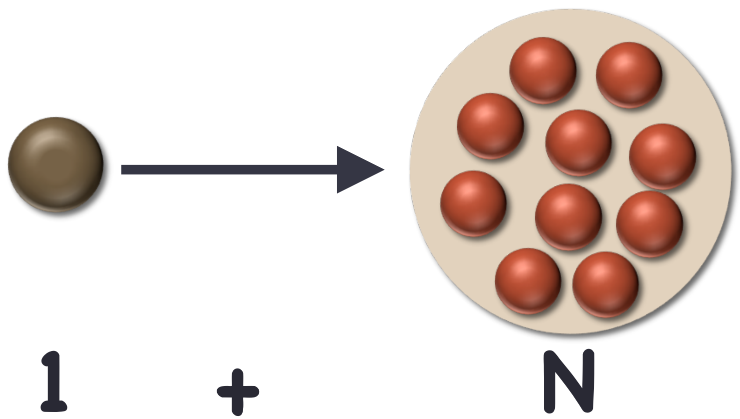
Purpose: Accurate description of 1+N reactions



- Elastic: 1+N
- Inelastic: 1+N*
- Transfer: 1*+N′
- Breakup: $N_1+N_2+\ldots+N_m=N+1$

TRIUMF — C. Romero-Redondo, *TRIUMF, Vancouver, Canada*

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CSIC Consejo Superior de Investigaciones Científicas — E. Garrido, *IEM-CSIC, Madrid, Spain*

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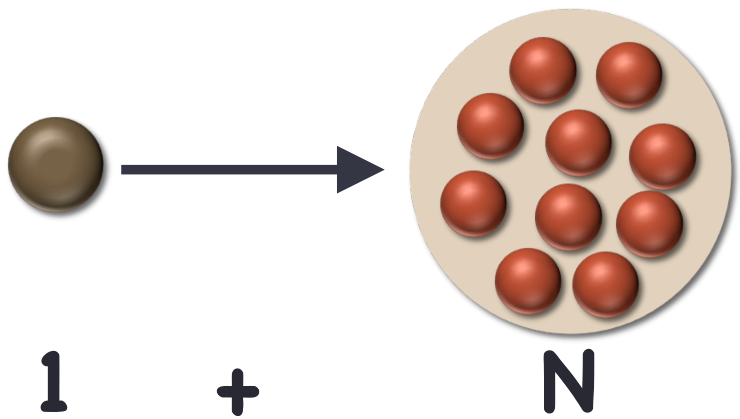

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N+1 wave function ⟶ $$H = T + V;\;\; (H - E)\,\Psi_{N+1} = 0$$

Coordinates: One radial coordinate ρ and 3N-1 angles

$$\Psi_{N+1} \xrightarrow{\rho\to\infty} \mathbb{I}\cdot F + S\cdot G \qquad (T-E)\,F,G = 0$$

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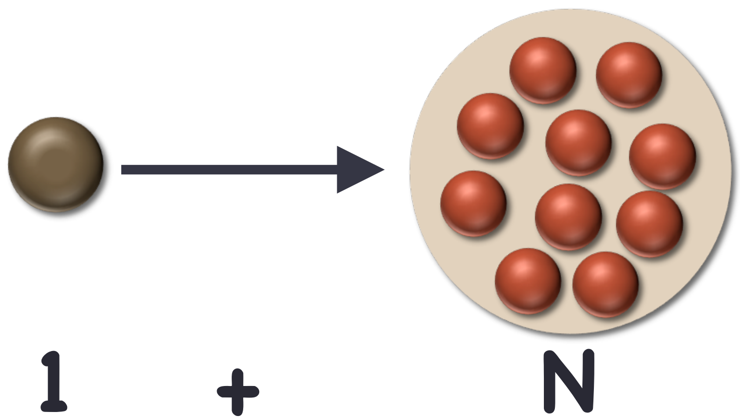

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Coo ... N-1 angles

$$\left(\Psi^{(i)}_{N+1}\right) \stackrel{\rho\to\infty}{\longrightarrow} \left(\sum_j F_j \delta_{ij} + S_{ij} G_j\right)$$

$$\Psi_{N+1} \stackrel{\rho\to\infty}{\longrightarrow} \mathbb{I}\cdot F + S \cdot G \qquad (T-E)\,F,G = 0$$

