Reactions in three body cluster states

Carolina Romero Redondo

Eduardo Garrido, Alejandro Kievsky and Michele Viviani

Petr Navratil, Sofia Quaglioni

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Eduardo Garrido, Alejandro Kievsky and Michele Viviani ⬅ Integral relations

Petr Navratil, Sofia Quaglioni ⬅ NCSM/RGM

Scattering in three-body cluster states

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TRIUMF
February 25th, 2012

Outline

Integral Relations

The Hyperspherical adiabatic expansion method

Studying scattering with HA method
Motivation
Particular Cases

Conclusions I

Three-body cluster NCSM/RGM

Scattering in three-body cluster states

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Introduction

Scattering properties are usually obtained from the long distance behavior of the wave function

Calculating **accurate** asymptotic wave functions can be complicated

Scattering in three-body cluster states

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Introduction

Scattering properties are usually obtained from the long distance behavior of the wave function

Calculating **accurate** asymptotic wave functions can be complicated

↓

Solution:

Extract the scattering matrix from the internal part of the wave function

We derived, from Kohn variational principle, a formalism in which the use of two integral relations solves this problem

* PRL **103,** 090402 (2009). One channel in s-wave

* PRA **83,** 022705 (2011). General form of the method

Integral relations

Asymptotic Behaviour

$$\Psi \rightarrow F - KG$$

Where F and G are asymptotic solutions of the Hamiltonian.

Integral relations

Asymptotic Behaviour

$$\boldsymbol{\Psi \rightarrow F - KG}$$

Where F and G are asymptotic solutions of the Hamiltonian.

Multichannel reaction

$$\boldsymbol{\Psi_n \rightarrow F_n - \sum_i K_{ni} G_i}$$

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Integral relations

Asymptotic Behaviour

$$\Psi \rightarrow F - KG$$

Undefined Normalization

$$\Psi \rightarrow AF + BG$$

Integral relations

Asymptotic Behaviour

$$\Psi \rightarrow F - KG$$

Undefined Normalization

$$\Psi \rightarrow AF + BG$$

$$\mathcal{K} = -A^{-1}B$$

We just need to calculate A and B!

Integral relations

General expressions for A and B

$$B = -\frac{2m}{\hbar^2}\left[\langle F|\hat{\mathcal{H}} - E|\Psi\rangle^T - \langle\Psi|\hat{\mathcal{H}} - E|F\rangle\right]$$

$$A = -\frac{2m}{\hbar^2}\left[\langle\Psi|\hat{\mathcal{H}} - E|G\rangle - \langle G|\hat{\mathcal{H}} - E|\Psi\rangle^T\right]$$

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Integral relations

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$$\boldsymbol{B = -\frac{2m}{\hbar^2}\left[\langle F|\hat{\mathcal{H}} - E|\Psi\rangle^T - \langle\Psi|\hat{\mathcal{H}} - E|F\rangle\right]}$$

$$\boldsymbol{A = -\frac{2m}{\hbar^2}\left[\langle\Psi|\hat{\mathcal{H}} - E|G\rangle - \langle G|\hat{\mathcal{H}} - E|\Psi\rangle^T\right]}$$

If ψ is the exact solution, then:

$$A = -\frac{2m}{\hbar^2}\langle\Psi|\hat{\mathcal{H}} - E|G\rangle$$

$$B = \frac{2m}{\hbar^2}\langle\Psi|\hat{\mathcal{H}} - E|F\rangle$$

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Integral relations

General expressions for A and B

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$$\boldsymbol{A = -\frac{2m}{\hbar^2}\left[\langle \Psi|\hat{\mathcal{H}} - E|G\rangle - \langle G|\hat{\mathcal{H}} - E|\Psi\rangle^T\right]}$$

If ψ is the exact solution, then:

$$A = -\frac{2m}{\hbar^2}\langle \Psi_t|\hat{\mathcal{H}} - E|G\rangle$$

$$B^{2^{nd}} = \frac{2m}{\hbar^2}\langle \Psi_t|\hat{\mathcal{H}} - E|F\rangle$$

$$\Psi_t = \Psi + \delta\Psi$$

Integral relations

Kohn Variational Principle

Stationary functional:

$$A^{-1}B^{2^{nd}} = A^{-1}B + \frac{2m}{\hbar^2}A^{-1}\langle\Psi_t|\hat{\mathcal{H}} - E|\Psi_t\rangle(A^{-1})^T$$

P. Barletta *et al.* PRL **103,** 090402 (2009).
C. Romero-Redondo *et al.* PRA **83,** 022705 (2011).

Integral relations

Kohn Variational Principle

Stationary functional:

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$$A = -\frac{2m}{\hbar^2}\langle\Psi_t|\hat{\mathcal{H}} - E|G\rangle$$

$$B^{2^{nd}} = \frac{2m}{\hbar^2}\langle\Psi_t|\hat{\mathcal{H}} - E|F\rangle$$

$$\mathcal{K} = -A^{-1}B^{2^{nd}}$$

$$\mathcal{S} = (1 + i\mathcal{K})(1 - i\mathcal{K})^{-1}$$

Integral relations

The integral relations are general:

* They can be used with wave functions calculated from different methods (in particular with HA method).

* Are extremely useful when the inner part of the wave function can be calculated much accurately than the asymptotic part

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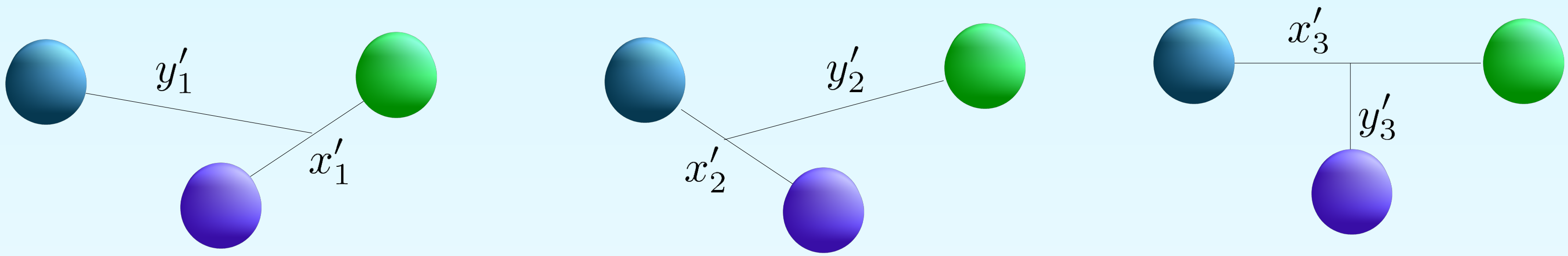
Adiabatic Approximation

Jacobi Coordinates



$$(T-E)\,\psi^{(1)}_{JM} + V_1\left(\psi^{(1)}_{JM} + \psi^{(2)}_{JM} + \psi^{(3)}_{JM}\right) = 0$$

$$(T-E)\,\psi^{(2)}_{JM} + V_2\left(\psi^{(1)}_{JM} + \psi^{(2)}_{JM} + \psi^{(3)}_{JM}\right) = 0$$

$$(T-E)\,\psi^{(3)}_{JM} + V_3\left(\psi^{(1)}_{JM} + \psi^{(2)}_{JM} + \psi^{(3)}_{JM}\right) = 0$$

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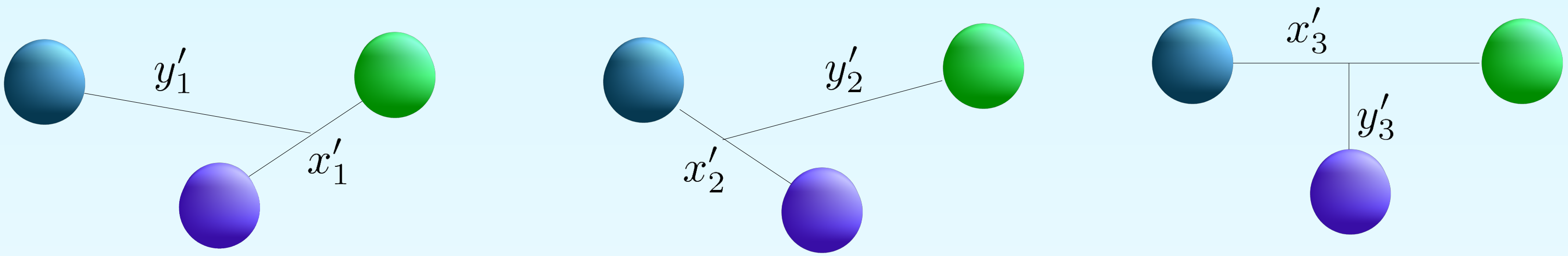
Adiabatic Approximation

Jacobi Coordinates



$$(T-E)\,\psi^{(1)}_{JM} + V_1\left(\psi^{(1)}_{JM}+\psi^{(2)}_{JM}+\psi^{(3)}_{JM}\right)=0$$

+

$$(T-E)\,\psi^{(2)}_{JM} + V_2\left(\psi^{(1)}_{JM}+\psi^{(2)}_{JM}+\psi^{(3)}_{JM}\right)=0$$

