Operator representation of realistic potentials for nuclear many-body calculations

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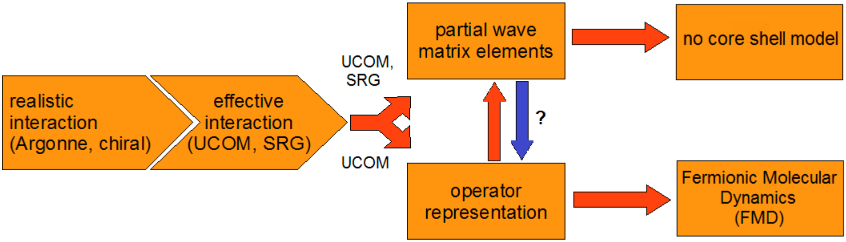
17.06.2010

Motivation

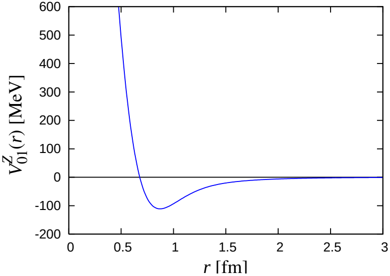
$$\left\langle k(LS)J;T \,\middle|\, \underset{\sim}{V}_{NN} \,\middle|\, k'(L'S)J;T \right\rangle$$



$$\begin{aligned}\underset{\sim}{V}_{NN} &= \sum_{S,T} V^{Z}_{ST}(\underset{\sim}{r})\, \underset{\sim}{\Pi}_{ST} \\ &+ \sum_{T} V^{LS}_{1T}(\underset{\sim}{r})\underset{\sim}{\vec{L}}\underset{\sim}{\vec{S}}\, \underset{\sim}{\Pi}_{1T} \\ &+ \cdots\end{aligned}$$

- operator representation:

$$\underset{\sim}{V}_{Arg} = \sum_{S,T} V_{ST}^{Z}(\underset{\sim}{r})\, \underset{\sim}{\Pi}_{ST} + \sum_{S,T} V_{ST}^{L2}(\underset{\sim}{r})\underset{\sim}{\vec{L}}^{2}\, \underset{\sim}{\Pi}_{ST} + \sum_{T} V_{1T}^{LS}(\underset{\sim}{r})\underset{\sim}{\vec{L}}\underset{\sim}{\vec{S}}\, \underset{\sim}{\Pi}_{1T} + \sum_{T} V_{1T}^{T}(\underset{\sim}{r})\underset{\sim}{S}_{12}\, \underset{\sim}{\Pi}_{1T} + \sum_{T} V_{1T}^{TLL}(\underset{\sim}{r})\underset{\sim}{s}_{12}(\vec{L},\vec{L})\, \underset{\sim}{\Pi}_{1T}$$



$$\underset{\sim}{S}_{12} = \frac{3}{\underset{\sim}{r}^{2}}\left(\underset{\sim}{\vec{r}}\cdot\underset{\sim}{\vec{\sigma}}_{1}\right)\left(\underset{\sim}{\vec{r}}\cdot\underset{\sim}{\vec{\sigma}}_{2}\right) - \underset{\sim}{\vec{\sigma}}_{1}\underset{\sim}{\vec{\sigma}}_{2}$$

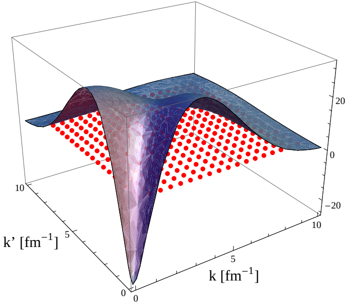
$$\underset{\sim}{s}_{12}(\vec{a},\vec{b}) = \frac{3}{2}\left[(\underset{\sim}{\vec{\sigma}}_{1}\cdot\underset{\sim}{\vec{a}})(\underset{\sim}{\vec{\sigma}}_{2}\cdot\underset{\sim}{\vec{b}}) + (\underset{\sim}{\vec{\sigma}}_{1}\cdot\underset{\sim}{\vec{b}})(\underset{\sim}{\vec{\sigma}}_{2}\cdot\underset{\sim}{\vec{a}})\right] - \frac{1}{2}(\underset{\sim}{\vec{\sigma}}_{1}\cdot\underset{\sim}{\vec{\sigma}}_{2})(\underset{\sim}{\vec{a}}\cdot\underset{\sim}{\vec{b}} + \underset{\sim}{\vec{b}}\cdot\underset{\sim}{\vec{a}})$$