Purpose: Accurate description of 1+N reactions

- ✓ **Problem 1:** Already for N=2 accurate calculation of the asymptotic part of the radial wave functions can be rather complicated.
- ✓ **Problem 2:** Even when done, it is not guaranteed that the extracted S-matrix is also accurate.
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N+1 wave function ⟶ $H = T + V; \; (H - E)\,\Psi_{N+1} = 0$

$$\Psi_{N+1} = \Psi_c + A \cdot F + B \cdot G, \qquad S = A^{-1}B$$

$$\Psi_{N+1} \xrightarrow{\rho\to\infty} \mathbb{I} \cdot F + S \cdot G \qquad (T - E)\,F, G = 0$$

$$W(\Psi_{N+1}, G) = \Psi_{N+1}(\nabla G) - (\nabla \Psi_{N+1})G = A$$
$$W(\Psi_{N+1}, F) = \Psi_{N+1}(\nabla F) - (\nabla \Psi_{N+1})F = -B$$

$$W(F, G) = F(\nabla G) - (\nabla F)G = \mathbb{I}$$

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N+1 wave function → $H = T + V; \ (H - E)\Psi_{N+1} = 0$

$$A = -\frac{2m}{\hbar^2}\left[\langle \Psi | H - E | G \rangle - \langle G | H - E | \Psi \rangle^T\right]$$
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If Ψ is an exact solution → $\begin{cases} \langle F|H-E|\Psi\rangle = 0 \\ \langle G|H-E|\Psi\rangle = 0 \end{cases}$

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Purpose: Accurate description of 1+N reactions

✓ The **Kohn Variational Principle** establishes that each matrix element of

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

is a stationary with respect to variations in the trial wave function

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✓ When using the trial functions the expressions of the matrices A and B are still valid **up to second order** $\delta\Psi = \Psi - \Psi_t$

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

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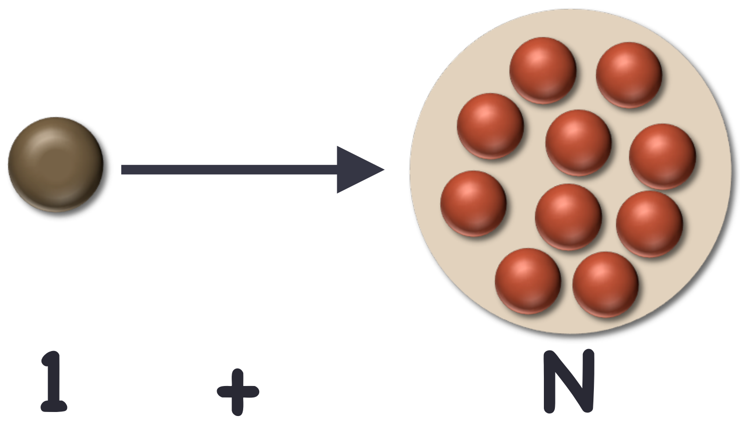

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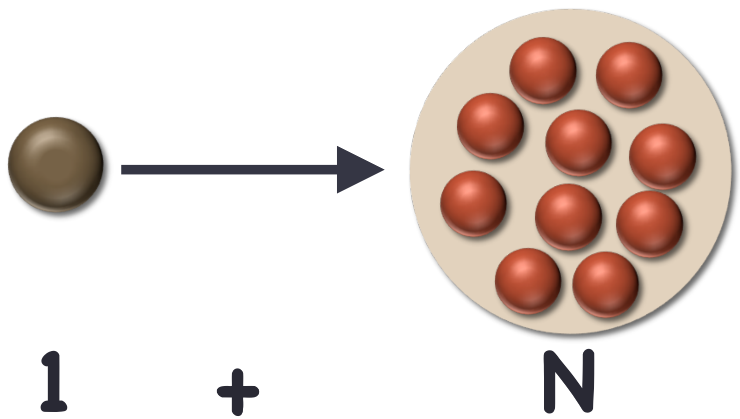