+

$$(T-E)\,\psi^{(3)}_{JM} + V_3\left(\psi^{(1)}_{JM}+\psi^{(2)}_{JM}+\psi^{(3)}_{JM}\right)=0$$

$$\boldsymbol{(T+V-E)\,\psi_{JM}=0}$$

Adiabatic Approximation

Hyperspherical coordinates

$$\rho = \sqrt{x^2 + y^2}, \qquad \alpha_i = \arctan(x_i/y_i), \qquad \Omega_{x_i},\ \Omega_{y_i}$$

Scattering in three-body cluster states

Adiabatic Approximation

Hyperspherical coordinates

$$\boldsymbol{\rho = \sqrt{x^2 + y^2}, \qquad \alpha_i = \arctan(x_i/y_i), \qquad \Omega_{x_i},\ \Omega_{y_i}}$$

Angular Equation

$$\hat{\Lambda}^2 \phi_n^{(i)} + \frac{2m\rho^2}{\hbar^2} V_{jk}(x_i) \left(\phi_n^{(i)} + \phi_n^{(j)} + \phi_n^{(k)} \right) = \lambda_n(\rho) \phi_n^{(i)}$$

Radial Equation

$$\left[-\frac{d^2}{d\rho^2} - \frac{2m}{\hbar^2} E + \frac{1}{\rho^2} \left(\lambda_n(\rho) + \frac{15}{4} \right) \right] f_n(\rho) + \sum_{n'} \left(-2P_{nn'} \frac{d}{d\rho} - Q_{nn'} \right) f_{n'}(\rho) = 0$$

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Adiabatic Approximation

Hyperspherical coordinates

$$\boldsymbol{\rho = \sqrt{x^2 + y^2}, \qquad \alpha_i = \arctan(x_i/y_i), \qquad \Omega_{x_i},\ \Omega_{y_i}}$$

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Adiabatic Approximation

$$\psi^{(i)} = \frac{1}{\rho^{5/2}} \sum_n f_n(\rho)\phi_n^{(i)}(\rho, \Omega_i)$$

Angular Equation

$$\hat{\Lambda}^2\phi_n^{(i)} + \frac{2m\rho^2}{\hbar^2}V_{jk}(x_i)\left(\phi_n^{(i)} + \phi_n^{(j)} + \phi_n^{(k)}\right) = \lambda_n(\rho)\phi_n^{(i)}$$

Radial Equation

$$\left[-\frac{d^2}{d\rho^2} - \frac{2m}{\hbar^2}E + \frac{1}{\rho^2}\left(\lambda_n(\rho) + \frac{15}{4}\right)\right] f_n(\rho) + \sum_{n'}\left(-2P_{nn'}\frac{d}{d\rho} - Q_{nn'}\right) f_{n'}(\rho) = 0$$

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Motivation

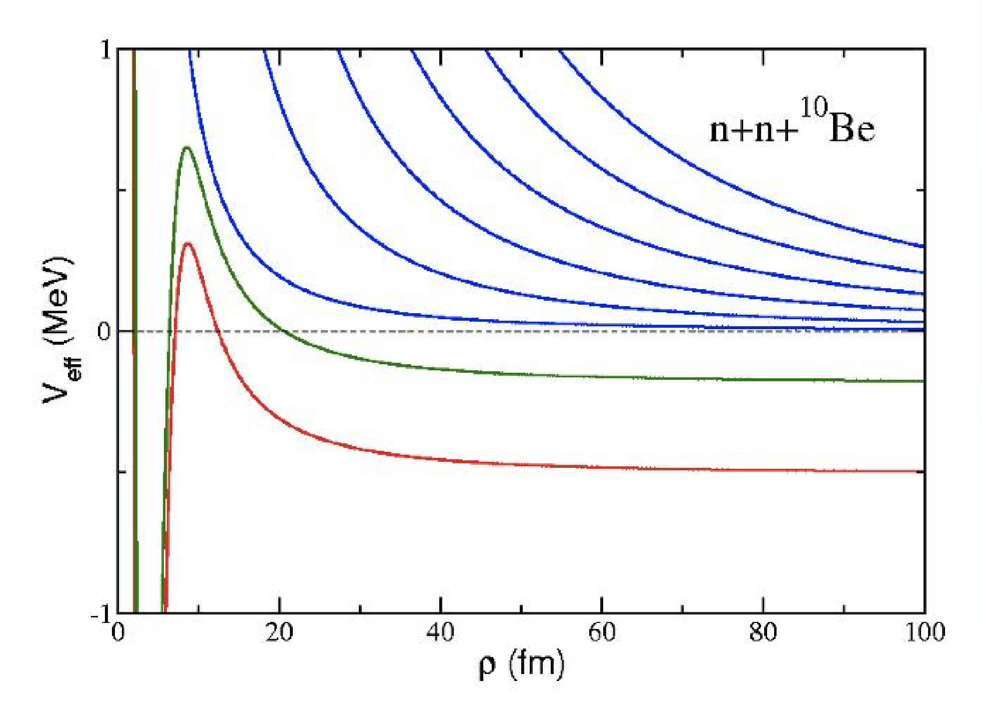
<u>Why</u> is it interesting to study reactions with this method?

Motivation

Advantage of the HA method

Differentiation of outgoing channel

in multi-channel scattering



Continuum states

^{11}Be*+n

^{11}Be+n

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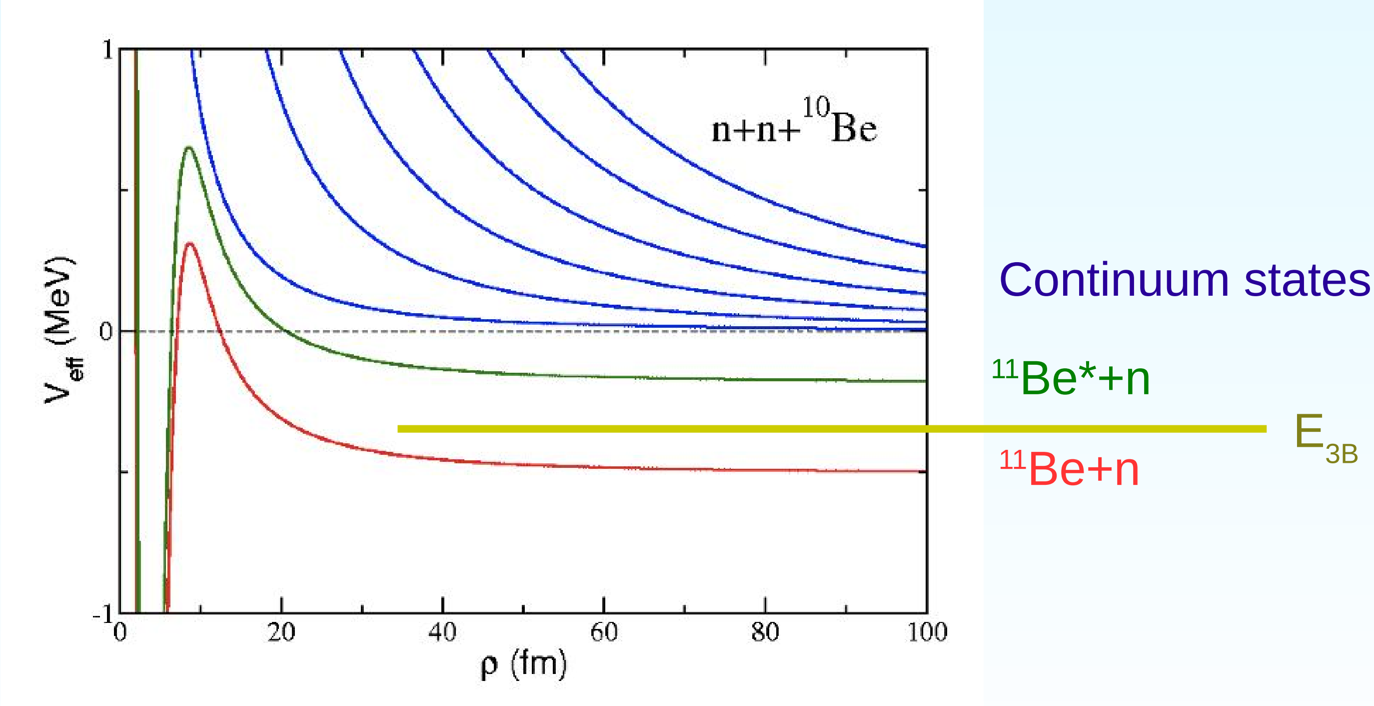

