# Three-body approach to $d + \alpha$ scattering and bound state using realistic forces in a separable or non-separable representation

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## Importance of $(d,p)$-reactions

- Probing single-particle structure of nuclei
- Extracting neutron-capture rates relevant for astrophysics

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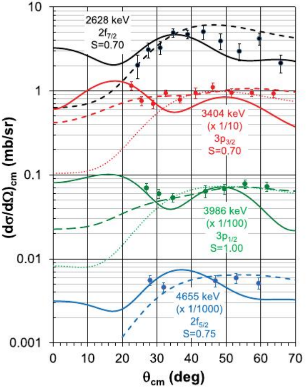
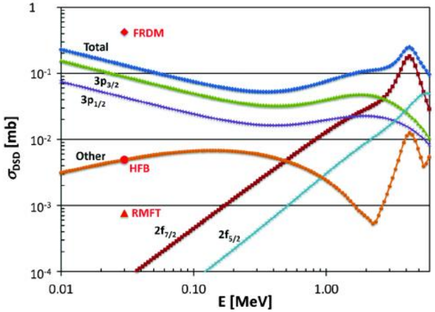
$^{130}$**Sn** $(d, p)^{131}$**Sn**




$\longrightarrow$

$^{130}$**Sn** $(n, \gamma)^{131}$**Sn**



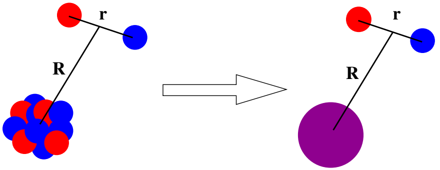

Kozub *et. al* PRL **109**, 172501 (2012)

# Three-Body Model for $(d, p)$ Reactions

## The many-body problem

- The deuteron $(d)$ + target $(A)$ system consists of $A + 2$ nucleons
- Solutions not feasible for reactions involving heavy targets

## Isolating relevant degrees of freedom




- Formulation of three-body problem by Faddeev
- Momentum space formulation: Faddeev-AGS equations

# The Effective Three-Body Hamiltonian

## np-system

- High precision NN potentials with $\chi^2 \approx 1$, e.g., **CD-Bonn** [R. Machleidt, Phys. Rev. C63, 024001 (2001)]
- NN potentials derived from chiral EFT

## $nA$ system

- Phenomenological fits of elastic scattering data to Woods-Saxon form, e.g.
  $$v(r) = -\frac{V_0}{1+\exp\left(\frac{r-R_0}{a_0}\right)} + \left(\frac{1}{r}\right)\frac{d}{dr}\frac{V_{so}}{1+\exp\left(\frac{r-R_{so}}{a_{so}}\right)}\,\mathbf{l}\cdot\boldsymbol{\sigma}$$
- Microscopically computed, e.g., J. Rotureau, Phys. Rev. C 95, 024315 (2017)

## $pA$ system

- Similar to $nA$ but with the Coulomb repulsion

# Solving the Faddeev-AGS Equations

## Challenges

1. Non-trivial singularities in the kernel of multivariate integral equations
2. Treatment of the Coulomb interaction in momentum space

## Remedy:

1. Employing **separable** two-body interactions
   (i.e. $v(r, r') = h_1(r)\ \lambda_{11}\ h_1(r') + h_1(r)\ \lambda_{12}\ h_2(r') + \ldots$)
   - Reduces the Faddeev-AGS equations into coupled integral equations in one variable
2. Formulation of Faddeev-AGS equations in the Coulomb basis (A. Mukhamedzhanov, *et al.* Phys.Rev. **C86**, 034001 (2012).)