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$$(T+V-E)\,F_j = V F_j$$

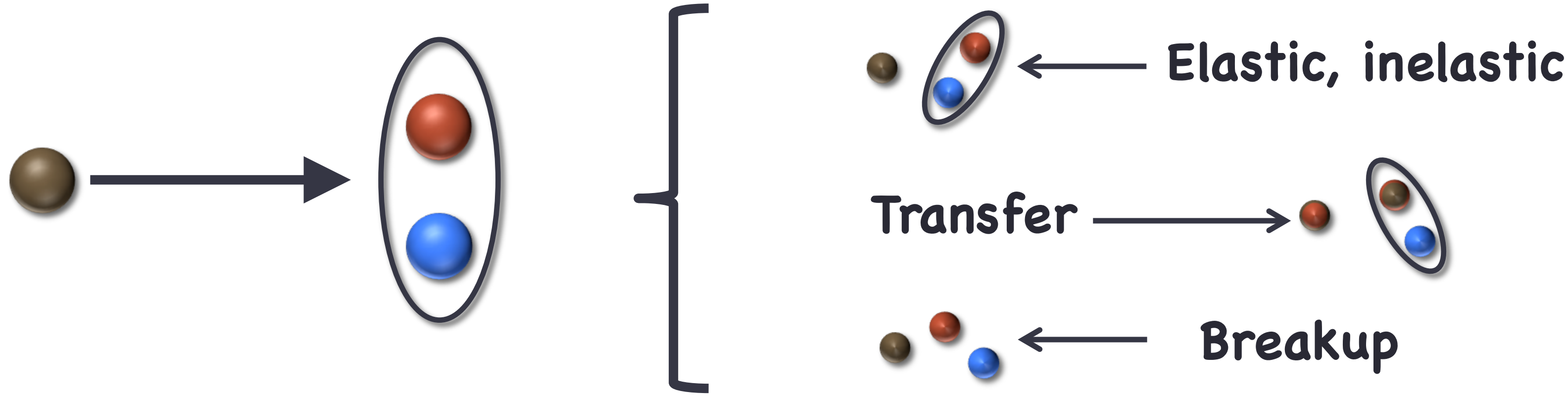
$$B_{ij} = \frac{2m}{\hbar^2}\int d\tau \Psi_t^i(\tau)(H-E)F_j(\tau)$$

Only the internal part of the trial function Ψ_t enters !!!!

$$S = A^{-1}B$$

$$A = -\frac{2m}{\hbar^2}\langle \Psi_t | H - E | G \rangle; \qquad B = \frac{2m}{\hbar^2}\langle \Psi_t | H - E | F \rangle$$

Results for 1+2 reactions with the adiabatic expansion method



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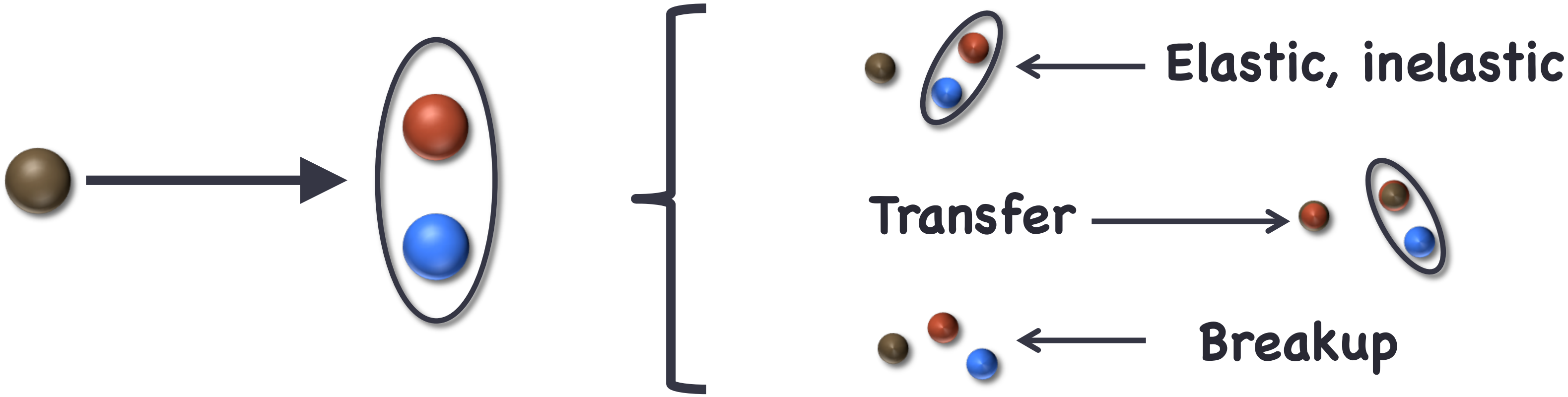