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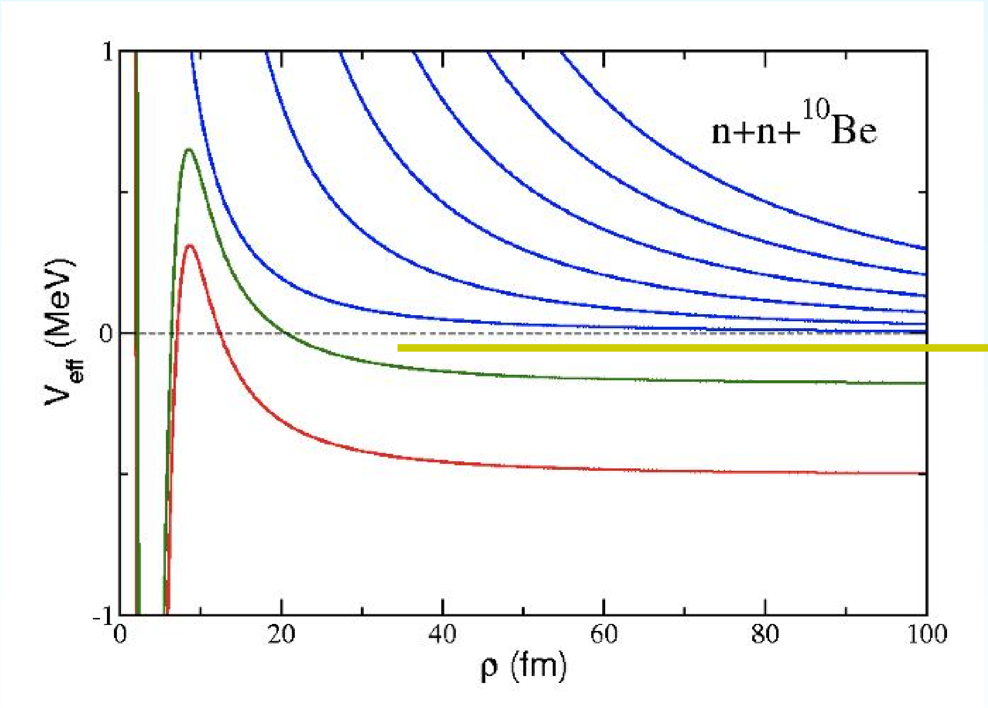


Continuum states

E_{3B}

^{11}Be*+n

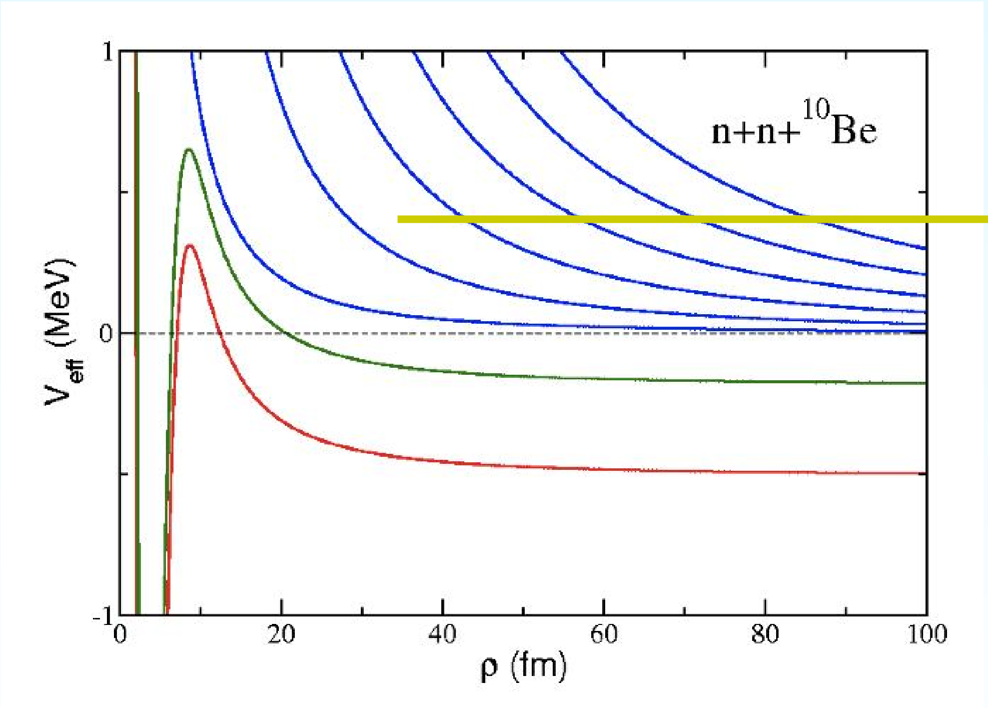
^{11}Be+n

Motivation

Advantage of the HA method

Differentiation of outgoing channel

in multi-channel scattering



E_{3B}

Continuum states

^{11}Be*+n

^{11}Be+n

Which processes could occur?

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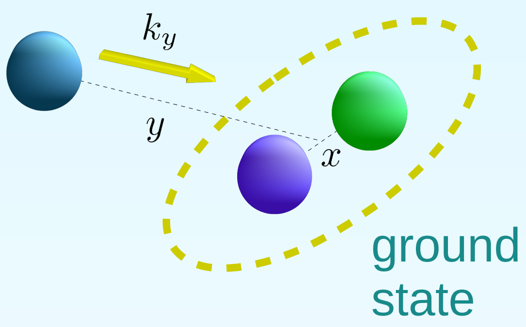

Incoming channel

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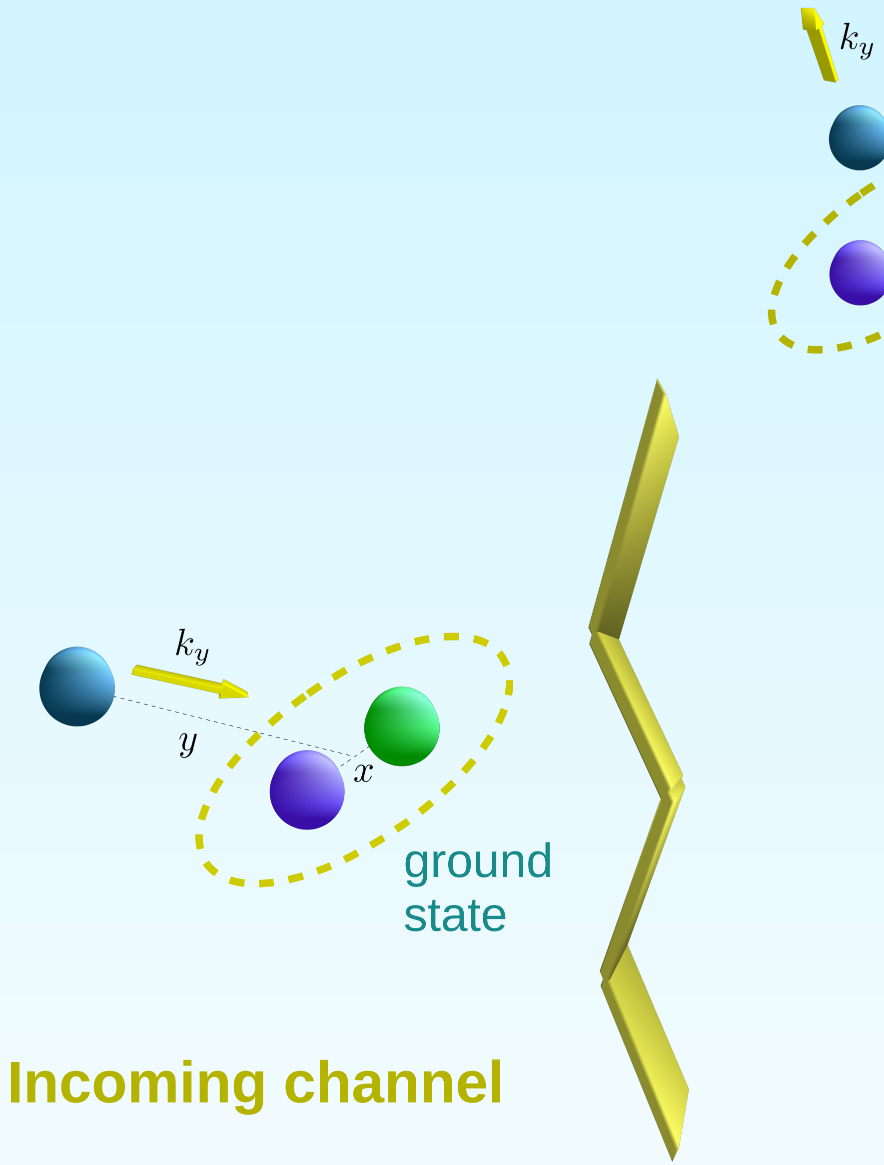
Elastic Scattering



