

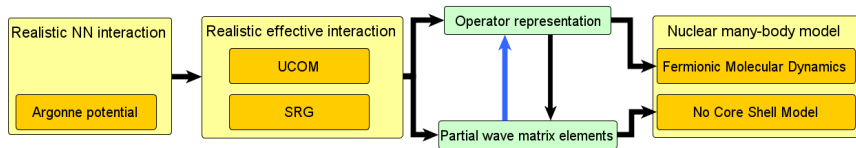
Operator representation for realistic effective interactions

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19.01.2012

Nuclear *ab-initio* calculations



Outline

- 1 Nuclear *ab-initio* calculations
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 - Unitary Correlation Operator Method
 - Similarity Renormalization Group
 - Fermionic Molecular Dynamics
- 2 Operator representation from partial wave matrix elements
- 3 Results
 - UCOM with reduced set of operators
 - SRG operator representation
- 4 Summary and conclusions

Argonne potential

Wiringa, Stoks, Schiavilla; Phys.Rev.C 51 1995



▶ Operator representation

$$\begin{aligned}
 \tilde{V}_{Argonne} = & \sum_{S,T} V_{ST}^Z(\tilde{r}) \tilde{\Pi}_{ST} \\
 & + \sum_{S,T} V_{ST}^{L^2}(\tilde{r}) \tilde{L}^2 \tilde{\Pi}_{ST} \\
 & + \sum_T V_{1T}^{LS}(\tilde{r}) \tilde{L} \tilde{S} \tilde{\Pi}_{1T} \\
 & + \sum_T V_{1T}^T(\tilde{r}) \tilde{S}_{12} \tilde{\Pi}_{1T} \\
 & + \sum_T V_{1T}^{TLL}(\tilde{r}) s_{12}(\tilde{L}, \tilde{L}) \tilde{\Pi}_{1T}
 \end{aligned}$$

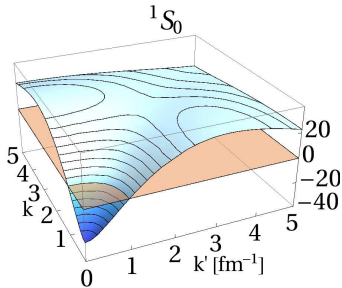
with

$$\tilde{S}_{12} = \frac{3}{\tilde{r}^2} (\tilde{r} \cdot \tilde{\sigma}_1) (\tilde{r} \cdot \tilde{\sigma}_2) - \tilde{\sigma}_1 \tilde{\sigma}_2$$

$$s_{12}(\vec{a}, \vec{b}) = \frac{3}{2} (\vec{\sigma}_1 \cdot \vec{a}) (\vec{\sigma}_2 \cdot \vec{b}) - \frac{1}{2} (\vec{\sigma}_1 \cdot \vec{\sigma}_2) \vec{a} \cdot \vec{b} + \vec{a} \leftrightarrow \vec{b}$$

▶ partial wave matrix elements

$$\langle k(LS)JM; TM_T | \tilde{V}_{Argonne} | k'(L'S)JM; TM_T \rangle$$



ME's in MeVfm³

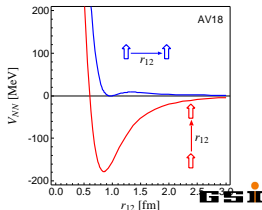
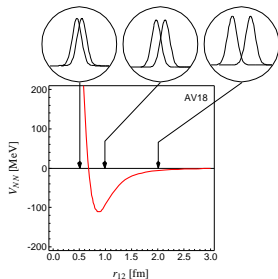
Unitary Correlation Operator Method

- ▶ nuclear interaction induces strong short-range correlations which cannot be described by “simple” many-body states $|\psi\rangle$
- ▶ “Unitary Correlation Operator Method” (UCOM):
Feldmeier, Neff, Roth, Schnack; Nucl.Phys. A632 1998
Roth, Neff, Feldmeier; Prog.Part.Nucl.Phys. 65 2010
 - ▶ imprint correlations onto uncorrelated states by unitary operator ζ :

$$|\hat{\psi}\rangle = \zeta|\psi\rangle$$

- ▶ correlated operator: $\hat{\mathcal{O}} = \zeta^\dagger \mathcal{O} \zeta$:

$$\langle \hat{\psi} | \hat{\mathcal{O}} | \hat{\psi}' \rangle = \langle \psi | \zeta^\dagger \mathcal{O} \zeta | \psi' \rangle = \langle \psi | \hat{\mathcal{O}} | \psi' \rangle$$