   – based on **separable** two-body potentials

# Objectives

1. **Construct separable expansions for:**
   - High precision NN interactions
   - Effective $nA$ and $pA$ potentials

2. **Benchmark for the three-body problem:**

   Faddeev-AGS equations with (1) original three-body Hamiltonian and (2) its separable expansion:

   (a) **3-body bound state:**
   - Compare 3-body binding energies and momentum distributions

   (b) **Benchmark for $d + A$ scattering:**
   - Compare angular distributions for elastic scattering as well as transfer and deuteron breakup reactions

# Separable expansion for 2-Body potentials: **EST** scheme

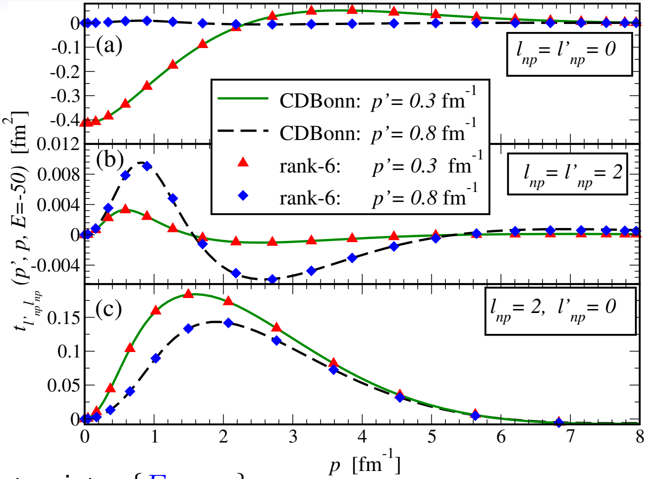
- Start from potential $V$, solve for eigenstates of Hamiltonian $H_0 + V$ at energies $E_i$: $H|\psi_i\rangle = E_i|\psi_i\rangle$
- Separable expansion: $v^{sep} = \sum_{ij}^{rank} V|\psi_i\rangle\, \lambda_{ij}\, \langle\psi_i|V$

$$[\lambda^{-1}]_{ij} = \langle\psi_i|V|\psi_j\rangle$$

- Momentum space: $|\psi_i\rangle = |p_i\rangle + G_0^{(+)}(E_i)\, V|\psi_i\rangle$
- Physical solutions: $p_i = \sqrt{2\mu E_i}$
- To accelerate convergence of observables: include off-shell solutions with independent $p_i$ and $E_i$
- Notation: $t$-matrix $t(E_i)|p_i\rangle = V|\psi_i\rangle \equiv |h_i\rangle$
- Matrix elements given as $v^{sep}(p', p) = \sum_{ij} h_i(p)\, \lambda_{ij}\, h_j(p)$

[Ernst *et al.*, Phys.Rev. C9, 1780 (1974)]

# The $np$ $t$-matrix for $J=S=1$ with CD-Bonn potential




- Support points: $\{E_m, p_m\} =$ $\{-60, 0.4\}, \{-60, 1.1\}, \{-60, 2.5\}, \{-5, 0.4\}, \{-5, 1.1\}, \{-5, 2.5\}$
- Shape of potential in $p$-space determines location of support momenta

# Removing Pauli-Forbidden States

- $S_{1/2}$ partial wave supports Pauli-forbidden state $|\phi\rangle$
- To project out the state $|\phi\rangle$: $V \longrightarrow \tilde{V} = V + \lim_{\Gamma\to\infty} |\phi\rangle\, \Gamma\, \langle\phi|$
- Corresponding $t$-matrix:

$$\tilde{t}(E) = t(E) - (E - H_0)\,\frac{|\phi\rangle\langle\phi|}{(E-E_b)[1-(E-E_b)/\Gamma]}(E - H_0)$$

- $\Gamma$ limit can be taken analytically

$$\tilde{t}(p', p; E) = t(p', p; E) - (E - E_{p'})\,\frac{\phi(p')\phi(p)}{E-E_b}(E - E_p)$$

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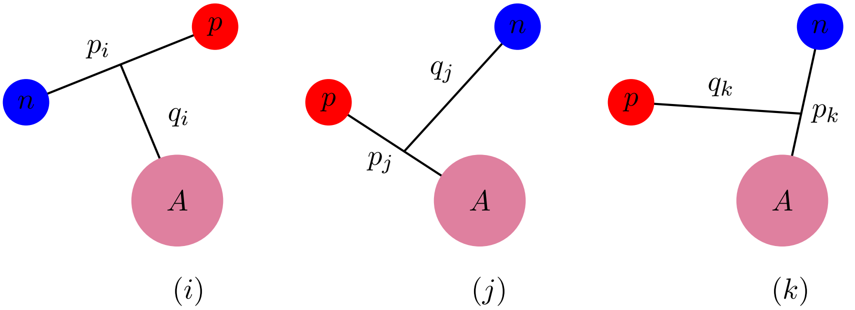
### Separable Expansion