$$\rho^2 = x^2 + y^2; \qquad \alpha = \arctan(x/y)$$

$$\hat{\mathcal{H}} = -\frac{\hbar^2}{2m}\hat{T}_\rho + \hat{\mathcal{H}}_\Omega$$

$$\hat{\mathcal{H}}_\Omega \Phi_n(\rho,\Omega) = \frac{\hbar^2}{2m}\frac{1}{\rho^2}\lambda_n(\rho)\Phi_n(\rho,\Omega)$$

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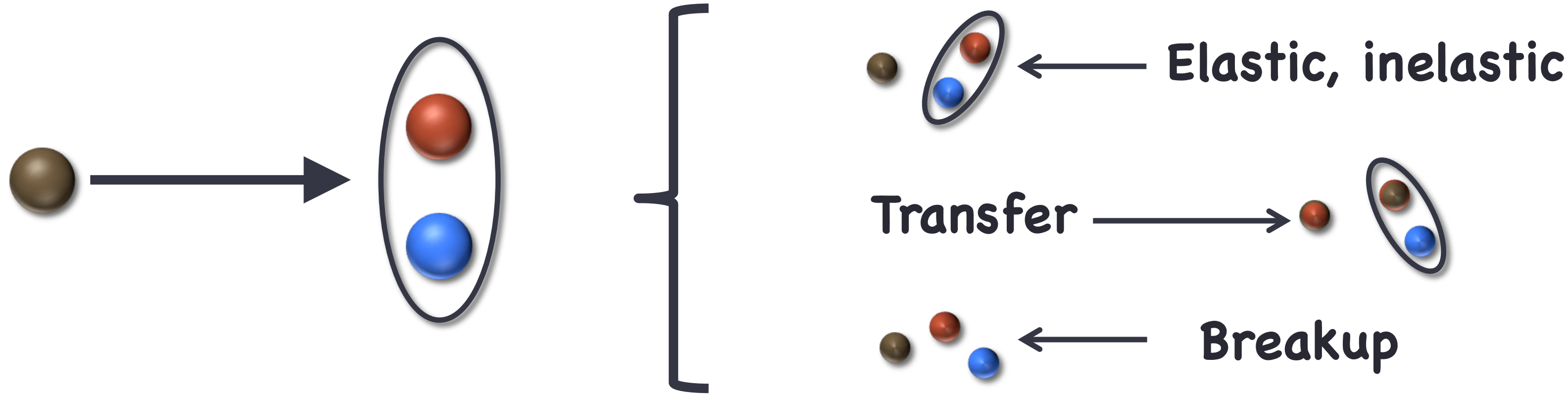

$$\Psi_t(\rho,\Omega) = \frac{1}{\rho^{5/2}} \sum_n f_n(\rho)\Phi_n(\rho,\Omega); \qquad \rho^2 = x^2 + y^2; \qquad \alpha = \arctan(x/y)$$

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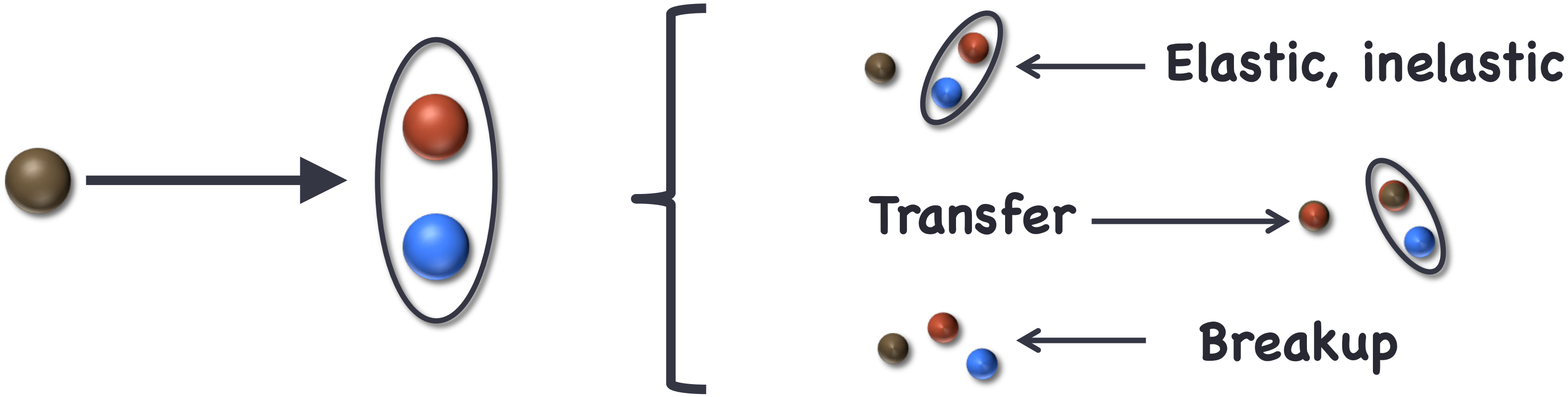