UCOM potential

Operator representation

operator representation:

$$\begin{aligned} \tilde{V}_{UCOM} = \tilde{C}^\dagger H \tilde{C} - \tilde{T} &= \sum_{S,T} V_{ST}^Z(\tilde{r}) \tilde{\Pi}_{ST} + \sum_{S,T} V_{ST}^{L2}(\tilde{r}) \tilde{L}^2 \tilde{\Pi}_{ST} \\ &+ \sum_{S,T} \frac{1}{2} (\tilde{p}^2 V_{ST}^{p2}(\tilde{r}) + V_{ST}^{p2}(\tilde{r}) \tilde{p}^2) \tilde{\Pi}_{ST} \\ &+ \sum_T V_{1T}^{LS}(\tilde{r}) \tilde{L} \tilde{S} \tilde{\Pi}_{1T} + \sum_T V_{1T}^{L2LS}(\tilde{r}) \tilde{L}^2 \tilde{L} \tilde{S} \tilde{\Pi}_{1T} \\ &+ \sum_T V_{1T}^T(\tilde{r}) \tilde{S}_{12} \tilde{\Pi}_{1T} + \sum_T V_{1T}^{TLL}(\tilde{r}) s_{12}(\tilde{L}, \tilde{L}) \tilde{\Pi}_{1T} \\ &+ \sum_T V_{1T}^{Tpp}(\tilde{r}) \tilde{s}_{12}(\tilde{p}_\Omega, \tilde{p}_\Omega) \tilde{\Pi}_{1T} \\ &+ \sum_T (\tilde{p}_r V_{1T}^{Trp}(\tilde{r}) + V_{1T}^{Trp}(\tilde{r}) \tilde{p}_r) s_{12}(\tilde{r}, \tilde{p}_\Omega) \tilde{\Pi}_{1T} \\ &+ \sum_T V_{1T}^{L2Tpp}(\tilde{r}) [\tilde{L}^2 \tilde{s}_{12}(\tilde{p}_\Omega, \tilde{p}_\Omega) + \tilde{s}_{12}(\tilde{p}_\Omega, \tilde{p}_\Omega) \tilde{L}^2] \tilde{\Pi}_{1T} \\ &+ \dots \end{aligned}$$

► more complicated, nonlocal structure

Similarity Renormalization Group

- ▶ decoupling of low and high momentum matrix elements by evolving potential to band-diagonal structure
- ▶ Similarity Renormalization Group (SRG)

Bogner, Furnstahl, Perry; Phys.Rev.C 75 2007

starting from initial Hamiltonian $\tilde{H}_0 = \tilde{T} + \tilde{V}_0$

flow equation:

$$\frac{d\tilde{H}_s}{ds} = [\tilde{\eta}_s, \tilde{H}_s]$$

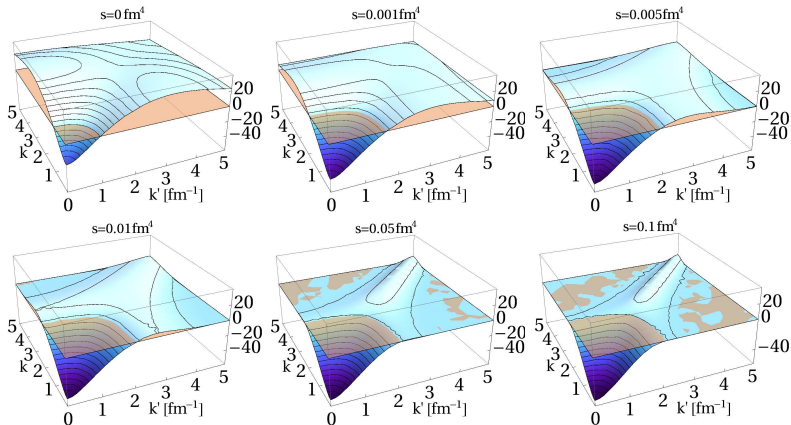
with flow parameter s and generator $\tilde{\eta}_s = [\tilde{T}, \tilde{H}_s] = [\tilde{T}, \tilde{V}_s]$