- Separable expansion of $V$ also supports bound state $|\phi\rangle$, must be removed
- Convenient approach: expand $\tilde{V}$ instead of $V$
- Advantages: (1) straightforward implementation and (2) does not increase rank

# Jacobi Coordinates: 3 different particles, 3 arrangement channels




- Pair momenta: $p_i$, $p_j$, $p_k$, spectator momenta $q_i$, $q_j$, $q_k$
- Notation: $V_i \equiv V_{np},\ V_j \equiv V_{pA},\ V_k \equiv V_{nA}$ $\Rightarrow$ 2-body potentials
- Free Hamiltonian $H_0 = p_i^2/2\mu_i + q_i^2/2M_i$
- 3-Body Hamiltonian: $H_{3b} = H_0 + V_i + V_j + V_k$

## Faddeev equations for a three-body bound state:

- Three-body wavefunction $|\Psi\rangle = |\psi_i\rangle + |\psi_j\rangle + |\psi_k\rangle$
- Faddeev components have definition $|\psi_i\rangle \equiv G_0(E_3) V_i |\Psi\rangle$

Coupled equations: $|\psi_i\rangle = G_0(E_3)\, t_i(E_3) \big[ |\psi_j\rangle + |\psi_k\rangle \big]$

- Two-body $t$-matrix: $t_i(E_3) = V_i + V_i\, G_0(E_3)\, t(E_3)$
- Explicit momentum space representation

$$\psi_i(p_i q_i \alpha_i) = G_0(E_{q_i}, p_i) \sum_{\alpha_{i'}} \int dp_i'\, {p_i'}^2\, t_i^{\alpha_i \alpha_i'}(p_i, p_i'; E_{q_i}) \times \big[ \psi_j(p_i' q_i \alpha_i') + \psi_k(p_i' q_i \alpha_i') \big]$$

♦ Coupled integral equations in two variables: $p_i$ and $q_i$

## Bound state Faddeev equations with separable potentials

- Separable potential $\Rightarrow$ $t$-matrix elements have form

$$t_i^{\alpha_i \alpha_i'}(p_i, p_i'; E_{q_i}) = \sum_{mn}^{rank} h^i_{m\alpha_i}(p_i)\, \tau_{mn}^{\alpha_i \alpha_i'}(E_{q_i})\, h^i_{n\alpha_i'}(p_i')$$

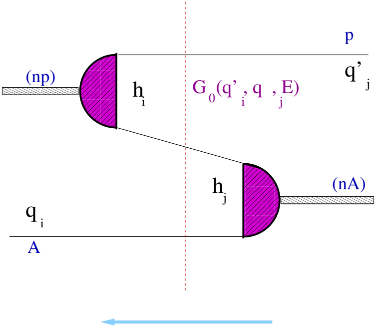
- Faddeev components become separable, e.g., if rank=1:

$$\psi_i(p_i q_i \alpha_i) = h^i(p_i)\, F^{(i)}_{\alpha_i}(q_i)$$

- Task is reduced to solving for functions $F^{(i)}(q_i)$ which fulfill

$$\begin{aligned} F^{(i)}_{\alpha_i}(q_i) &= \sum_{\alpha_j \alpha_j'} \int dq_j{}'\, {q_j'}^2\, Z^{(ij)}_{\alpha_i \alpha_j'}(q_i, q_j'; E_{3b})\, \tau^{\alpha_j \alpha_j'}(q_j')\, F^{(j)}_{\alpha_j'}(q_j') \\ &+ \sum_{\alpha_k \alpha_k'} \int dq_k'\, {q_k'}^2\, Z^{(ik)}_{\alpha_i \alpha_k'}(q_i, q_k'; E_{3b})\, \tau^{\alpha_k \alpha_k'}(q_k')\, F^{(k)}_{\alpha_k'}(q_k') \end{aligned}$$