Argonne potential

partial wave matrix elements

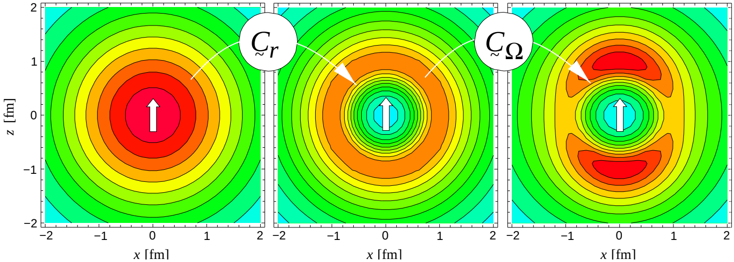
- for each L, L', S, J, T:

$$\left\langle\, k(LS)J;\, T \,\middle|\, \underset{\sim}{V} \,\middle|\, k'(L'S)J;\, T \,\right\rangle$$



matrix elements in MeV fm^3 for $S{=}0$, $T{=}1$ and $L_1{=}L_2{=}0$

Unitary Correlation Operator Method



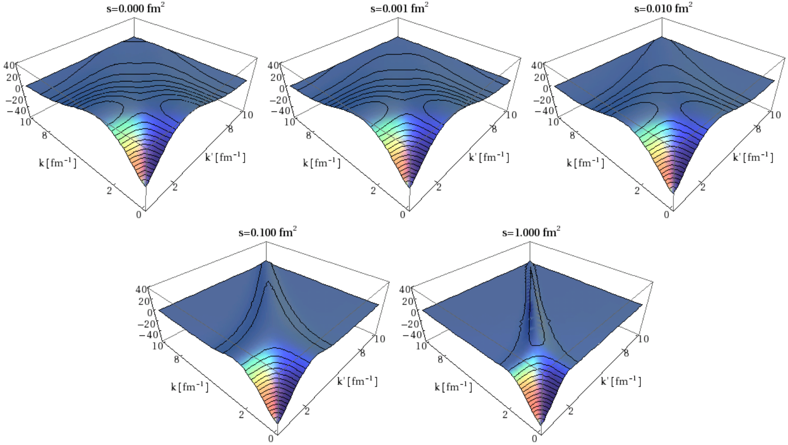
taken fom T. Neff, H. Feldmeier, Nucl. Phys. A713

- correlations introduced explicitly by the 'Unitary Correlation Operator Method' UCOM:
  - correlated state
    $\left| \widehat{\Psi} \right\rangle = \underset{\sim}{\mathcal{C}} \left| \Psi \right\rangle = \underset{\sim}{\mathcal{C}}_\Omega \underset{\sim}{\mathcal{C}}_r \left| \Psi \right\rangle$
  - correlated operator
    $\left\langle \widehat{\Psi}' \middle| \underset{\sim}{B} \middle| \widehat{\Psi} \right\rangle = \left\langle \Psi' \middle| \underset{\sim}{\mathcal{C}}^\dagger \underset{\sim}{B} \underset{\sim}{\mathcal{C}} \middle| \Psi \right\rangle \equiv \left\langle \Psi' \middle| \widehat{\underset{\sim}{B}} \middle| \Psi \right\rangle$

- operator representation:

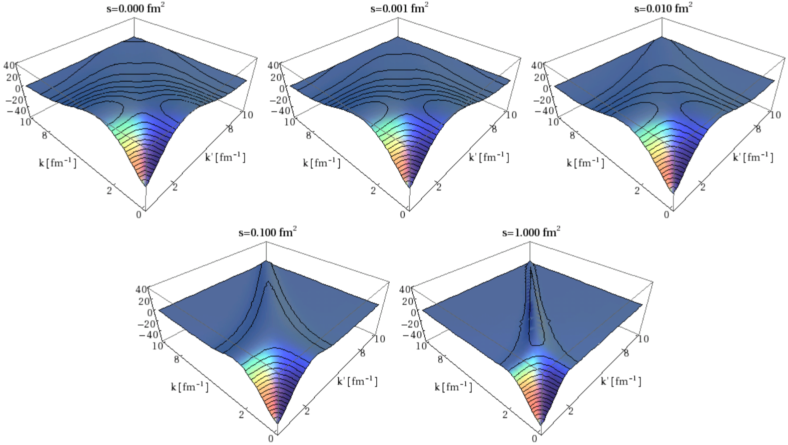
$$
\begin{aligned}
\underset{\sim}{V}_{UCOM} = \underset{\sim}{\widehat{H}}^{[2]} = \underset{\sim}{\widehat{T}}^{[2]} + \underset{\sim}{\widehat{V}}^{[2]} \quad = \quad & \sum_{S,T} V^{Z}_{ST}(\underset{\sim}{r})\,\underset{\sim}{\Pi}_{ST} \\
+ \quad & \sum_{S,T} V^{L2}_{ST}(\underset{\sim}{r})\underset{\sim}{\vec{L}}^{2}\underset{\sim}{\Pi}_{ST} \\
+ \quad & \sum_{S,T} \frac{1}{2}(\underset{\sim}{\vec{p}}^{\,2} V^{p2}_{ST}(\underset{\sim}{r}) + V^{p2}_{ST}(\underset{\sim}{r})\underset{\sim}{\vec{p}}^{\,2})\underset{\sim}{\Pi}_{ST} \\
+ \quad & \sum_{T} V^{LS}_{1T}(\underset{\sim}{r})\underset{\sim}{\vec{L}}\underset{\sim}{\vec{S}}\,\underset{\sim}{\Pi}_{1T} \\
+ \quad & \sum_{T} V^{L2LS}_{1T}(\underset{\sim}{r})\underset{\sim}{\vec{L}}^{2}\,\underset{\sim}{\vec{L}}\underset{\sim}{\vec{S}}\,\underset{\sim}{\Pi}_{1T} \\
+ \quad & \sum_{T} V^{T}_{1T}(\underset{\sim}{r})\underset{\sim}{S}_{12}\,\underset{\sim}{\Pi}_{1T} \\
+ \quad & \sum_{T} V^{TLL}_{1T}(\underset{\sim}{r})\underset{\sim}{s}_{12}(\vec{L},\vec{L})\,\underset{\sim}{\Pi}_{1T} \\
+ \quad & \sum_{T} V^{Tpp}_{1T}(\underset{\sim}{r})\underset{\sim}{\bar{s}}_{12}(p_{\Omega},p_{\Omega})\underset{\sim}{\Pi}_{1T} \\
+ \quad & \sum_{T} (\underset{\sim}{p}_{r} V^{Trp}_{1T}(\underset{\sim}{r}) + V^{Trp}_{1T}(\underset{\sim}{r})\underset{\sim}{p}_{r})\underset{\sim}{s}_{12}(r,p_{\Omega})\underset{\sim}{\Pi}_{1T} \\
+ \quad & \ldots
\end{aligned}
$$