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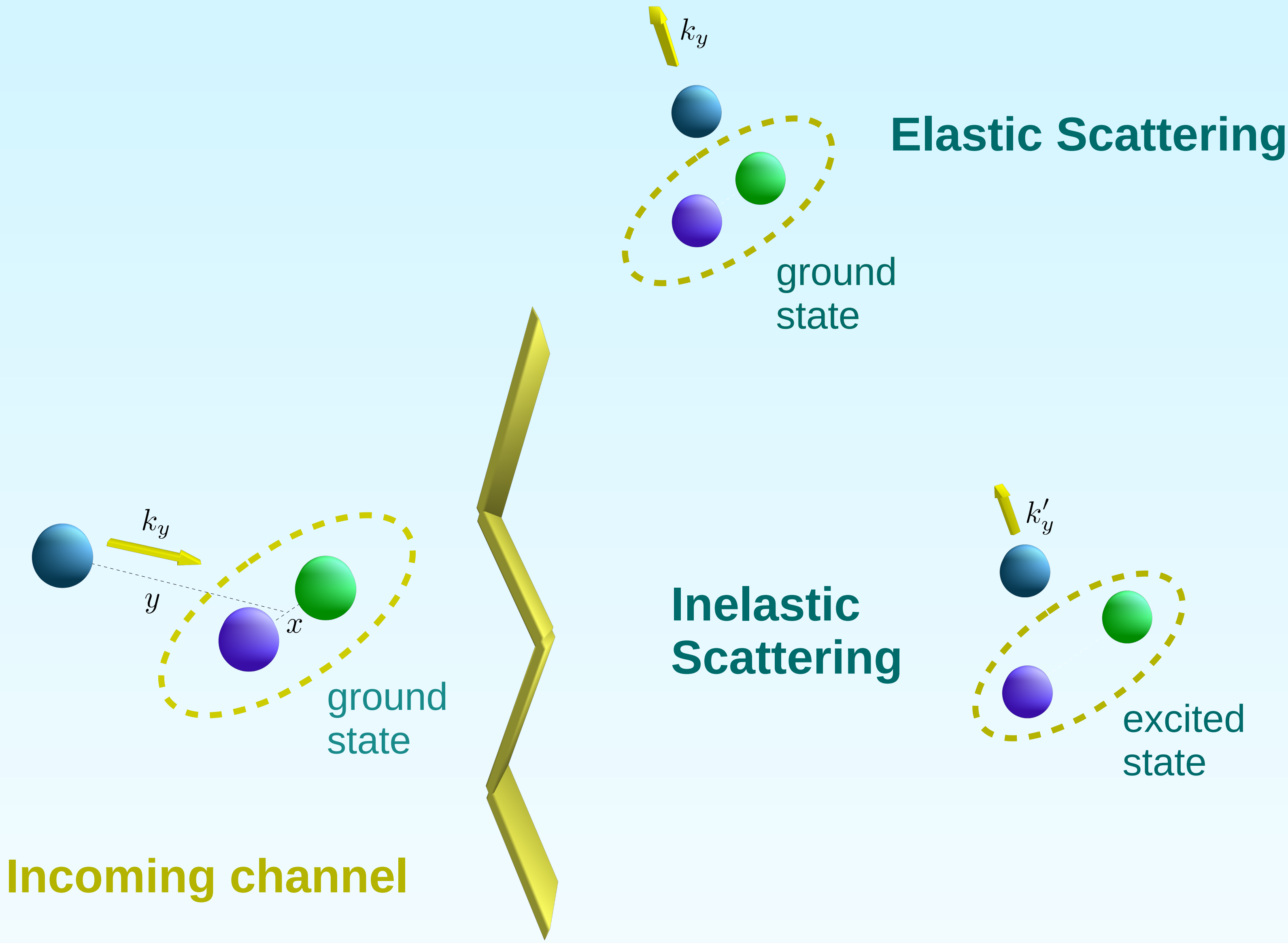

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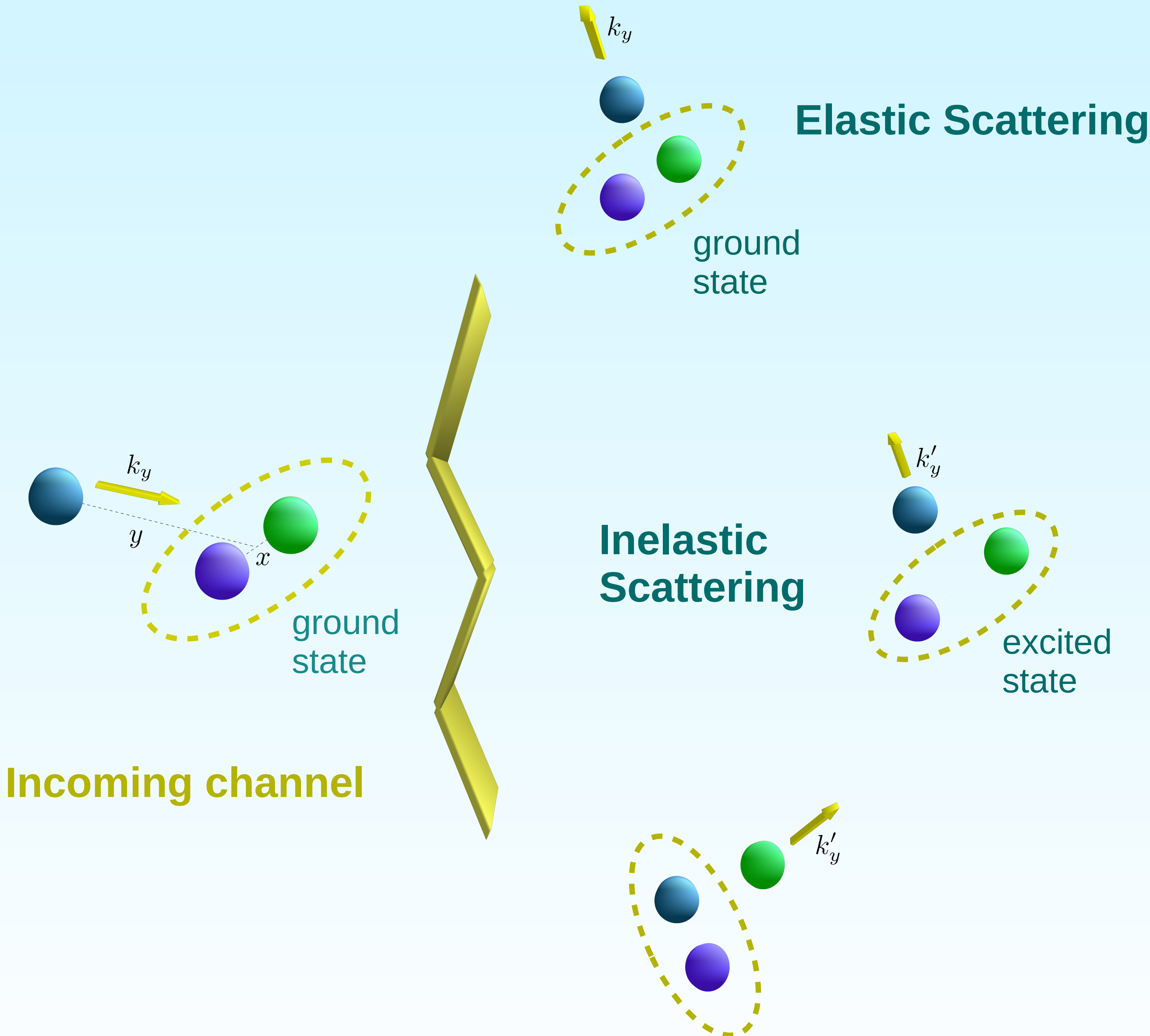
Scattering in three-body cluster states



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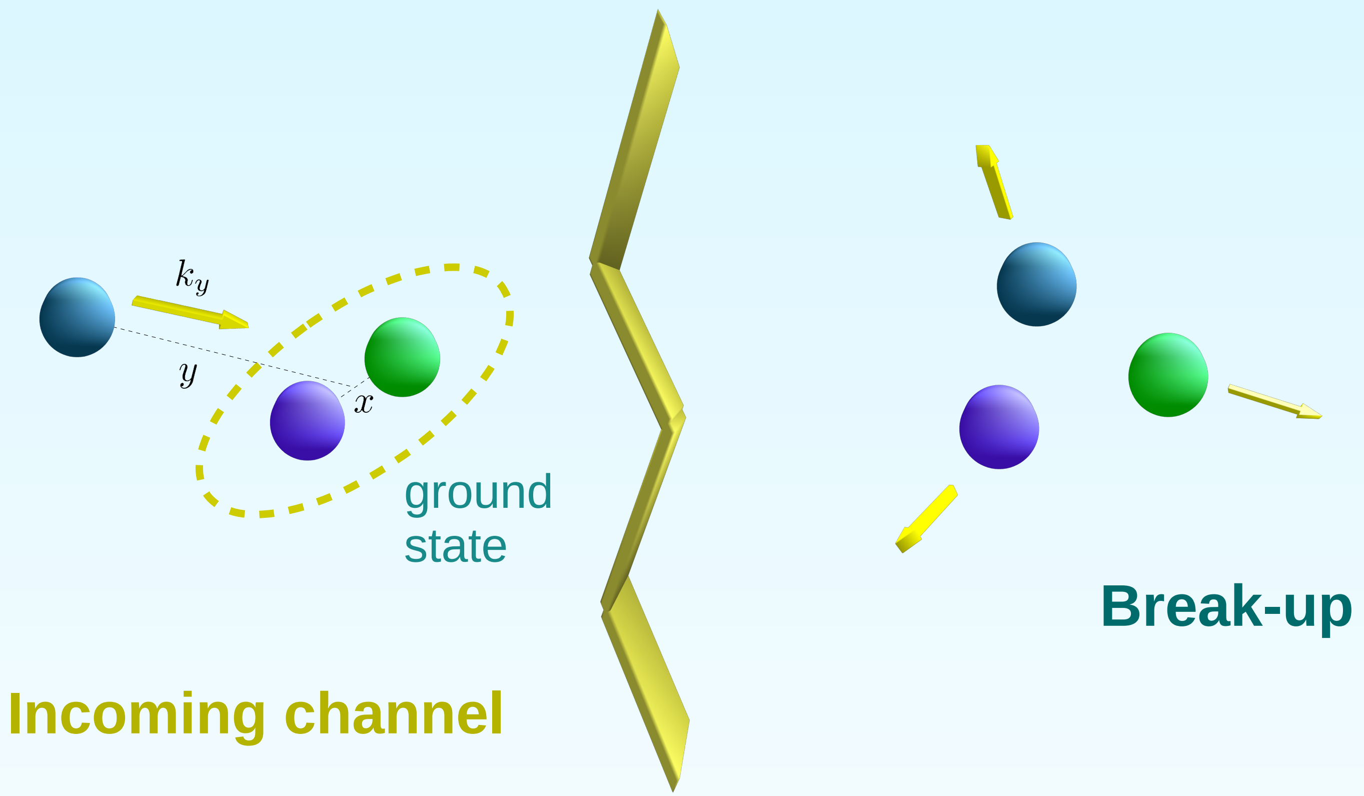
Scattering in three-body cluster states