- ▶ evolution towards $[\tilde{T}, \tilde{H}_s] = 0$: $\tilde{H}_s \rightarrow$ band-diagonal

Similarity Renormalization Group

SRG flow

▶ SRG evolution



▶ partial wave matrix elements, **no operator representation**

Fermionic Molecular Dynamics (FMD)

Feldmeier, Nucl.Phys. A515 1990



- ▶ microscopic model to describe nuclei and nuclear reactions
- ▶ model states: antisymmetrized gaussian wave packets:

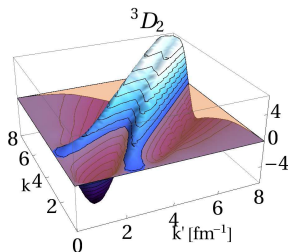
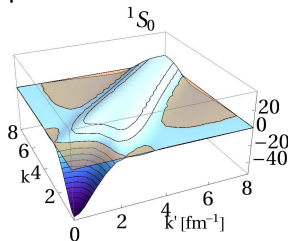
$$|Q\rangle = \mathcal{A}(|q_1\rangle \otimes \cdots \otimes |q_A\rangle)$$
$$\langle \vec{r} | q \rangle = \sum_i c_i \exp\left\{-\frac{(\vec{r} - \vec{b}_i)^2}{2a_i}\right\} \otimes |\chi_i^\uparrow, \chi_i^\downarrow\rangle \otimes |\xi\rangle$$

- ▶ complex parameters \vec{b}_i encode mean position and momentum
- ▶ width parameter a_i
- ▶ description of exotic phenomena like halos, cluster-states, ...
- ▶ interaction matrix elements in FMD basis calculated analytically: **operator representation needed!**

From partial wave matrix elements to operator representation



partial wave matrix elements



Fit
←
 $\gamma_{ST,j}^i$

operator representation

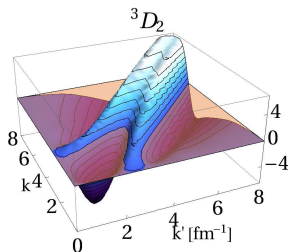
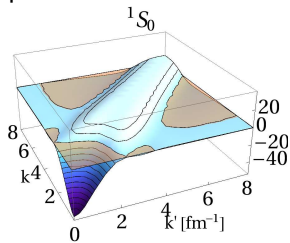
- ▶ choose appropriate set of operators

$$\underline{V}_{\text{ansatz}} = \sum_{ST,i} v_{ST}^i(\underline{r}, \underline{p}) \underline{Q}_i \underline{\Pi}_{ST}$$

From partial wave matrix elements to operator representation



partial wave matrix elements



Fit
←
 $\gamma_{ST,j}^i$

operator representation

- ▶ choose appropriate set of operators

$$\underline{V}_{ansatz} = \sum_{ST,i} \mathcal{V}_{ST}^i(\underline{r}, \underline{p}) \mathcal{O}_i \Pi_{ST}$$

- ▶ representation of (unknown!) radial functions by a sum of gaussians:

$$\mathcal{V}_{ST}^i(\underline{r}) = \sum_k \gamma_{ST,k}^i \cdot e^{-\frac{\tilde{r}^2}{2\kappa_k}}$$

$$\mathcal{V}_{ST}^i(\underline{r}, \underline{p}) =$$

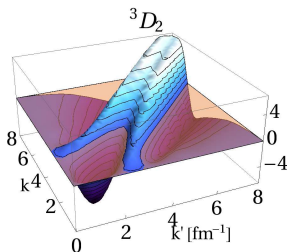
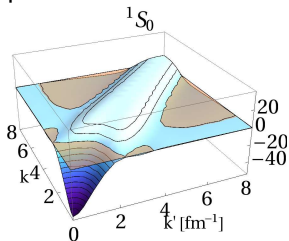
$$\sum_{k,l} \gamma_{ST,kl}^i \cdot e^{-\frac{\lambda_l}{4} \tilde{p}^2} e^{\frac{-\tilde{r}^2}{2(\kappa_k - \lambda_l/4)}} e^{-\frac{\lambda_l}{4} \tilde{p}^2}$$