- SRG evolution



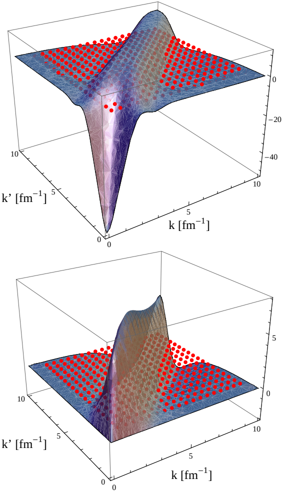
- matrix elements, but no operator representation

- SRG evolution



- matrix elements, but no operator representation

Operator representation and matrix elements partial wave matrix elements



?

operator representation

$$
\begin{aligned}
\underset{\sim}{V}_{NN} &= \sum_{ST,i} V^{i}_{ST}(\underset{\sim}{r})\, \underset{\sim}{\mathcal{O}}_i\, \underset{\sim}{\Pi}_{ST} \\
&= \sum_{S,T} V^{Z}_{ST}(\underset{\sim}{r})\, \underset{\sim}{\Pi}_{ST} \\
&+ \sum_{T} V^{LS}_{1T}(\underset{\sim}{r})\, \underset{\sim}{\vec{L}}\underset{\sim}{\vec{S}}\, \underset{\sim}{\Pi}_{1T} \\
&+ \cdots
\end{aligned}
$$

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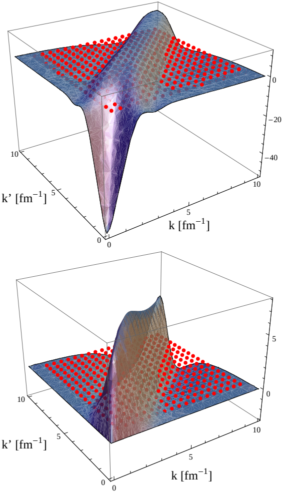
From partial wave matrix elements
to operator representation

partial wave matrix elements



Fit

$\gamma^{i}_{ST,j}$

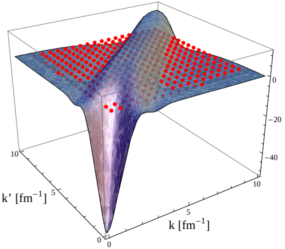
operator representation

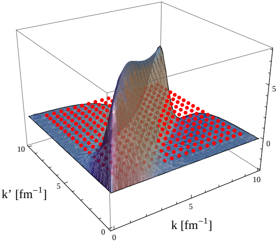
- choose appropriate set of operators

$$\underset{\sim}{V}_{Ansatz} = \sum_{ST,i} V^{i}_{ST}(\underset{\sim}{r})\,\underset{\sim}{O}_i\underset{\sim}{\Pi}_{ST}$$

From partial wave matrix elements
to operator representation

partial wave matrix elements





Fit

$\gamma^{i}_{ST,j}$

operator representation

- choose appropriate set of operators

$$\underset{\sim}{V}_{Ansatz} = \sum_{ST,i} V^{i}_{ST}(\underset{\sim}{r})\, \underset{\sim}{\mathcal{O}}_i \underset{\sim}{\Pi}_{ST}$$

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

$$V^{i}_{ST}(r) = \sum_j \gamma^{i}_{ST,j} \exp\left\{-\frac{r^2}{2\kappa_j}\right\}$$

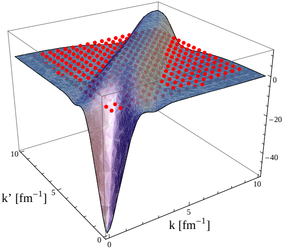
- choose parameters: $\kappa_j = \kappa_1 \cdot b^{j-1}$

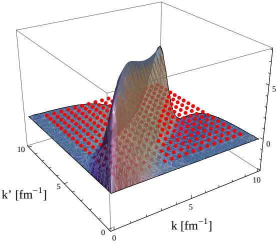
$$\kappa = \{0.05,\, 0.05 \cdot \sqrt{2},\, 0.1,\, \cdots 6.4\}\,\text{fm}^2$$