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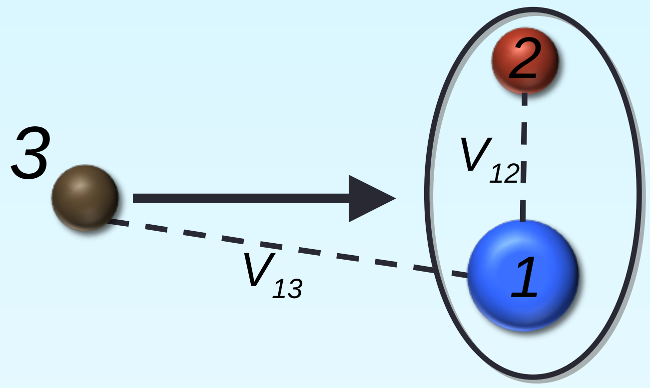
Particular Cases

A test case



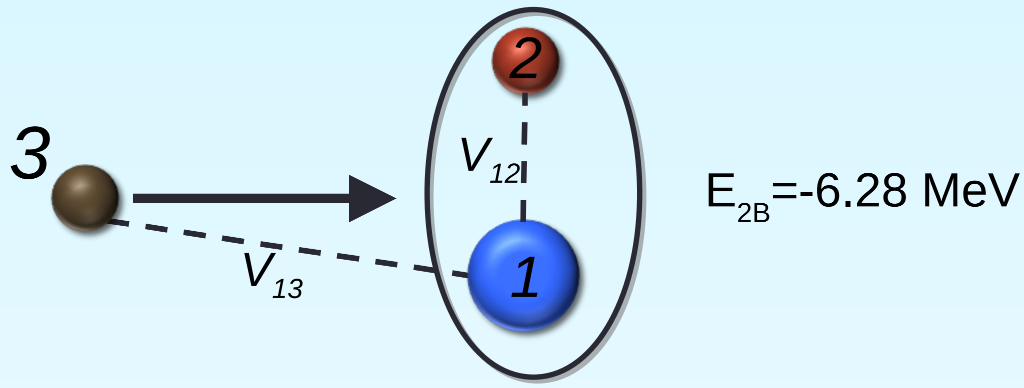
Particles 2 and 3 do not interact

Particle 1 with infinite mass

Only 1 and 2 form a bound state

The process is equivalent to a two-body collision between particles 1 and 3

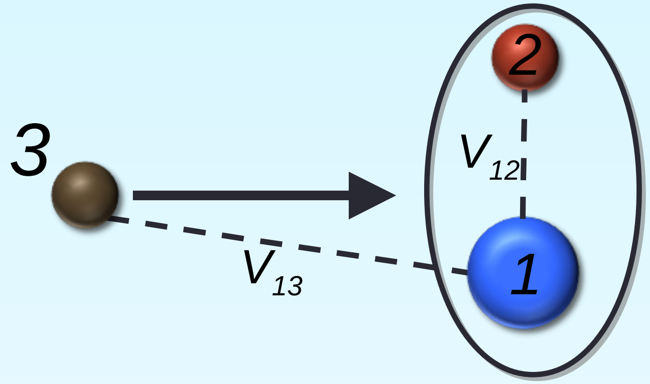
A test case

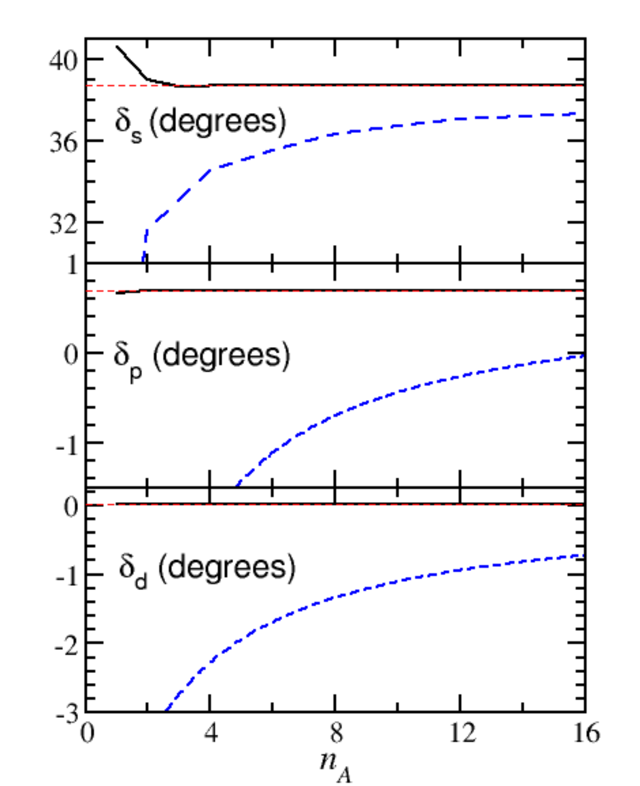


$E_{incident}$= 3 MeV (only elastic process allowed)

n_A	δ_s	δ_p	δ_d
1	40.554	0.6658	0.0136
2	38.988	0.6892	0.0113
3	38.642	0.6921	0.0121
5	38.693	0.6911	0.0119
8	38.702	0.6918	0.0118
10	38.701	0.6918	0.0118
two-body	38.699	0.6917	0.0117

A test case





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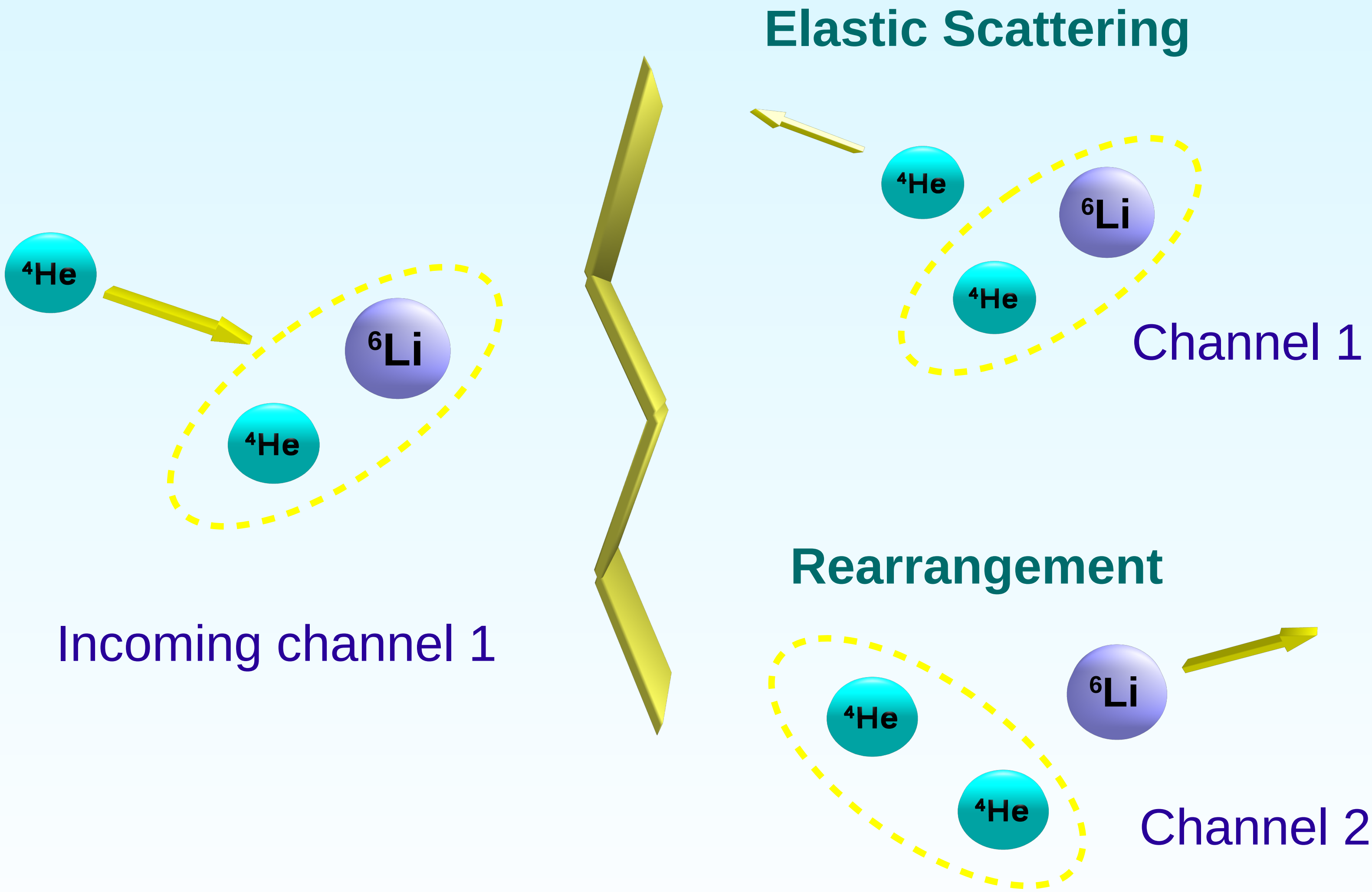
A multichannel collision: ^{4}He - ^{6}Li - ^{4}He