- ▶ choose parameters κ_j and λ_l on a grid

From partial wave matrix elements to operator representation



partial wave matrix elements



Fit
←
 $\gamma_{ST,j}^i$

operator representation

- ▶ choose appropriate set of operators

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$$\sum_{k,l} \gamma_{ST,kl}^i \cdot e^{-\frac{\lambda_l}{4} \tilde{p}^2} e^{\frac{-\tilde{r}^2}{2(\kappa_k - \lambda_l/4)}} e^{-\frac{\lambda_l}{4} \tilde{p}^2}$$

- ▶ choose parameters κ_j and λ_l on a grid
- ▶ calculate **analytically** matrix elements
 $\langle k(LS)JT | \underline{V}_{ansatz} | k'(L'S)JT \rangle$

UCOM - with a reduced set of operators



$$\begin{aligned}
 \tilde{V}_{UCOM} &= \sum_{S,T} V_{ST}^Z(\underline{r}) \tilde{\Pi}_{ST} \\
 &+ \sum_{S,T} V_{ST}^{L2}(\underline{r}) \tilde{L}^2 \tilde{\Pi}_{ST} \\
 &+ \sum_{S,T} \frac{1}{2} (\tilde{\rho}^2 V_{ST}^{\rho^2}(\underline{r}) + V_{ST}^{\rho^2}(\underline{r}) \tilde{\rho}^2) \tilde{\Pi}_{ST} \\
 &+ \sum_T V_{1T}^{LS}(\underline{r}) \tilde{L} \tilde{S} \tilde{\Pi}_{1T} \\
 &+ \sum_T V_{1T}^{L2LS}(\underline{r}) \tilde{L}^2 \tilde{L} \tilde{S} \tilde{\Pi}_{1T} \\
 &+ \sum_T V_{1T}^T(\underline{r}) \tilde{S}_{12} \tilde{\Pi}_{1T} \\
 &+ \sum_T V_{1T}^{TLL}(\underline{r}) \tilde{S}_{12}(\vec{L}, \vec{L}) \tilde{\Pi}_{1T} \\
 &+ \sum_T V_{1T}^{TPP}(\underline{r}) \tilde{S}_{12}(\rho_\Omega, \rho_\Omega) \tilde{\Pi}_{1T} \\
 &+ \sum_T (\rho_r V_{1T}^{Trp}(\underline{r}) + V_{1T}^{Trp}(\underline{r}) \rho_r) \tilde{S}_{12}(r, \rho_\Omega) \tilde{\Pi}_{1T} \\
 &+ \sum_T V_{1T}^{L2TPP}(\underline{r}) \tilde{L}^2 \tilde{S}_{12}(\rho_\Omega, \rho_\Omega) + \tilde{S}_{12}(\rho_\Omega, \rho_\Omega) \tilde{L}^2 \tilde{\Pi}_{1T} \\
 &+ \dots
 \end{aligned}
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UCOM - with a reduced set of operators