GSI

From partial wave matrix elements
to operator representation

partial wave matrix elements





Fit ←

$\gamma^{i}_{ST,j}$

operator representation

- choose appropriate set of operators

$$\underset{\sim}{V}_{Ansatz} = \sum_{ST,i} V^{i}_{ST}(\underset{\sim}{r})\, \underset{\sim}{\mathcal{O}}_i \underset{\sim}{\Pi}_{ST}$$

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- choose parameters: $\kappa_j = \kappa_1 \cdot b^{j-1}$

$$\kappa = \{0.05,\ 0.05\cdot\sqrt{2},\ 0.1,\ \cdots 6.4\}\ \mathrm{fm}^2$$

- calculate analytically matrix elements $\left\langle k(LS)JT \left| \underset{\sim}{V}_{Ansatz} \right| k'(L'S)JT \right\rangle$

Applications

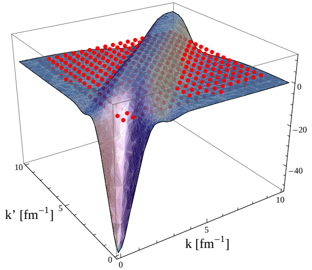
Results

UCOM - reduced set of operators

- Which operators do we really need?
- procedure:
  - fitting Ansatz with less operators to 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

- Ansatz

$$
\begin{aligned}
\underset{\sim}{V}_{Ansatz} &= \sum_{S,T} V^{Z}_{ST}(\underset{\sim}{r})\,\underset{\sim}{\Pi}_{ST} \\
&+ \sum_{S,T} V^{L2}_{ST}(\underset{\sim}{r})\underset{\sim}{\vec{L}}^{2}\underset{\sim}{\Pi}_{ST} \\
&+ \sum_{S,T} \frac{1}{2}(\underset{\sim}{\vec{p}}^{\,2} V^{p2}_{ST}(\underset{\sim}{r}) + V^{p2}_{ST}(\underset{\sim}{r})\underset{\sim}{\vec{p}}^{\,2})\underset{\sim}{\Pi}_{ST} \\
&+ \sum_{T} V^{LS}_{1T}(\underset{\sim}{r})\underset{\sim}{\vec{L}}\underset{\sim}{\vec{S}}\,\underset{\sim}{\Pi}_{1T} \\
&+ \sum_{T} V^{L2LS}_{1T}(\underset{\sim}{r})\underset{\sim}{\vec{L}}^{2}\underset{\sim}{\vec{L}}\underset{\sim}{\vec{S}}\,\underset{\sim}{\Pi}_{1T} \\
&+ \sum_{T} V^{T}_{1T}(\underset{\sim}{r})\underset{\sim}{S}_{12}\,\underset{\sim}{\Pi}_{1T} \\
&+ \sum_{T} V^{TLL}_{1T}(\underset{\sim}{r})\underset{\sim}{s}_{12}(\vec{L},\vec{L})\,\underset{\sim}{\Pi}_{1T} \\
&+ \sum_{T} V^{Tpp}_{1T}(\underset{\sim}{r})\underset{\sim}{\bar{s}}_{12}(p_{\Omega},p_{\Omega})\underset{\sim}{\Pi}_{1T} \\
&+ \sum_{T} (\underset{\sim}{p}_{r} V^{Trp}_{1T}(\underset{\sim}{r}) + V^{Trp}_{1T}(\underset{\sim}{r})\underset{\sim}{p}_{r})\underset{\sim}{s}_{12}(r,p_{\Omega})\underset{\sim}{\Pi}_{1T}
\end{aligned}
$$



- Ansatz

$$
\begin{aligned}
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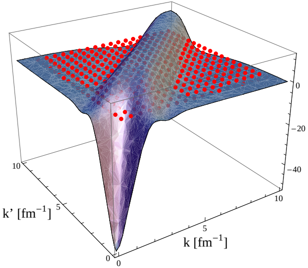
\end{aligned}
$$



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- Ansatz

$$
\begin{aligned}
\underset{\sim}{V}_{Ansatz} = & \sum_{S,T} V^{Z}_{ST}(\underset{\sim}{r})\,\underset{\sim}{\Pi}_{ST} \\
+ & \sum_{S,T} V^{L2}_{ST}(\underset{\sim}{r})\underset{\sim}{\vec{L}}^{2}\underset{\sim}{\Pi}_{ST} \\
+ & \sum_{S,T} \frac{1}{2}(\underset{\sim}{\vec{p}}^{\,2} V^{p2}_{ST}(\underset{\sim}{r}) + V^{p2}_{ST}(\underset{\sim}{r})\underset{\sim}{\vec{p}}^{\,2})\underset{\sim}{\Pi}_{ST} \\
+ & \sum_{T} V^{LS}_{1T}(\underset{\sim}{r})\underset{\sim}{\vec{L}}\underset{\sim}{\vec{S}}\,\underset{\sim}{\Pi}_{1T} \\
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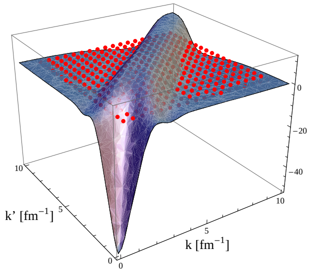
+ & \sum_{T} (\underset{\sim}{p}_{r} V^{Trp}_{1T}(\underset{\sim}{r}) + V^{Trp}_{1T}(\underset{\sim}{r})\underset{\sim}{p}_{r})\underset{\sim}{s}_{12}(r,p_{\Omega})\underset{\sim}{\Pi}_{1T}
\end{aligned}
$$