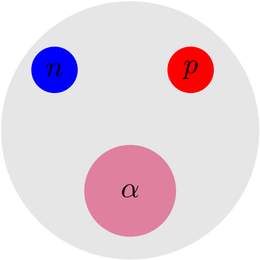
# The "transition potential" $Z^{(ij)}(q_i, q'_j; E_{3b})$




$Z^{(ij)}(q_i, q'_j)$ all contains three-body dynamics

$$= \int_{-1}^{1} dx \;\; h^i_{m\alpha_i}(\pi_i)\, G_{\alpha_i\alpha_j}(q_i, q_j, x)\, \frac{1}{E - \frac{q_i^2}{2M_i} - \frac{\pi_i^2}{2\mu_i} + i\varepsilon}\, h^j_{n\alpha_j}(\pi_j)$$

# Test Case I: 3-Body model for $^6$Li ground state




Three-body model for $^6\text{Li} \equiv n + p + \alpha$

- Alpha particle tightly bound $E_4$ $[\alpha]$= -28.3 MeV
- Two nucleons loosely bound with $E_3$ $[^6\text{Li}]$= -3.7 MeV
- Several Faddeev-type calculations exist for $^6$Li
  $\Rightarrow$ ideal case for benchmarking [e.g. Thompson *et al.*, Phys. Rev. **C61**, 024318 (2000), Eskandarian *et al.* , Phys. Rev. **C46**, 2344 (1992)]

# The effective $n+p+\alpha$ Hamiltonian

## $np$ potential $(J^\pi = 1^+, S = 1)$

- CD-Bonn potential [R. Machleidt, Phys. Rev. C63, 024001 (2001)]

## $n/p - \alpha$ potential $(S_{1/2}, P_{1/2}, P_{3/2})$

- The Bang potential [J. Bang *et al.*, Nucl. Phys. A405, 126 (1983)]:

$$v(r) = -\frac{V_0}{1+\exp\left(\frac{r-R_0}{a_0}\right)} + \left(\frac{1}{r}\right)\frac{d}{dr}\frac{V_{so}}{1+\exp\left(\frac{r-R_{so}}{a_{so}}\right)}\,\mathbf{l}\cdot\boldsymbol{\sigma}$$

$V_0 = 44$ MeV $a_0 = 0.65$ fm, $R_0 = 2$ fm, $V_{so} = 40$ MeVfm
$a_{so} = 0.37$ fm, $R_{so} = 1.5$ fm

## $p - \alpha$ Coulomb potential: charged sphere

$$V_c(r) = \begin{cases} \frac{Ze^2}{2R_c}\left[3 - \left(\frac{r}{R_c}\right)^2\right] & r \le R_c \\ \frac{Ze^2}{r} & R_c < r < R_{cutoff} \end{cases}$$

Sharp cutoff

# Convergence of the Three-Body Binding Energy

CD-Bonn $np$ potential

| label | rank | $E_3$ [MeV] |
|---|---|---|
| EST5-1 | 5 | -**3.78**47 |
| EST5-2 | 5 | -**3.78**48 |
| EST5-3 | 5 | -**3.78**55 |
| EST6-1 | 6 | -**3.78**67 |
| EST6-2 | 6 | -**3.78**68 |
| EST6-3 | 6 | -**3.78**71 |
| EST7-1 | 7 | -**3.7867** |
| EST7-2 | 7 | -**3.7867** |
| EST7-3 | 7 | -**3.7867** |
| **EXACT:** | | -3.787 |

[L. Hlophe, Jin Lei, *et al.*, Phys. Rev. **C 96**, 2017 ]