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 \end{aligned}$$

UCOM - with a reduced set of operators



$$\begin{aligned}
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Fit



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$$\begin{aligned}
 \tilde{V}_{ansatz} = & \sum_{S,T} V_{ST}^Z(\underline{r}) \tilde{\Pi}_{ST} \\
 & + \sum_{S,T} V_{ST}^{L2}(\underline{r}) \tilde{L}^2 \tilde{\Pi}_{ST} \\
 & + \sum_{S,T} \frac{1}{2} (\tilde{\rho}^2 V_{ST}^{\rho^2}(\underline{r}) + V_{ST}^{\rho^2}(\underline{r}) \tilde{\rho}^2) \tilde{\Pi}_{ST} \\
 & + \sum_T V_{1T}^{LS}(\underline{r}) \tilde{L} \tilde{S} \tilde{\Pi}_{1T} \\
 & + \sum_T V_{1T}^{L2LS}(\underline{r}) \tilde{L}^2 \tilde{L} \tilde{S} \tilde{\Pi}_{1T} \\
 & + \sum_T V_{1T}^T(\underline{r}) \tilde{S}_{12} \tilde{\Pi}_{1T} \\
 & + \sum_T V_{1T}^{TLL}(\underline{r}) \tilde{S}_{12}(\tilde{L}, \tilde{L}) \tilde{\Pi}_{1T} \\
 & + \sum_T V_{1T}^{TPP}(\underline{r}) \tilde{S}_{12}(\rho_\Omega, \rho_\Omega) \tilde{\Pi}_{1T} \\
 & + \sum_T (\rho_r V_{1T}^{Trp}(\underline{r}) + V_{1T}^{Trp}(\underline{r}) \rho_r) \tilde{S}_{12}(r, \rho_\Omega) \tilde{\Pi}_{1T} \\
 & + \sum_T V_{1T}^{L2TPP}(\underline{r}) \tilde{L}^2 \tilde{S}_{12}(\rho_\Omega, \rho_\Omega) + \tilde{S}_{12}(\rho_\Omega, \rho_\Omega) \tilde{L}^2 \tilde{\Pi}_{1T} \\
 & + \dots
 \end{aligned}$$

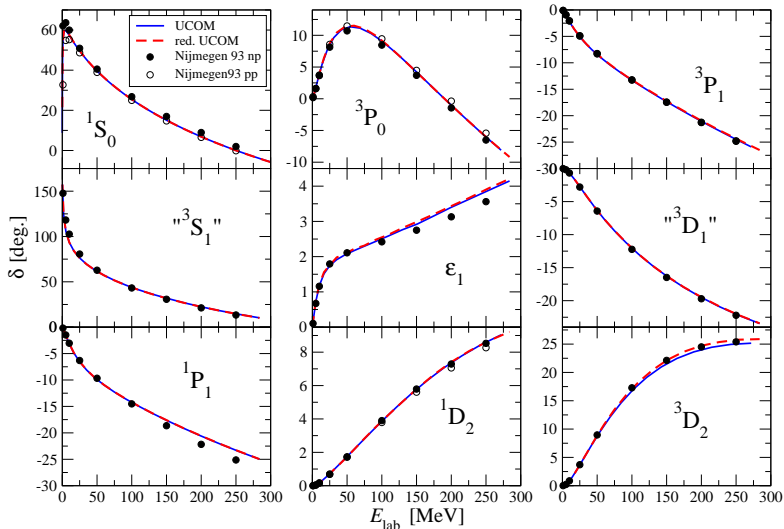
Results

UCOM - reduced set of operators

- ▶ fitting ansatz with **reduced** set of operators to the matrix elements containing **full** set of operators
- ▶ optimized for 'low' angular momenta, contributions from neglected terms 'absorbed' in other terms
- ▶ reduced set of operators has to describe two-nucleon data correctly