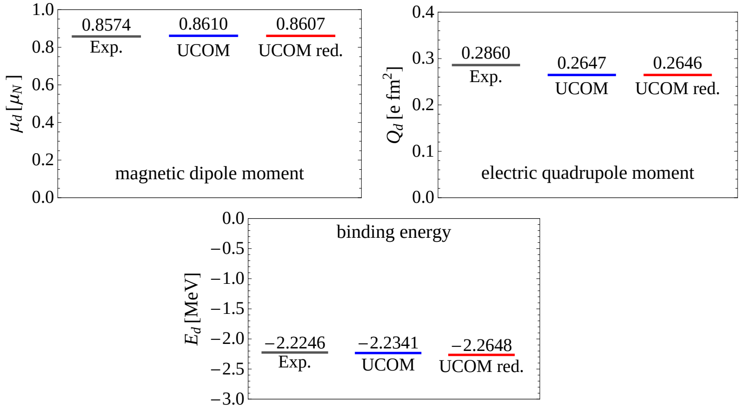


- Does the reduced set of operators keep the features of the interaction?
  - deuteron
  - phase-shifts
  - few-nucleon systems

Results

UCOM - reduced set of operators

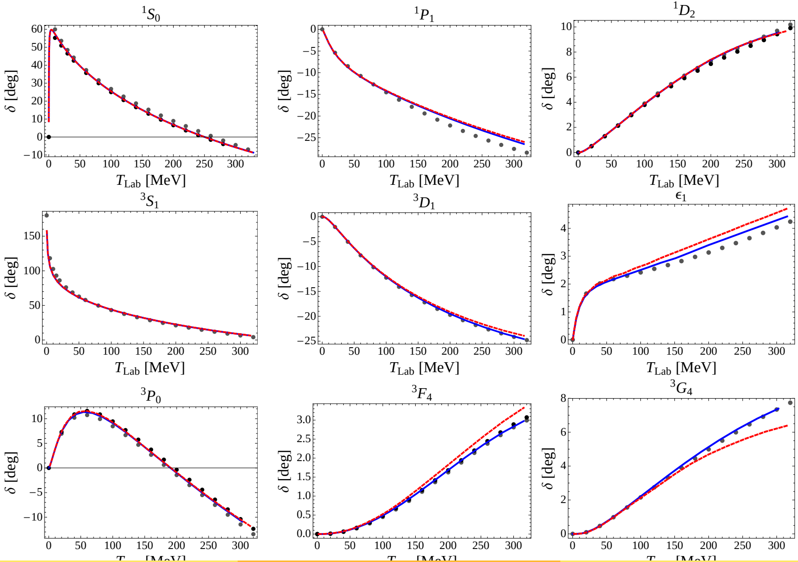
- deuteron properties:



μ_d and Q_d calculated with uncorrelated operators

Results

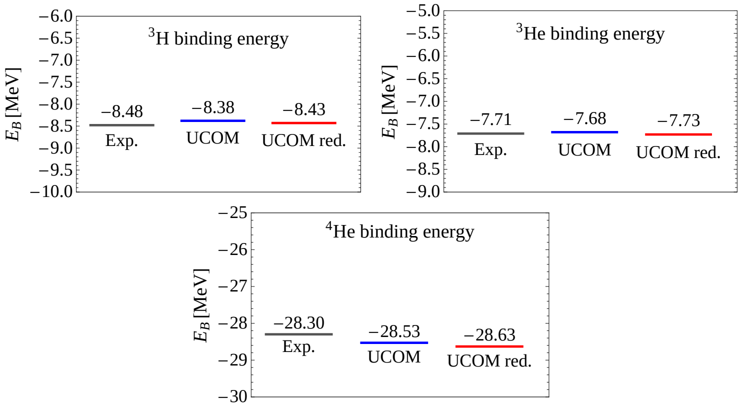
UCOM - reduced set of operators



Results

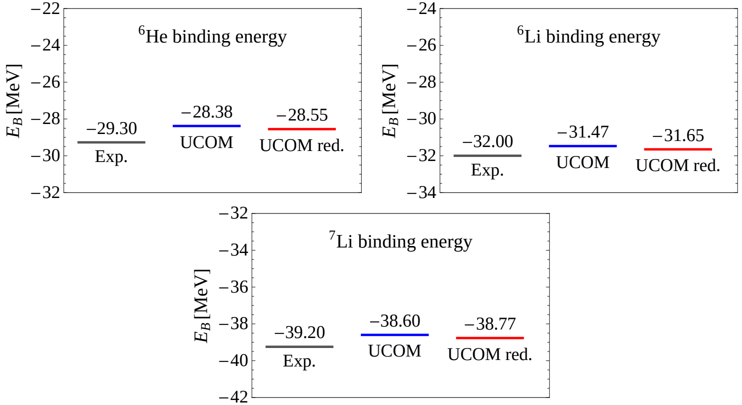
UCOM - reduced set of operators

- 'no core shell model' calculations for light nuclei



Results

UCOM - reduced set of operators



- results for full UCOM and reduced operator form in good agreement
- neglecting more terms changes few-nucleon properties