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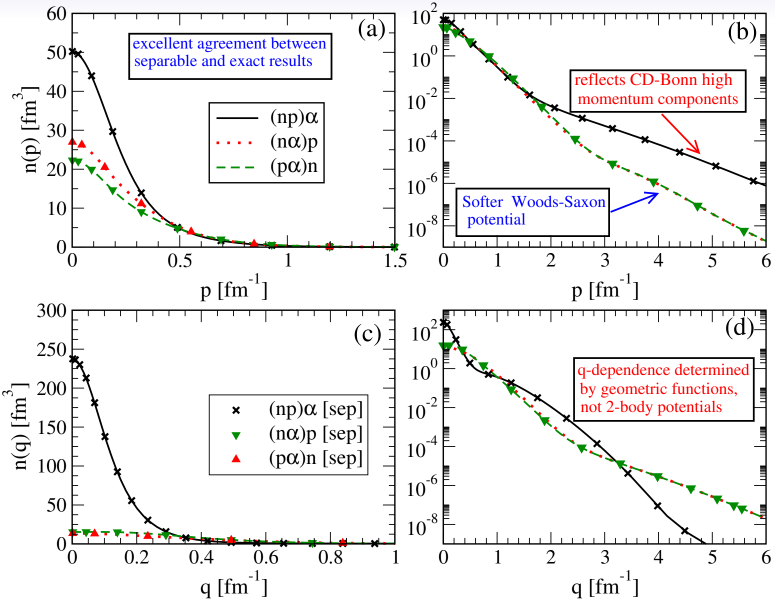
| EST7-3 | 7 | **-3.7867** |
| **EXACT:** | | **-3.787** |

**Bang $n\alpha$ potential**

| label | rank | $E_{3b}$ [MeV] |
|---|---|---|
| EST6-1 | 6 | -**3.785**6 |
| EST6-2 | 6 | -**3.785**2 |
| EST6-3 | 6 | -**3.785**2 |
| EST7-1 | 7 | -**3.786**8 |
| EST7-2 | 7 | -**3.786**4 |
| EST7-3 | 7 | -**3.786**7 |
| EST8-1 | 8 | -**3.78**70 |
| EST8-2 | 8 | -**3.78**70 |
| EST8-3 | 8 | -**3.78**66 |
| **EXACT:** | | **-3.787** |

♦ **Four significant figures** stable w.r.t (1) choice of $\{E_m\}$ and (2) rank; agrees with **exact** calculation; with Coulomb $E_3 = -2.777$ MeV

# Momentum distributions: separable vs non-separable



# **Faddeev-AGS equations:** processes treated on equal footing

- Observables: $\sigma_{i\leftarrow j} \propto \left|\langle\Phi_i|V_j + V_k|\Psi_j^{(+)}\rangle\right|^2 = \left|\langle\Phi_i|U^{ij}|\Phi_j\rangle\right|^2$

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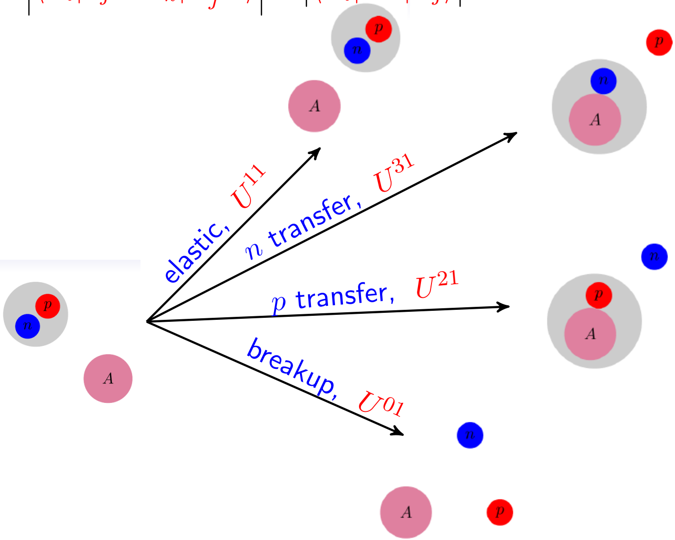


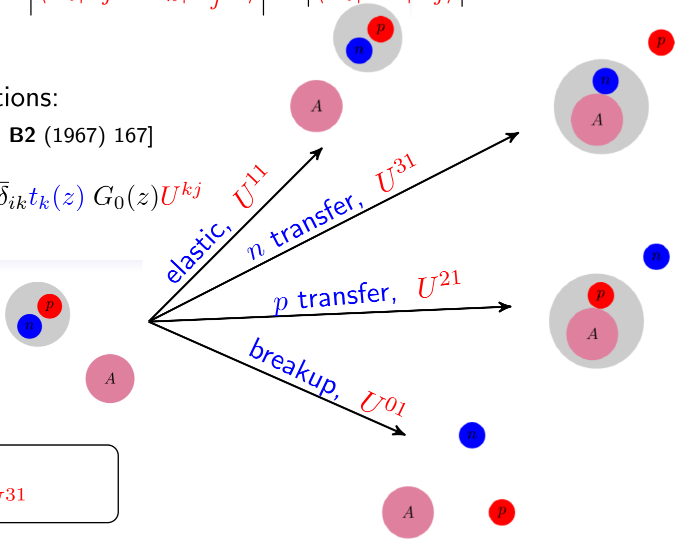
# Faddeev-AGS equations: processes treated on equal footing