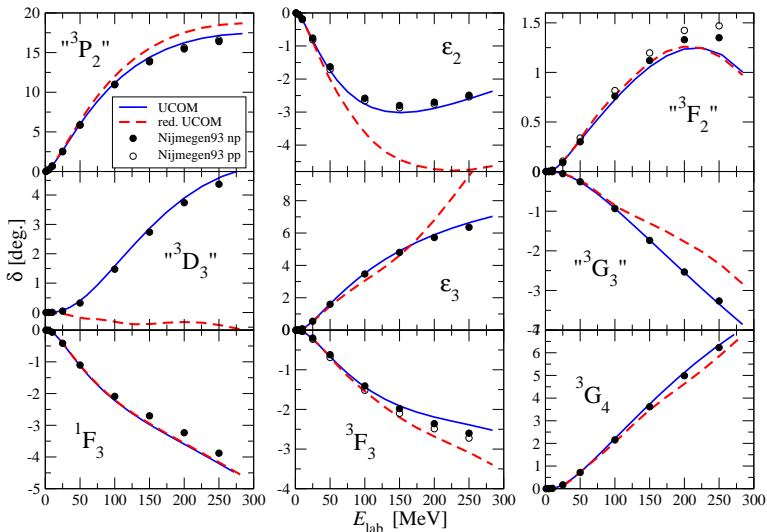
Reduced UCOM potential

NN phase shifts



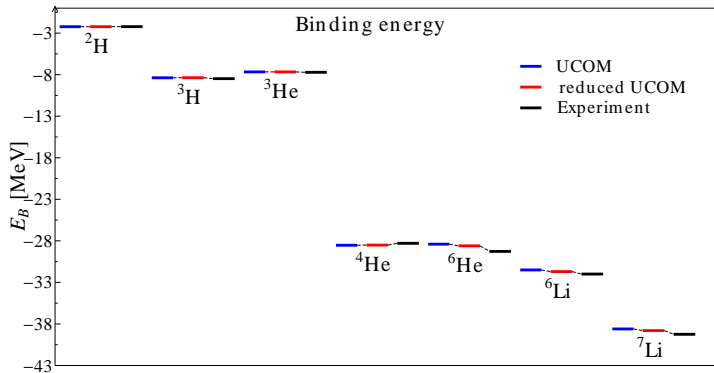
Reduced UCOM potential

NN phase shifts



Reduced UCOM potential

Binding energies

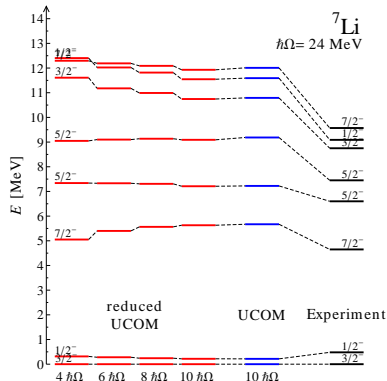
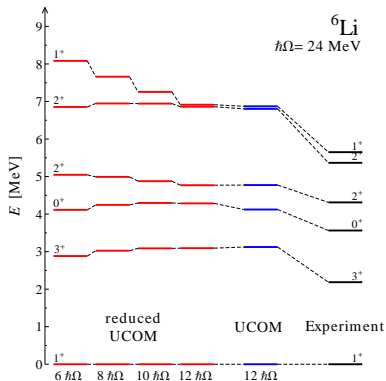


Binding energy [MeV]

| | ^2H | ^3H | ^3He | ^4He | ^6He | ^6Li | ^7Li |
|------------|--------------|--------------|---------------|---------------|---------------|---------------|---------------|
| UCOM | 2.23 | 8.38(1) | 7.67(1) | 28.53(1) | 28.4(2) | 31.5(2) | 38.6(4) |
| red. UCOM | 2.23 | 8.37(1) | 7.67(1) | 28.51(2) | 28.6(2) | 31.7(2) | 38.8(4) |
| Experiment | 2.2246 | 8.482 | 7.718 | 28.296 | 29.269 | 31.995 | 39.245 |

Reduced UCOM potential

Spectra and other observables from the NCSM



Properties of ${}^6\text{Li}$

| | R_p [fm] | μ [μ_N] | Q [$e \text{ fm}^2$] |
|------------|------------|-------------------|--------------------------|
| UCOM | 2.1(1) | 0.843(2) | -0.04(2) |
| red. UCOM | 2.1(1) | 0.842(1) | -0.03(3) |
| Experiment | 2.41(3) | 0.8220 | -0.0818(17) |

Properties of ${}^7\text{Li}$

| | R_p [fm] | μ [μ_N] | Q [$e \text{ fm}^2$] |
|------------|------------|-------------------|--------------------------|
| UCOM | 2.0(1) | 2.988(3) | -2.6(3) |
| red. UCOM | 2.0(1) | 2.987(2) | -2.5(3) |
| Experiment | 2.26(2) | 3.2564 | -4.06(8) |