- UCOM fit: local potential, parameterized by gaussians

$$V(\underset{\sim}{r}) \propto \sum_k \gamma_k \exp\left\{-\frac{\vec{\underset{\sim}{r}}^2}{2\kappa_k}\right\}$$

(+ quadratic momentum dependence)

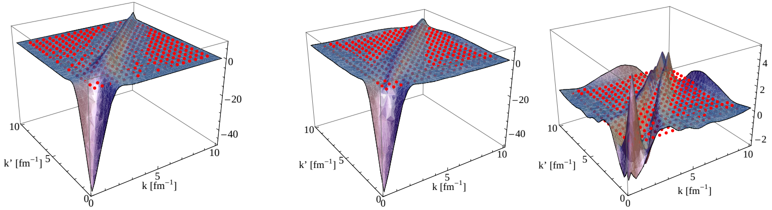
- SRG momentum dependence more complicated: fit with nonlocal potential

$$V(\vec{\underset{\sim}{r}}^2, \vec{\underset{\sim}{p}}^2) \propto \sum_{k,l} \gamma_{kl} \exp\left\{-\frac{\lambda_l}{4}\vec{\underset{\sim}{p}}^2\right\} \exp\left\{-\frac{\vec{\underset{\sim}{r}}^2}{2(\kappa_k - \lambda_l/4)}\right\} \exp\left\{-\frac{\lambda_l}{4}\vec{\underset{\sim}{p}}^2\right\}$$

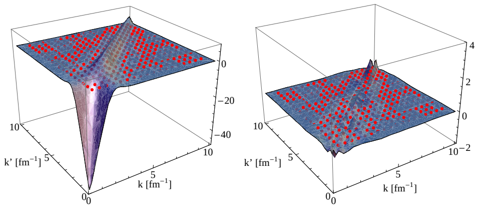
- λ shows how 'local' the potential is:
  - $\lambda = 0$: local
  - $\lambda k_f^2 \ll 1$: quadratic momentum dependence

$$V(\vec{\underset{\sim}{r}}^2, \vec{\underset{\sim}{p}}^2) \longrightarrow V^Z(\underset{\sim}{r}) + \frac{1}{2}(\vec{\underset{\sim}{p}}^2 V^{p2}(\underset{\sim}{r}) + V^{p2}(\underset{\sim}{r})\vec{\underset{\sim}{p}}^2)$$

- SRG matrix element fit with local $(+p^2)$



- and nonlocal Ansatz



$s = 1.0\,\mathrm{fm}^2$

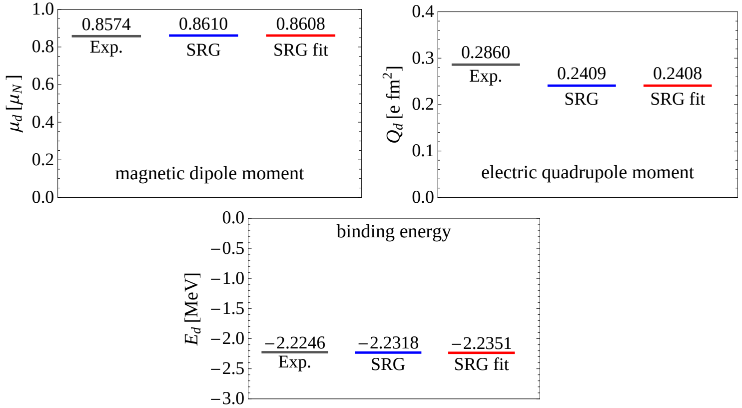
matrix elements in *MeV fm*^{3}

- operators of Argonne potential, but $V^i_{ST}(\underset{\sim}{r}) \to V^i_{ST}(\underset{\sim}{\vec{r}}^2, \underset{\sim}{\vec{p}}^2)$

$$
\begin{aligned}
\underset{\sim}{V}_{Ansatz} &= \sum_{S,T} V^{Z}_{ST}(\underset{\sim}{\vec{r}}^2, \underset{\sim}{\vec{p}}^2)\,\underset{\sim}{\Pi}_{ST} \\
&+ \sum_{S,T} V^{L2}_{ST}(\underset{\sim}{\vec{r}}^2, \underset{\sim}{\vec{p}}^2)\underset{\sim}{\vec{L}}^2\,\underset{\sim}{\Pi}_{ST} \\
&+ \sum_{T} V^{LS}_{1T}(\underset{\sim}{\vec{r}}^2, \underset{\sim}{\vec{p}}^2)\underset{\sim}{\vec{L}}\underset{\sim}{\vec{S}}\,\underset{\sim}{\Pi}_{1T} \\
&+ \sum_{T} V^{T}_{1T}(\underset{\sim}{\vec{r}}^2, \underset{\sim}{\vec{p}}^2)\underset{\sim}{S}_{12}\,\underset{\sim}{\Pi}_{1T} \\
&+ \sum_{T} V^{TLL}_{1T}(\underset{\sim}{\vec{r}}^2, \underset{\sim}{\vec{p}}^2)\underset{\sim}{s}_{12}(\vec{L}, \vec{L})\,\underset{\sim}{\Pi}_{1T} \\
&+ \cdots \underset{\sim}{s}_{12}(r, p_\Omega)?
\end{aligned}
$$

