)}{K_{\lambda}(k_0)}$ .

• Look for plateaus for  $q \gtrsim 2 \text{fm}^{-1}$ 



- Singular value decomposition
  - quantitatively analyze the extent to which *U* factorizes
  - outer product expansion

$$G = \sum_{i}^{r} d_{i} \mathbf{u}_{i} \mathbf{v}_{i}^{t}$$

where r is the rank and the  $d_i$  are decreasing singular values

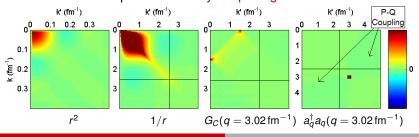
Example: results for λ = 2 fm<sup>-1</sup>, for q > λ and k < λ</li>

	<sup>1</sup> S <sub>0</sub>		
Potential	<b>d</b> <sub>1</sub>	<b>d</b> <sub>2</sub>	<b>d</b> 3
AV18	0.763	0.033	0.007
N3LO 500 MeV	1.423	0.221	0.015
N3LO 550/600 MeV	3.074	0.380	0.061
	<sup>3</sup> S <sub>1</sub> - <sup>3</sup> S <sub>1</sub>		
AV18	0.671	0.015	0.008
N3LO 500 MeV	1.873	0.225	0.044
N3LO 550/600 MeV	4.195	0.587	0.089

Dick Furnstahl SRG and Many-Body Operators

## Practical use of factorization

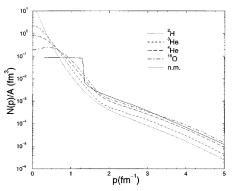
• Decoupling implies  $\langle \psi_{\lambda} | U_{\lambda} \widehat{O} U_{\lambda}^{\dagger} | \psi_{\lambda} \rangle \cong \int_{0}^{\lambda} dk' \int_{0}^{\infty} dq' \int_{0}^{\infty} dq \int_{0}^{\lambda} dk \ \psi_{\lambda}^{\dagger}(k') U_{\lambda}(k',q') \widehat{O}(q',q) U_{\lambda}^{\dagger}(q,k) \psi_{\lambda}(k)$ • Factorization: set  $U_{\lambda}(k,q) \to K_{\lambda}(k) Q_{\lambda}(q)$ , where  $k < \lambda$  and  $q \gg \lambda$   $\Rightarrow \int_{0}^{\lambda} \int_{0}^{\lambda} \psi_{\lambda}^{\dagger}(k') \left[ \int_{0}^{\lambda} \int_{0}^{\lambda} \underbrace{U_{\lambda}(k',q') \widehat{O}(q',q) U_{\lambda}^{\dagger}(q,k) + I_{QOQ} K_{\lambda}(k') K_{\lambda}(k)}{Low Momentum Structure} \right] \psi_{\lambda}(k)$ = Valid when initial operators weakly couple high and low momentum:



Dick Furnstahl SRG and Many-Body Operators

## **Factorization in few-body nuclei:** *n*(*k*) **at large** *k*

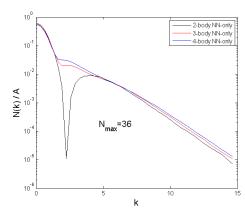
#### AV14 NN with VMC



From Pieper, Wiringa, and Pandharipande (1992).

 Conventional explanation: Dominance of NN potential and short-range correlations (Frankfurt et al.)

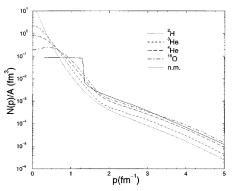
#### A bosons in 1D model



• Alternative: factorization  $\int_{0}^{\lambda} \int_{0}^{\lambda} \psi_{\lambda}^{\dagger}(k') \left[ I_{QOQ} K_{\lambda}(k') K_{\lambda}(k) \right] \psi_{\lambda}(k)$ 

## **Factorization in few-body nuclei:** *n*(*k*) **at large** *k*

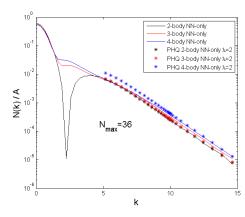
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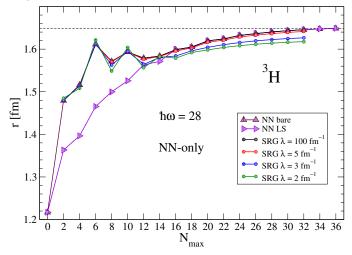
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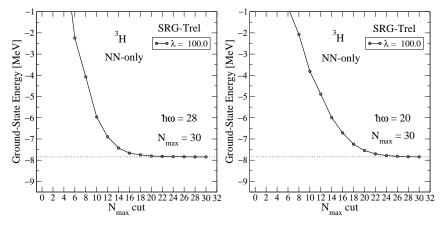