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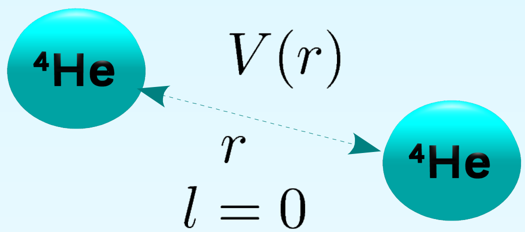
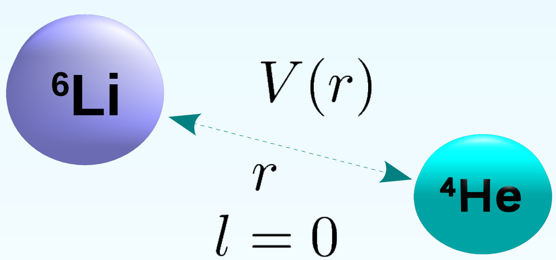
A multichannel collision: ^{4}He - ^{6}Li - ^{4}He

The two body potentials



$$V_{(^4He-^4He)}(r) = -1.227K \cdot \; e^{-r^2/(10.03a.u.)^2}$$

Bound state: E_{2B}= -1.2959mK



$$V^{*}_{(^6Li-^4He)}(r) = -0.27368K \cdot \; e^{-r^2/(20.14a.u.)^2}$$

Bound state: E_{2B}= -1.4225mK

*The parameters have been adjusted to give a scattering length of -173.5 a.u. and an effective range of 26.475 a.u. in agreement with the values obtained in U. Kleinekathöfer *et al.*, Phys. Rev. Lett. **83**, 4717 (1999)

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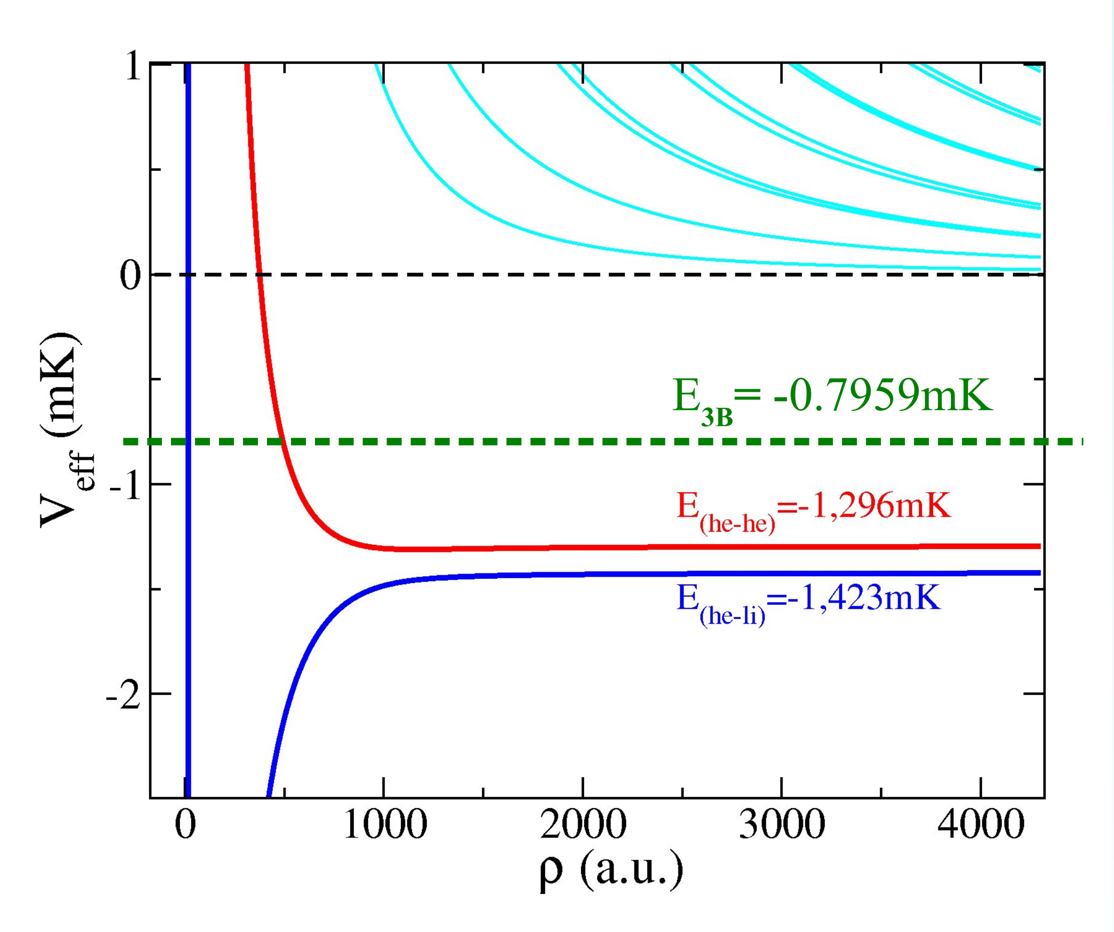
A multichannel collision: ^{4}He - ^{6}Li - ^{4}He

Results



Incident energy with { incoming channel 1: 0.6266mK
incoming channel 2: 0.5mK

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A multichannel collision: ^{4}He - ^{6}Li - ^{4}He

Results

K – matrix elements

n_A	$\mathcal{K}_{11}$	$\mathcal{K}_{12}$	$\mathcal{K}_{21}$	$\mathcal{K}_{22}$
2	-2.460	-0.650	-0.648	-1.411
3	-2.765	-0.821	-0.801	-1.496
4	-2.691	-0.775	-0.776	-1.468
6	-2.699	-0.781	-0.781	-1.471
8	-2.702	-0.783	-0.783	-1.471
10	-2.710	-0.787	-0.787	-1.473
14	-2.714	-0.790	-0.789	-1.474
18	-2.712	-0.791	-0.790	-1.474

$$\mathcal{K} = -A^{-1}B$$

A multichannel collision: ^{4}He - ^{6}Li - ^{4}He

Results

K – matrix elements

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10	-2.710	-0.787	-0.787	-1.473
14	-2.714	-0.790	-0.789	-1.474
18	-2.712	-0.791	-0.790	-1.474

$$\mathcal{K} = -A^{-1}B$$

A multichannel collision: ^4He - ^6Li - ^4He

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Results

S – matrix

$$\mathcal{S} = (1 + i\mathcal{K})(1 - i\mathcal{K})^{-1}$$

A multichannel collision: ^{4}He - ^{6}Li - ^{4}He

Results

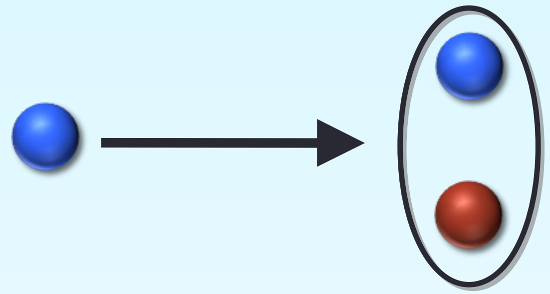
S – matrix

$$\mathcal{S} = (1 + i\mathcal{K})(1 - i\mathcal{K})^{-1}$$

Elastic scattering probability: $|\mathcal{S}_{11}|^2 = |\mathcal{S}_{22}|^2 = 0.892$

Rearrangement probability: $|\mathcal{S}_{12}|^2 = |\mathcal{S}_{21}|^2 = 0.108$

A break-up process: n+d



s-waves. S=3/2

J.L. Friar et al., PRC 42 (1990) 1838, PRC 51 (1995) 2356

$$V(r) = (-626.885e^{-1.55r} + 1438.72e^{-3.11r})/r$$

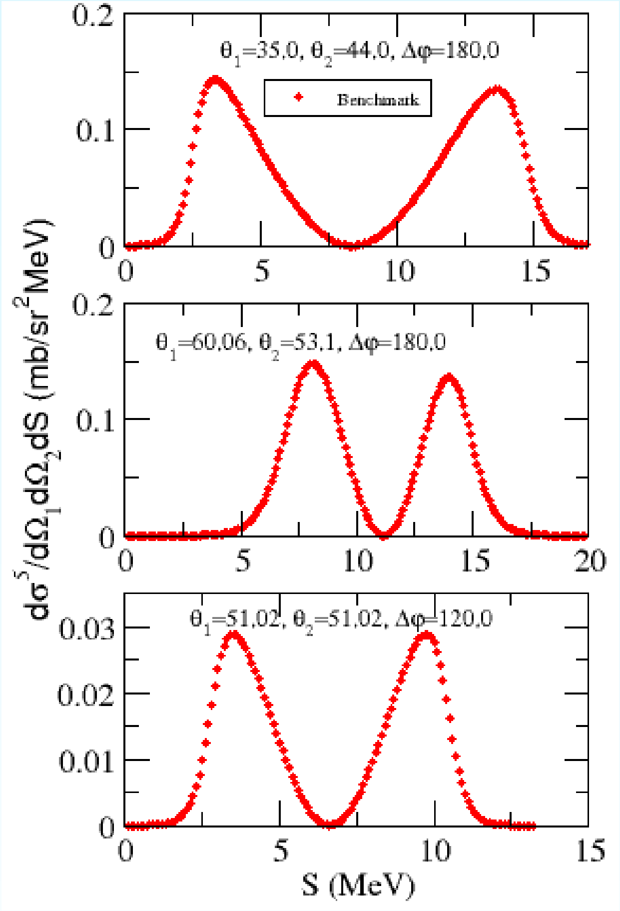
$$E_d = -2.2307\mathrm{MeV}$$

A break-up process: n+d

s-waves. S=3/2

E_{lab}=14.1 MeV	$\lvert S_{11}\rvert$	Re(δ_{11})
4 adiabs.	0.979	68.77
8 adiabs.	0.978	68.85
12 adiabs.	0.978	68.86
16 adiabs.	0.978	68.86
Benchmark	0.978	68.95