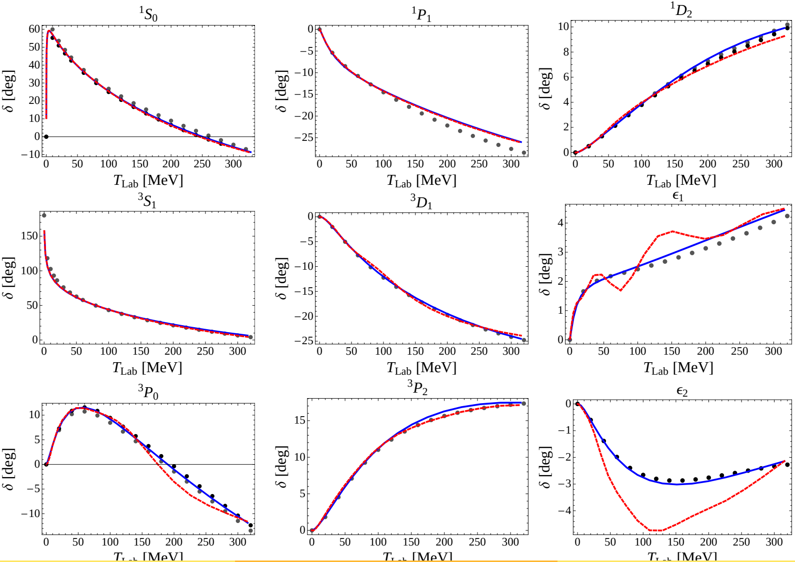
Results
SRG fit - deuteron

- deuteron properties:



Results

SRG fit - phase-shifts



Summary

- operator representation of potentials needed for FMD, AMD
- operator representation starting from partial wave matrix elements
- UCOM interaction with reduced set of operators
  - less complicated structure, but same features
- operator representation for SRG potentials
  - nonlocal Ansatz
  - improve fit of nonlocal matrix elements

Thanks to my collaborators
H.Feldmeier
T.Neff

- which operators do we really need?
- Ansatz

$$
\begin{aligned}
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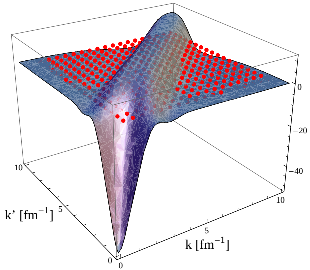
\end{aligned}
$$

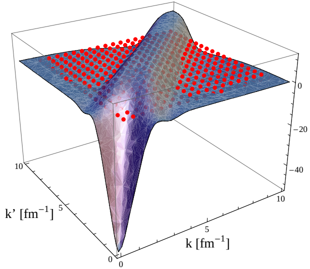


Results

UCOM - reduced set of operators 2

- which operators do we really need?
- Ansatz

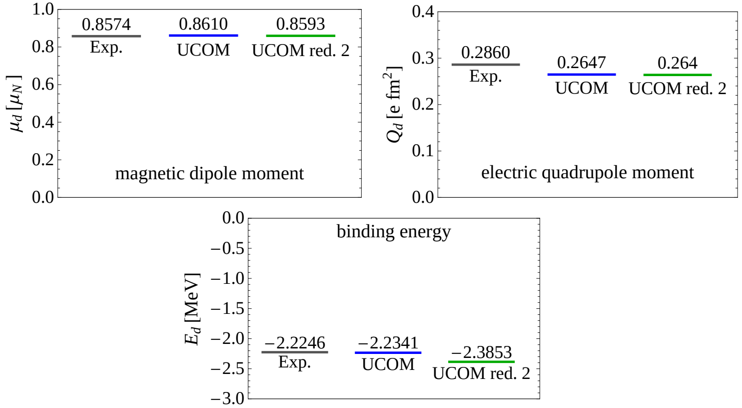
$$
\begin{aligned}
\underset{\sim}{V}_{Ansatz} &= \sum_{S,T} V^{Z}_{ST}(\underset{\sim}{r})\,\underset{\sim}{\Pi}_{ST} \\
&+ \sum_{S,T} V^{L2}_{ST}(\underset{\sim}{r})\underset{\sim}{\vec{L}}^2\underset{\sim}{\Pi}_{ST} \\
&+ \sum_{S,T} \frac{1}{2}(\underset{\sim}{\vec{p}}^{\,2} V^{p2}_{ST}(\underset{\sim}{r}) + V^{p2}_{ST}(\underset{\sim}{r})\underset{\sim}{\vec{p}}^{\,2})\underset{\sim}{\Pi}_{ST} \\
&+ \sum_{T} V^{LS}_{1T}(\underset{\sim}{r})\underset{\sim}{\vec{L}}\underset{\sim}{\vec{S}}\,\underset{\sim}{\Pi}_{1T} \\
&+ \sum_{T} V^{L2LS}_{1T}(\underset{\sim}{r})\underset{\sim}{\vec{L}}^2\,\underset{\sim}{\vec{L}}\underset{\sim}{\vec{S}}\,\underset{\sim}{\Pi}_{1T} \\
&+ \sum_{T} V^{T}_{1T}(\underset{\sim}{r})\underset{\sim}{S}_{12}\,\underset{\sim}{\Pi}_{1T} \\
&+ \sum_{T} V^{TLL}_{1T}(\underset{\sim}{r})\underset{\sim}{s}_{12}(\vec{L},\vec{L})\,\underset{\sim}{\Pi}_{1T} \\
&+ \sum_{T} V^{Tpp}_{1T}(\underset{\sim}{r})\underset{\sim}{\bar{s}}_{12}(p_{\Omega},p_{\Omega})\underset{\sim}{\Pi}_{1T} \\
&+ \sum_{T} (\underset{\sim}{p}_r V^{Trp}_{1T}(\underset{\sim}{r}) + V^{Trp}_{1T}(\underset{\sim}{r})\underset{\sim}{p}_r)\underset{\sim}{s}_{12}(r,p_{\Omega})\underset{\sim}{\Pi}_{1T}
\end{aligned}
$$