- Observables: $\sigma_{i \leftarrow j} \propto \left| \langle \Phi_i | V_j + V_k | \Psi_j^{(+)} \rangle \right|^2 = \left| \langle \Phi_i | U^{ij} | \Phi_j \rangle \right|^2$

- Faddeev-AGS equations:

  [Alt *et al.*, Nucl. Phys. **B2** (1967) 167]

$$U^{ij} = \bar{\delta}_{ij} \, G_0^{-1}(z) + \sum_k \bar{\delta}_{ik} t_k(z) \, G_0(z) U^{kj}$$




**Breakup amplitude:**
$U^{01} = U^{11} + U^{21} + U^{31}$

# Faddeev-AGS equations with separable two-body potentials

- Define amplitudes $X^{ij}_{mn}$ so that $\langle\Phi_i|U^{ij}|\Phi_j\rangle \equiv \sum_{mn}^{rank} c_m c_n \langle q_i|X^{ij}_{mn}|q_j\rangle$

- Amplitudes $X^{ij}_{mn}(q_i,q_j)$ fulfill, e.g., if rank=1

$$X^{ij}(q_i,q_j) = Z^{ij}(q_i,q_j;E_{3b}) + \sum_k \int dq_k\, q_k^2\, Z^{ik}(q_i,q_k;E_{3b})\, \tau^{(k)}(E_{q_k})\, X^{kj}(q_k,q_j)$$

[C. Lovelace, Phys.Rev. 135 (1964) B1225]

## Below 3-body breakup:

- Only bound state singularities exist
- So-called 'transition potentials' $Z^{ij}(q_i,q_j;E_{3b}) \equiv \langle h_i|G_0(E_{3b}|h_j\rangle)$ can be computed
- Faddeev-AGS equations $\Rightarrow$ multichannel Lippmann-Schwinger-type equations

## Above three-body breakup threshold

- Propagator has moving singularities since

$$G_0(E, p_i, q_i) = [E_{3b} - p_i^2/2M_i - q_i^2/2\mu_i + i\epsilon]^{-1}$$

- Transition potentials $Z^{ij}(q_i, q_j; E_{3b})$ cannot be evaluated for $q_i < \sqrt{2M_i E_{3b}}$ and $q_j < \sqrt{2M_i E_{3b}}$

- Faddeev-AGS equations are rewritten with explicit integration over pair momenta $p$
  - two-body bound state and three-body breakup poles are treated by the simple subtraction method
  - coupled integral equations depend on both $p$ and $q$ variables, but solution $X^{ij}$ depends only on spectator momenta $q$

# Faddeev-AGS equations above breakup

$$X^{ij}_{\alpha_i,\alpha_j}(q_i,q_j;z) = Z^{ij}_{\alpha_i,\alpha_j}(q_i,q_j,z)$$

$$+ \sum_{k\alpha_k\alpha'_k} \int dq_k\, q_k^2\, \bar{Z}^{ik}_{\alpha_i,\alpha_k}(q_i,q_k,z)\, \tau^{\alpha_k\alpha'_k}(E_{q_k})\, X^{kj}_{\alpha'_k,\alpha_j}(q_k,q_j;z)$$

$$+ \int dp_i\, p_i\, \frac{1}{\beta q_i}\, h^i_{\alpha_i}(p_i)\, \frac{2\mu_i}{p^2_{0i}(q_i) - p_i + i\varepsilon} \Bigg[ \sum_{k\alpha_k\alpha'_k} \bar{\delta}_{ik}$$