$$S_{11} = e^{2i\delta_{11}}$$



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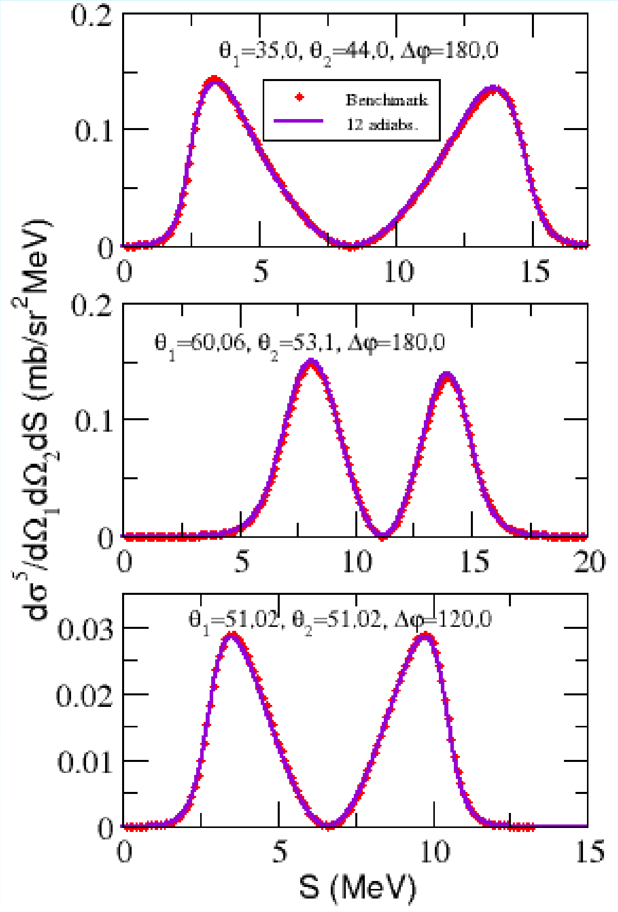
Benchmark	0.978	68.95

$$S_{11} = e^{2i\delta_{11}}$$



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Conclusions
(Integral Relations)

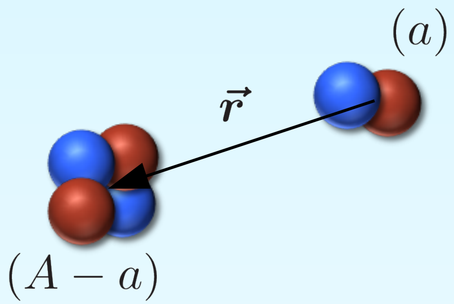
The integral relations derived from Kohn's variational principle permit obtaining the S-matrix from the internal part of the wave function

They can be applied to wave functions calculated with different methods. In particular, they permit using the HA method

We have tested the method in different cases below and over the breakup energy finding it to be a powerful tool to study reactions.

NCSM/RGM

Binary cluster

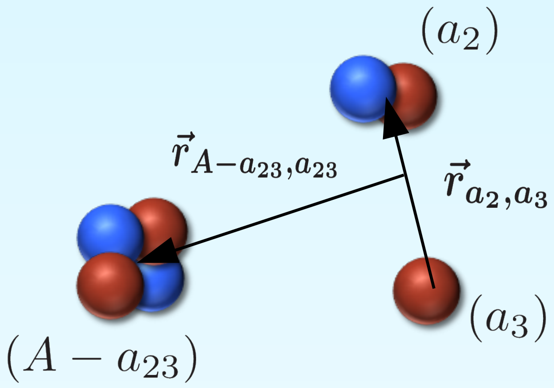


S. Quaglioni and P. Navratil

- PRL 101, 092501 (2008)
- PRC 79, 044606 (2009)

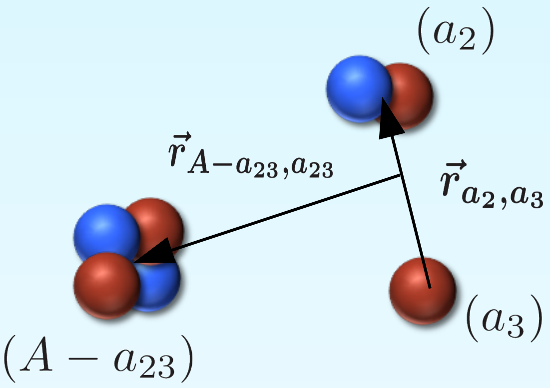
NCSM/RGM

Three-body cluster



NCSM/RGM

Three-body cluster



$$|\Psi^{J^\pi T}\rangle = \sum_\nu \int dx x^2 \int dy y^2 \hat{A}_\nu |\Phi^{J^\pi T}_{\nu x y}\rangle G^{J^\pi T}_\nu(x,y)$$

$$|\Phi^{J^\pi T}_{\nu x y}\rangle = \Big\{ \Big[|A-a_{23}\alpha_1 I_1^{\pi_1} T_1\rangle \left(|a_2 \alpha_2 I_2^{\pi_2} T_2\rangle |a_3 \alpha_3 I_3^{\pi_3} T_3\rangle\right)^{S_{23}T_{23}} \Big]^{sT} \left(Y_{\ell_x}(\hat{r}_{a_2,a_3}) Y_{\ell_x}(\hat{r}_{A-a_{23},a_{23}})\right)^L \Big\}^{J^\pi T} \frac{\delta(x-r_{a_2,a_3})}{x r_{a_2,a_3}} \frac{\delta(y-r_{A-a_{23},a_{23}})}{y r_{A-a_{23},a_{23}}}$$

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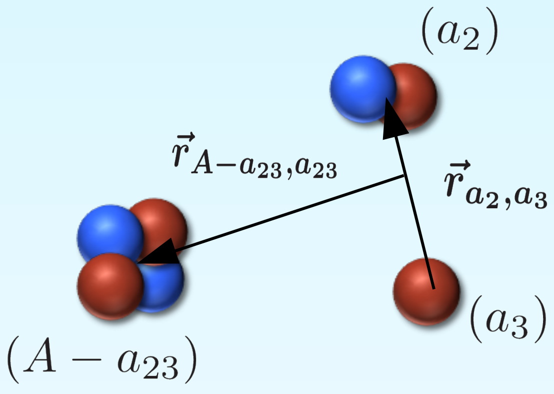

$$|\Psi^{J^\pi T}\rangle = \sum_\nu \int dx x^2 \int dy y^2 \hat{A}_\nu |\Phi^{J^\pi T}_{\nu x y}\rangle G^{J^\pi T}_\nu(x,y)$$

NCSM wave functions

$$|\Phi^{J^\pi T}_{\nu x y}\rangle = \Big\{ \Big[|A-a_{23}\alpha_1 I_1^{\pi_1} T_1\rangle \left(|a_2\alpha_2 I_2^{\pi_2} T_2\rangle |a_3\alpha_3 I_3^{\pi_3} T_3\rangle \right)^{S_{23}T_{23}} \Big]^{sT}$$

$$\left(Y_{\ell_x}(\hat{r}_{a_2,a_3}) Y_{\ell_x}(\hat{r}_{A-a_{23},a_{23}})\right)^L \Big\}^{J^\pi T} \frac{\delta(x-r_{a_2,a_3})}{x r_{a_2,a_3}} \frac{\delta(y-r_{A-a_{23},a_{23}})}{y r_{A-a_{23},a_{23}}}$$

NCSM/RGM

$$|\Psi^{J^\pi T}\rangle = \sum_\nu \int dx x^2 \int dy y^2 \hat{A}_\nu |\Phi^{J^\pi T}_{\nu x y}\rangle G^{J^\pi T}_\nu(x,y)$$

$$\sum_\nu \int dx dy x^2 y^2 \left[\mathcal{H}_{\nu'\nu}(x,y,x',y') - E\mathcal{N}_{\nu'\nu}(x,y,x',y')\right] G^{J^\pi T}_\nu(x,y) = 0$$

$$\mathcal{N}_{\nu'\nu}(x,y,x',y') = \langle \Phi^{J^\pi T}_{\nu' x' y'} | \hat{A}^2 | \Phi^{J^\pi T}_{\nu x y}\rangle$$

$$\mathcal{H}_{\nu'\nu}(x,y,x',y') = \langle \Phi^{J^\pi T}_{\nu' x' y'} | \hat{A}_{\nu'} \mathcal{H} \hat{A}_\nu | \Phi^{J^\pi T}_{\nu x y}\rangle$$