• Alternative: factorization  $\int_{0}^{\lambda} \int_{0}^{\lambda} \psi_{\lambda}^{\dagger}(k') \left[ I_{QOQ} K_{\lambda}(k') K_{\lambda}(k) \right] \psi_{\lambda}(k)$ 

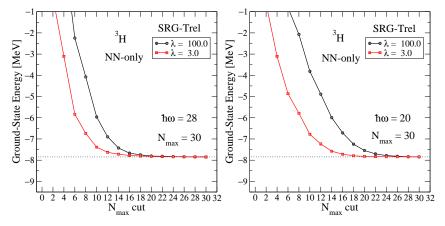
#### Long-distance observables: radius



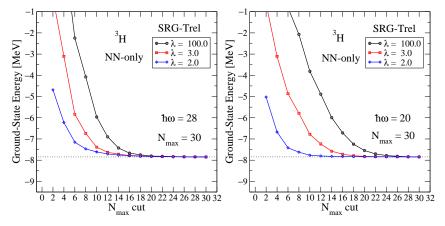
- Unevolved operator
- Harmonic oscillator basis is problematic!



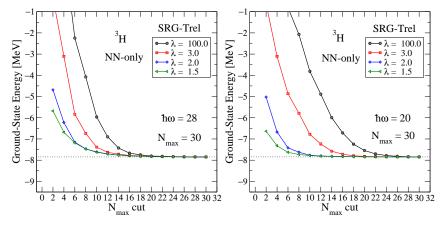
- $\hbar\omega = 28$  is optimal for the bare interaction
- $\hbar \omega = 20$  is optimal for  $\lambda = 2$  evolution
- No improvement in convergence for small  $\lambda$



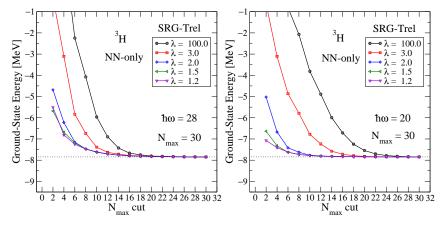
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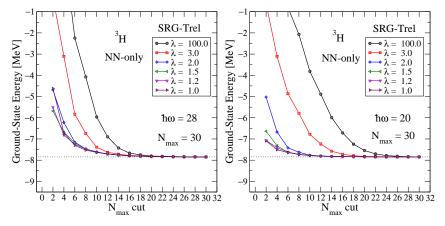
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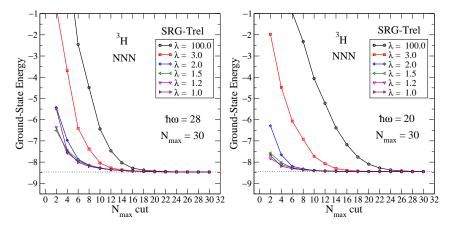


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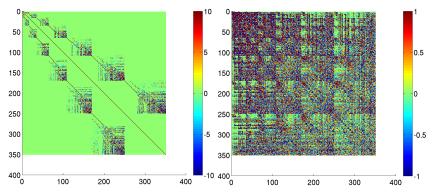
## Evolving NN + NNN in NCSM A=3 space



- Same plots but now including an initial 3NF from N2LO
- No improvement in convergence for small  $\lambda$

## Using other SRG Generators

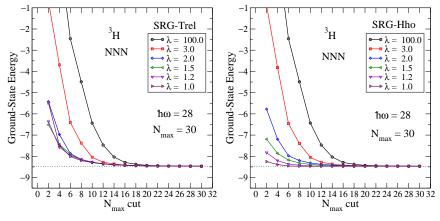
• 1D matrices  $T_{\rm rel}$  and V in NCSM basis:



- In this basis *T<sub>rel</sub>* will not drive *H* to diagonal form
- But harmonic oscillator Hamiltonian will!
  - $H_{\rm ho} = T_{\rm rel} + V_{\rm ho}$  is diagonal in this basis

# Evolving with $H_{\rm ho}$ in HO Basis

• Using  $G = H_{ho}$  improves convergence dramatically



- Compare  $T_{rel}$  on the left with  $H_{ho}$  on the right
- But: 1D study indicates spurious bound states contaminate evolution with *H*<sub>ho</sub> with many-body truncation

## Summary of open questions and issues

- Power counting for evolved many-body interactions
- Do many-body interactions flow to universal form?
- Operator issues
  - Scaling of many-body operators
  - Factorization for few-body systems
- Can choices for G<sub>s</sub> ...
  - reduce the many-body forces?
  - improve convergence in HO basis?