$$\times \int_{q_k=|p_i-\beta q_i|}^{q_k=p_i+\beta q_i} dq_k\, q_k\;\; h^k_{\alpha_k}(\pi_k)\, \frac{1}{\epsilon_k + \frac{{\pi_k}^2}{2\mu_k}}\, G_{\alpha_i\alpha_k}(q_i,q_k,x_0)\, \tilde{\tau}^{\alpha_k\alpha'_k}(E_{q_k})$$

$$\times \;\; X^{kj}_{\alpha'_k,\alpha_j}(q_k,q_j;z) \Bigg]$$

**additional term due to pole**

## The effective $n + p + \alpha$ Hamiltonian

$np$ potential $(J = 0, 1, 2, 3,\ l_{max} = 2)$

- CD-Bonn potential [R. Machleidt, Phys. Rev. C63, 024001 (2001)]

Above three-body breakup threshold

$n/p - \alpha$ potential $(S_{1/2}, P_{1/2}, P_{3/2},\ D_{3/2}, D_{5/2})$

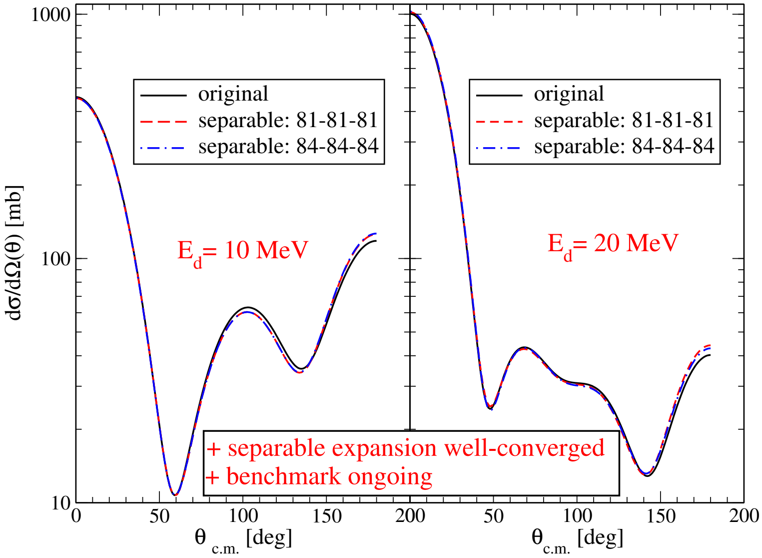
- The Bang potential [J. Bang *et al.*, Nucl. Phys. A405, 126 (1983)]:

$$v(r) = -\frac{V_0^l}{1+\exp\left(\frac{r-R_0}{a_0}\right)} + \left(\frac{1}{r}\right)\frac{d}{dr}\frac{V_{so}}{1+\exp\left(\frac{r-R_{so}}{a_{so}}\right)}\,\mathbf{l}\cdot\boldsymbol{\sigma}$$

$V_0^{l=0,1} = 43$ MeV, $V_0^{l=2} = 21.6$ MeV, $a_0 = 0.65$ fm, $R_0 = 2$ fm, $V_{so} = 40$ MeVfm, $a_{so} = 0.37$ fm, $R_{so} = 1.5$ fm

## Test Case II: 3-Body model for $d+\alpha$ Scattering

Coulomb potential omitted



## Summary

- Calculated $^6$Li ground state properties by
  (a) directly solving of the Faddeev equations with realistic two-body potentials
  (b) performing a separable expansion of two-body potentials/$t$-matrices and solving one-dimensional coupled equations
- Support energies and momenta are chosen independently
  $\Rightarrow$ essential for attaining precise results
- Three-body binding energy predictions using separable expansion agrees perfectly with exact result within four digits
- Calculated elastic $d+\alpha$ scattering wavefunctions with EST-type multi-rank separable potentials:
  (a) Rank-8 sufficient to obtain converged results
  (b) Agreement with calculations carried out with original Hamiltonian is good, but benchmarking still ongoing

## Outlook

- Complete benchmarking for $d + \alpha$ scattering, extend to heavier systems such as Ca and Pb isotopes
- Full incorporation of the Coulomb potential in Faddeev-AGS equations
- Include target excitations: can be readily incorporated within existing machinery
- **Ultimate goal:** Perform $d + A$ scattering calculations for
  - neutron-rich nuclei from He $(Z = 4)$ to Pb $(Z = 82)$
  - energies between 0 and $100$ MeV/nucleon (relevant range e.g. for FRIB)