Scattering in three-body cluster states

NCSM/RGM

$$|\Psi^{J^\pi T}\rangle = \sum_\nu \int dx x^2 \int dy y^2 \hat{A}_\nu |\Phi^{J^\pi T}_{\nu x y}\rangle G^{J^\pi T}_\nu(x,y)$$

$$\sum_\nu \int dxdy x^2 y^2 \left[\mathcal{H}_{\nu'\nu}(x,y,x',y') - E\mathcal{N}_{\nu'\nu}(x,y,x',y')\right] G^{J^\pi T}_\nu(x,y) = 0$$

Orthogonalization

$$\sum_\nu \int dxdy x^2 y^2 \left[\mathbb{H}_{\nu'\nu}(x,y,x',y') - E\delta\nu'\nu \frac{\delta(x'-x)}{x'x}\frac{\delta(y'-y)}{y'y}\right] \chi^{J^\pi T}_\nu(x,y) = 0$$

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$$\sum_{\nu}\int dxdyx^2y^2\left[\mathbb{H}_{\nu'\nu}(x,y,x',y') - E\delta\nu'\nu\frac{\delta(x'-x)}{x'x}\frac{\delta(y'-y)}{y'y}\right]\chi_{\nu}^{J^{\pi}T}(x,y)=0$$

Hyperspherical coordinates: $\rho = \sqrt{x^2+y^2}, \quad \alpha = \arctan(x/y)$

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$$\sum_{\nu} \int dx dy x^2 y^2 \left[\mathbb{H}_{\nu'\nu}(x,y,x',y') - E\delta\nu'\nu \frac{\delta(x'-x)}{x'x} \frac{\delta(y'-y)}{y'y} \right] \chi_{\nu}^{J^\pi T}(x,y) = 0$$

Hyperspherical coordinates: $\rho = \sqrt{x^2 + y^2}, \quad \alpha = \arctan(x/y)$

$$\chi_{\nu}^{J^\pi T}(x,y) = \sum_k C_{k\nu}(\rho) \phi_k^{\ell_x \ell_y}(\alpha)$$

$$\phi_k^{\ell_x \ell_y}(\alpha) = N_k \sin^{\ell_x}(\alpha) \cos^{l_y}(\alpha) P_{k/2}^{\ell_x+1/2, \ell_y+1/2}(\cos 2\alpha)$$

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$$\sum_{\nu} \int dx dy x^2 y^2 \left[\mathbb{H}_{\nu'\nu}(x,y,x',y') - E\delta\nu'\nu \frac{\delta(x'-x)}{x'x} \frac{\delta(y'-y)}{y'y} \right] \chi_{\nu}^{J^\pi T}(x,y) = 0$$

Hyperspherical coordinates: $\rho = \sqrt{x^2+y^2}, \quad \alpha = \arctan(x/y)$

$$\chi_{\nu}^{J^\pi T}(x,y) = \sum_k C_{k\nu}(\rho) \phi_k^{\ell_x \ell_y}(\alpha)$$

After changing to hyperspherical coordinates and integrating in α,α':

$$\sum_{\nu k} \int d\rho \rho^5 \left[\bar{\mathcal{H}}_{\nu'\nu}^{k'k}(\rho',\rho) - E \frac{\delta(\rho-\rho')}{\rho^5} \delta_{\nu'\nu} \delta_{k'k} \right] C_{k\nu}^{J^\pi T}(\rho) = 0$$

NCSM/RGM

$$\sum_{\nu} \int dx dy x^2 y^2 \left[\mathbb{H}_{\nu'\nu}(x,y,x',y') - E\delta\nu'\nu \frac{\delta(x'-x)}{x'x} \frac{\delta(y'-y)}{y'y} \right] \chi_{\nu}^{J^\pi T}(x,y) = 0$$

Hyperspherical coordinates: $\rho = \sqrt{x^2+y^2}, \quad \alpha = \arctan(x/y)$

$$\chi_{\nu}^{J^\pi T}(x,y) = \sum_k C_{k\nu}(\rho) \phi_k^{\ell_x \ell_y}(\alpha)$$

After changing to hyperspherical coordinates and integrating in α,α':

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Coupled-channel microscopic R-matrix method on a Lagrange mesh

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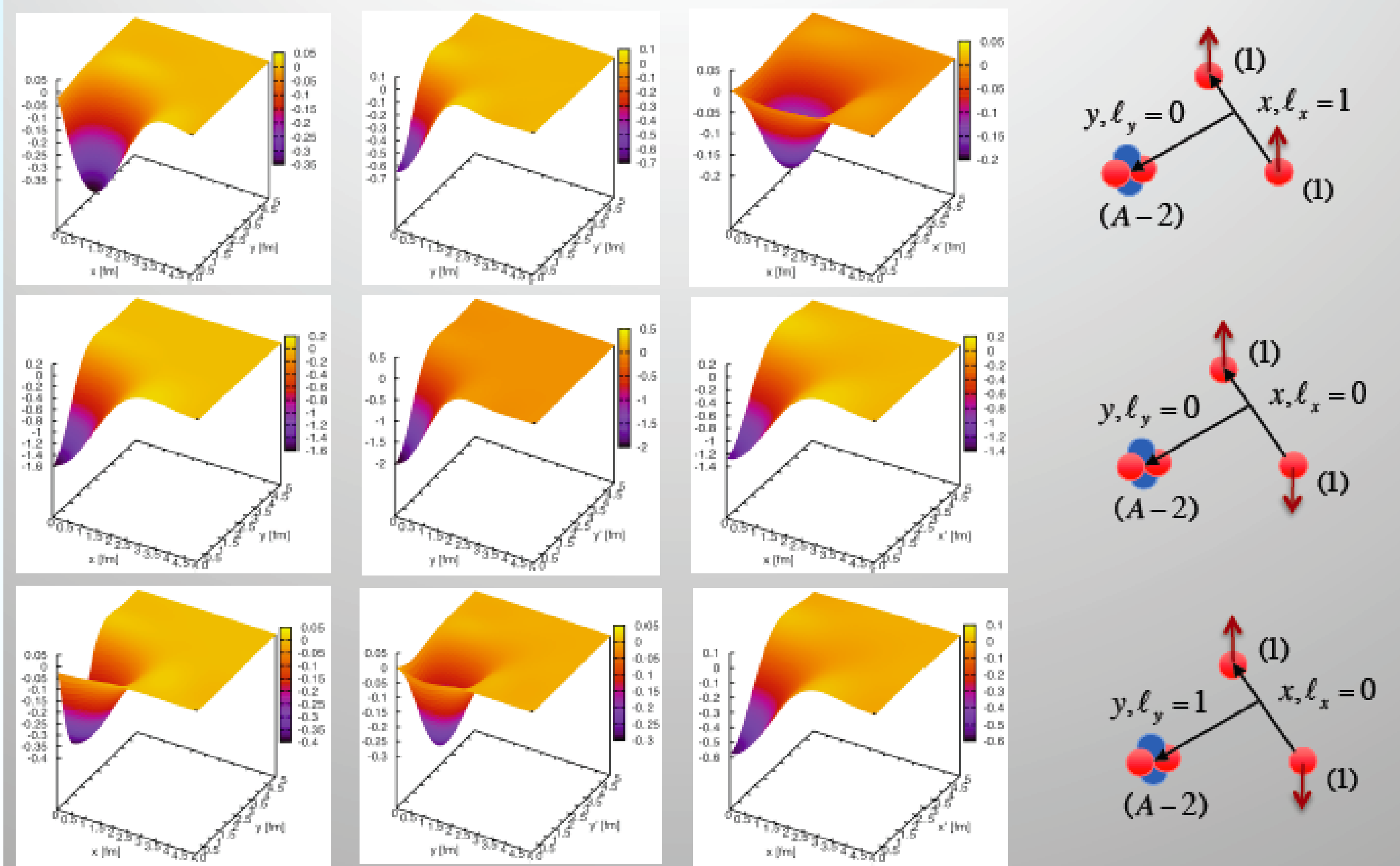
Scattering in three-body cluster states

NCSM/RGM

Work in progress: n+n+^{4}He

Norm Kernel $\mathcal{N}_{\nu'\nu}(x,y,x',y')$



Summary

NCSM/RGM

NCSM/RGM is an *Ab initio* many-body approach capable of studying both scattering and bound states

Extension to three-body cluster is in progress and will permit studying a wide range of systems, for example:

- Transfer reactions: ^{3}H(^{3}H,2n)^{4}He, ^{3}He(^{3}He,2p)^{4}He

- Bound and resonant states in two-neutron halo systems: ^{6}He (^{4}He+n+n), ^{11}Li (^{9}Li+n+n)

The End

Collaborators

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Scattering in three-body cluster states

Outline

Introduction

Integral relations

HA method

*Motivation

*Results

*Conclusions

NCSM/RGM

*n+n+4He

*Summary

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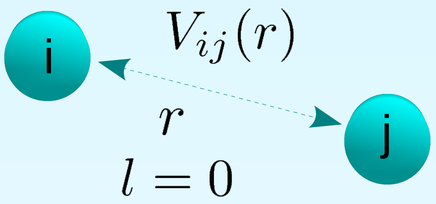
A break-up process: Three identical bosons

$$V_{ij}(r) = -51.5\, e^{-(r/1,6)^2}\ MeV$$

$$E_{2B} = -0.397742\ MeV$$

$$\hbar^2/m = 41.4696\ MeV\ fm^2$$



Incident energy of the projectile greater than $|E_{2B}|$

↓

Break-up may occur

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