SRG operator representation

Ansatz

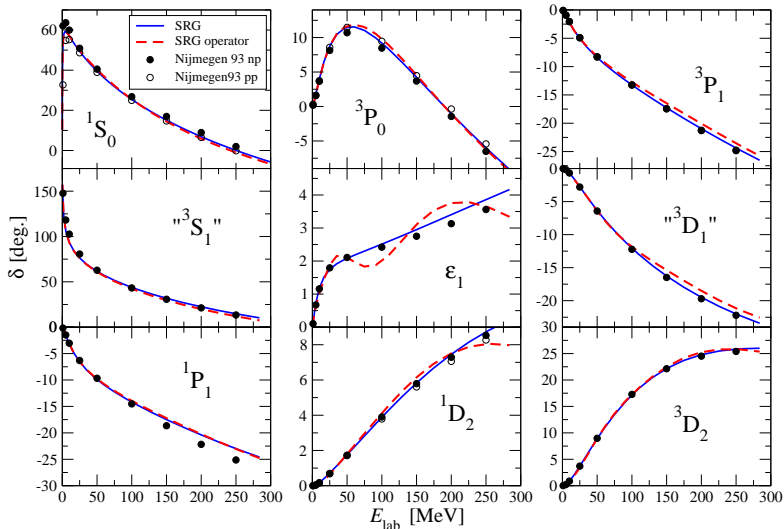
- ▶ complicated momentum dependence
- ▶ operators of Argonne potential, but $\mathcal{V}_{ST}^i(\underline{r}) \rightarrow \mathcal{V}_{ST}^i(\underline{r}, \underline{p})$

$$\begin{aligned}\tilde{\mathcal{V}}_{ansatz} &= \sum_{S,T} \mathcal{V}_{ST}^Z(\underline{r}, \underline{p}) \tilde{\Pi}_{ST} \\ &+ \sum_{S,T} \mathcal{V}_{ST}^{L^2}(\underline{r}, \underline{p}) \tilde{\underline{L}}^2 \tilde{\Pi}_{ST} \\ &+ \sum_T \mathcal{V}_{1T}^{LS}(\underline{r}, \underline{p}) \tilde{\underline{L}} \tilde{\underline{S}} \tilde{\Pi}_{1T} \\ &+ \sum_T \frac{1}{2} \left(\mathcal{S}_{12} \mathcal{V}_{1T}^T(\underline{r}, \underline{p}) + \mathcal{V}_{1T}^T(\underline{r}, \underline{p}) \mathcal{S}_{12} \right) \tilde{\Pi}_{1T} \\ &+ \sum_T \mathcal{V}_{1T}^{TLL}(\underline{r}, \underline{p}) \mathcal{S}_{12}(\tilde{\underline{L}}, \tilde{\underline{L}}) \tilde{\Pi}_{1T}\end{aligned}$$

- ▶ SRG transforms each partial wave differently for a given flow parameter: more complicated L and J dependence?