# Acknowledgments

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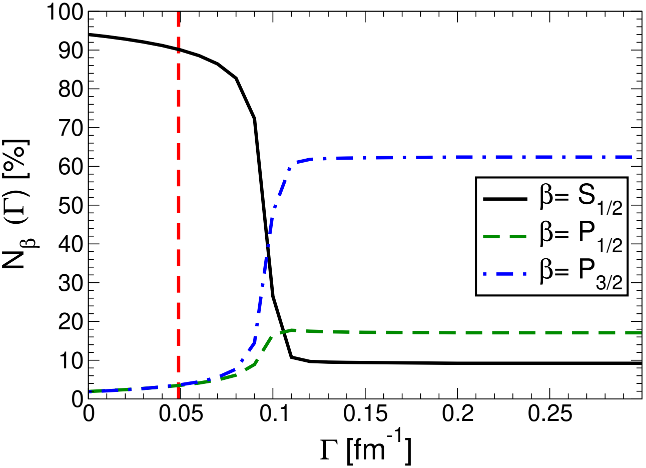
# Probability of the $S_{1/2}$ State

Define probability: $N_\beta(\Gamma) = \sum_\gamma \int_0^\infty dp\, dq\, p^2 q^2 \left|\Psi_{\alpha=\{\beta,\gamma\}}(p,q;\Gamma)\right|^2$

- 3-body wavefunction initially dominated by $S_{1/2}$ wave, which supports forbidden state

- Around $\Gamma = 0.1$ fm$^{-1}$ $S_{1/2}$ probability falls drastically, increases rapidly for $P_{1/2}$ and $P_{3/2}$



## Treatment of Bound State and Breakup Poles

- General singularity structure:

$$\text{S.T.} \quad = \quad \frac{1}{E_{3b} - \frac{{q_k}^2}{2M_k} - \frac{{p_k}^2}{2\mu_k} + i\varepsilon} \; \frac{1}{E_{3b} - \frac{{q_k}^2}{2M_k} + \epsilon_k + i\varepsilon}$$

- Separate the two poles, partial fractions:

$$\begin{aligned}
\text{S.T.} \quad &= \quad \frac{1}{E_{3b} - \frac{{q_k}^2}{2M_k} - \frac{{p_k}^2}{2\mu_k} + i\varepsilon} \; \frac{1}{E_{3b} - \frac{{q_k}^2}{2M_k} + \epsilon_k + i\varepsilon} \\
&= \quad \frac{1}{\epsilon_k + \frac{{p_k}^2}{2\mu_k}} \; \frac{1}{E_{3b} - \frac{{q_k}^2}{2M_k} - \frac{{p_k}^2}{2\mu_k} + i\varepsilon} - \frac{1}{\epsilon_k + \frac{{p_k}^2}{2\mu_k}} \; \frac{1}{E_{3b} - \frac{{q_k}^2}{2M_k} + \epsilon_k + i\varepsilon} \\
&= \quad \frac{1}{\epsilon_k + \frac{{p_k}^2}{2\mu_k}} \; \frac{2\mu_k}{p_{0k}^2(q_k) - p_i^2 + i\varepsilon} - \frac{1}{\epsilon_k + \frac{{p_k}^2}{2\mu_k}} \; \frac{2M_k}{q_{0k}^2 - q_k^2 + i\varepsilon},
\end{aligned}$$

## Taking the limit $v_{sep} \to V$

Potential $V$ on momentum grid $[p_1, p_2, ..., p_N]$, $V(p_m, p_n)$:

Eigenstates of $V(p_m, p_n)$:

$$V|\varphi_n\rangle = \lambda_n|\varphi_n\rangle \quad (1)$$

Eigenstates of $V$:

$$V(p', p) = \sum_{n=1}^{N} \varphi_n(p')\tilde{\lambda}_n\varphi_n(p),$$

$$\equiv \sum_{n,m=1}^{N} \varphi(p')\, \lambda_{nm}\, \varphi_m(p), \quad (2)$$