Results

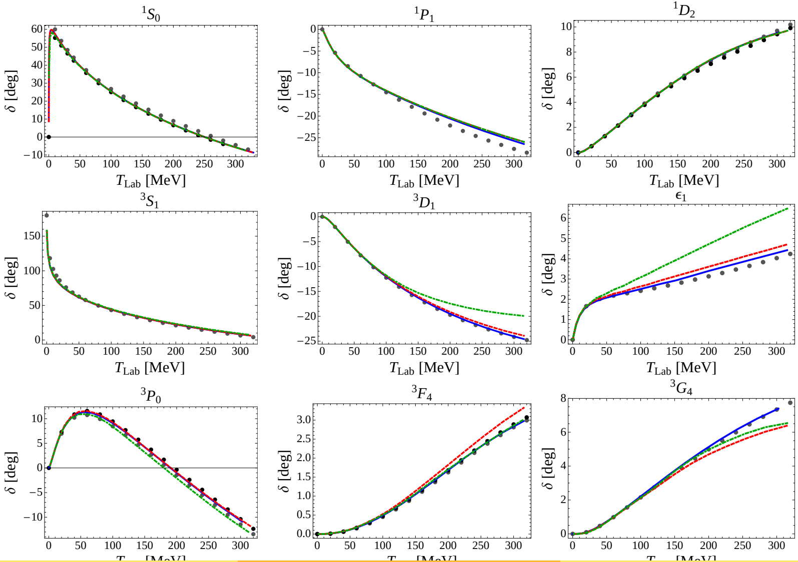
UCOM - reduced set of operators 2

- deuteron properties:

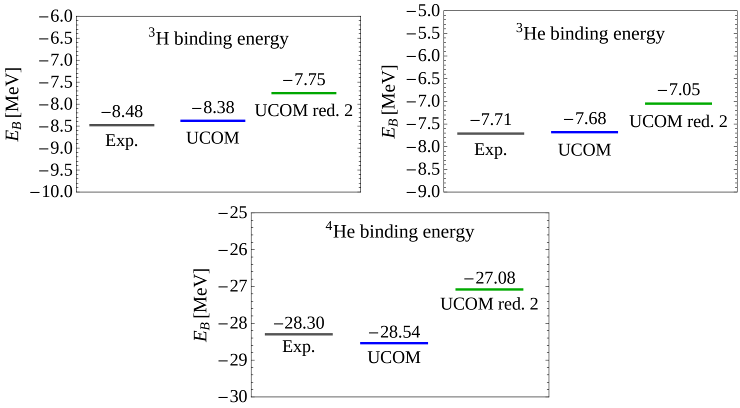


Results

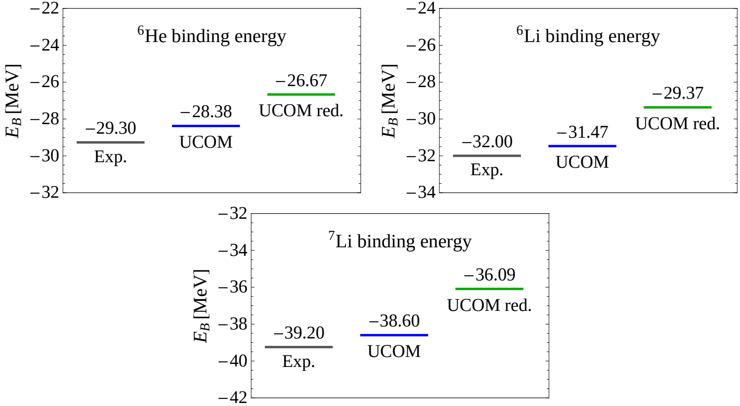
UCOM - reduced set of operators 2



- 'no core shell model' calculations for light nuclei



- A=6,7 nuclei


^{6}He binding energy
E_B [MeV]
−22
−24
−26
−28
−30
−32
−29.30
Exp.
−28.38
UCOM
−26.67
UCOM red.
^{6}Li binding energy
E_B [MeV]
−24
−26
−28
−30
−32
−34
−32.00
Exp.
−31.47
UCOM
−29.37
UCOM red.
^{7}Li binding energy
E_B [MeV]
−32
−34
−36
−38
−40
−42
−39.20
Exp.
−38.60
UCOM
−36.09
UCOM red.