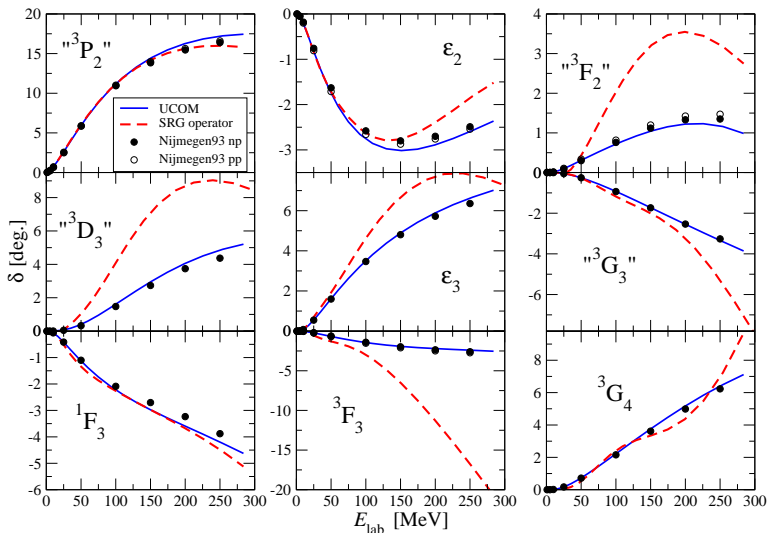
SRG operator representation

NN phase shifts



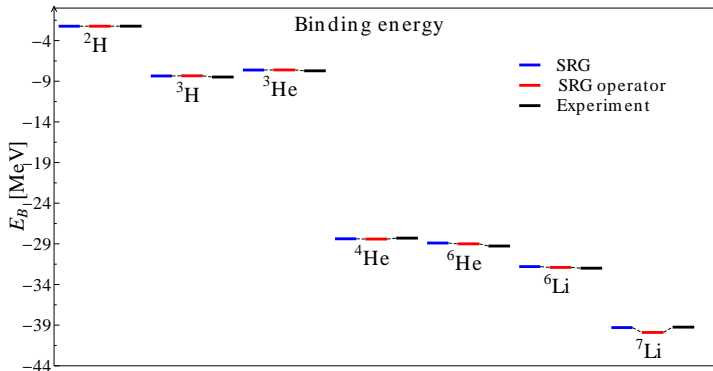
SRG operator representation

NN phase shifts



SRG operator representation

Binding energies

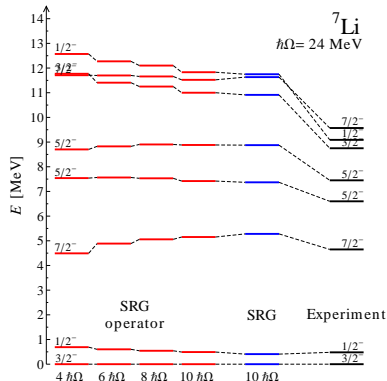
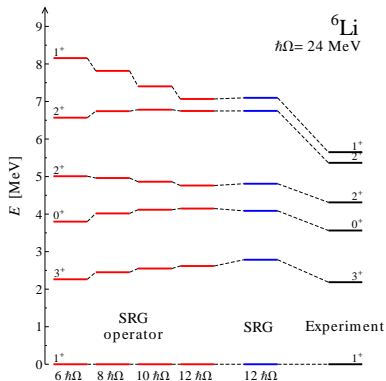


Binding energy [MeV]

| | ^3H | ^3H | ^3He | ^4He | ^6He | ^6Li | ^7Li |
|--------------|--------------|--------------|---------------|---------------|---------------|---------------|---------------|
| SRG | 2.23 | 8.35(1) | 7.62(1) | 28.38(1) | 28.9(4) | 31.8(3) | 39.3(5) |
| SRG operator | 2.23 | 8.33(1) | 7.61(1) | 28.41(2) | 29.0(5) | 31.9(3) | 39.9(5) |
| Experiment | 2.2246 | 8.482 | 7.718 | 28.296 | 29.269 | 31.995 | 39.245 |

SRG operator representation

Spectra and other observables from the NCSM



Properties of ${}^6\text{Li}$

| | R_p [fm] | μ [μ_N] | Q [$e \text{ fm}^2$] |
|--------------|------------|-------------------|--------------------------|
| SRG | 2.0(2) | 0.839(1) | 0.01(1) |
| SRG operator | 2.0(1) | 0.840(2) | 0.02(2) |
| Experiment | 2.41(3) | 0.8220 | -0.0818(17) |

Properties of ${}^7\text{Li}$

| | R_p [fm] | μ [μ_N] | Q [$e \text{ fm}^2$] |
|--------------|------------|-------------------|--------------------------|
| SRG | 2.0(1) | 2.983(3) | -2.4(2) |
| SRG operator | 2.0(1) | 2.997(2) | -2.4(3) |
| Experiment | 2.26(2) | 3.2564 | -4.06(8) |

Summary and conclusions

- ▶ Fermionic (Antisymmetric) Molecular Dynamics require operator representation of the interaction
- ▶ method to derive an operator representation starting from the partial wave matrix elements of the interaction
- ▶ UCOM potential with a reduced set of operators
 - ▶ operator form with less operators, but same accuracy in few-nucleon calculations
 - ▶ quadratic momentum dependent operators
- ▶ operator representation for SRG transformed Argonne potential
 - ▶ nonlocal radial functions
 - ▶ exact description of low angular momentum phase shifts
 - ▶ good agreement with few-nucleon properties calculated with the exact SRG interaction