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$$\left[-\frac{d^2}{d\rho^2} + \frac{2m}{\hbar^2}\left(V_n(\rho) - E\right)\right] f_n(\rho) + \sum_{n'} \left(-2P_{nn'}\frac{d}{d\rho} - Q_{nn'}\right) f_{n'}(\rho) = 0$$

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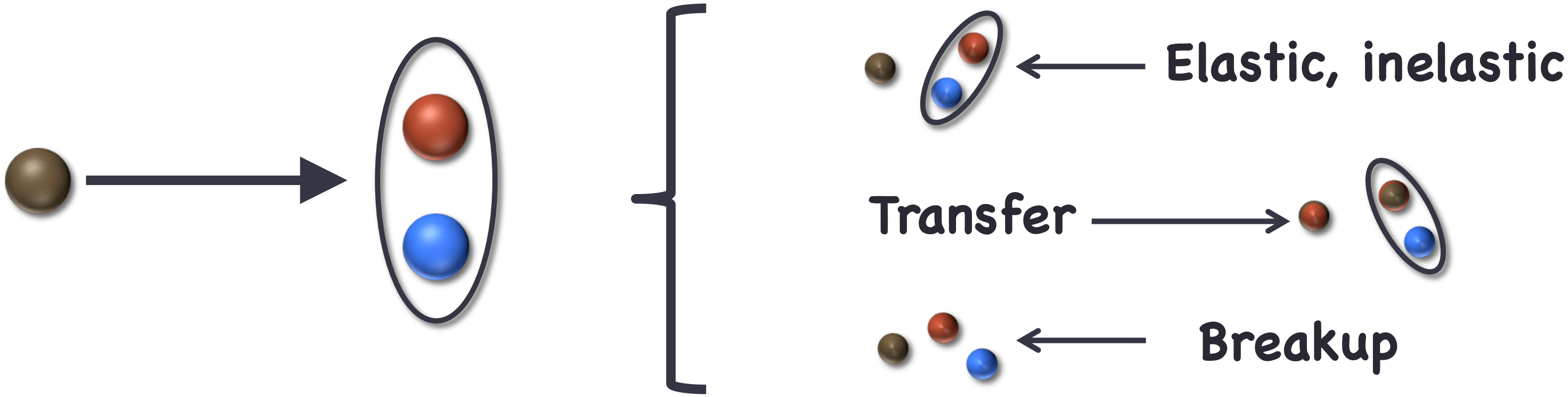

$$\Psi_t(\rho,\Omega) = \frac{1}{\ldots} \ldots + y^2; \qquad \alpha = \arctan(x/y)$$

$$P_{nn'} = \langle \Phi_n(\rho,\Omega) | \frac{\partial}{\partial\rho} | \Phi_{n'}(\rho,\Omega) \rangle_\Omega$$

$$Q_{nn'} = \langle \Phi_n(\rho,\Omega) | \frac{\partial^2}{\partial\rho^2} | \Phi_{n'}(\rho,\Omega) \rangle_\Omega$$

$$\hat{\mathcal{H}} = -\frac{\ldots}{2m} \ldots$$

$$\ldots \frac{\hbar^2}{2m}\frac{1}{\rho^2}\lambda_n(\rho)\Phi_n(\rho,\Omega)$$

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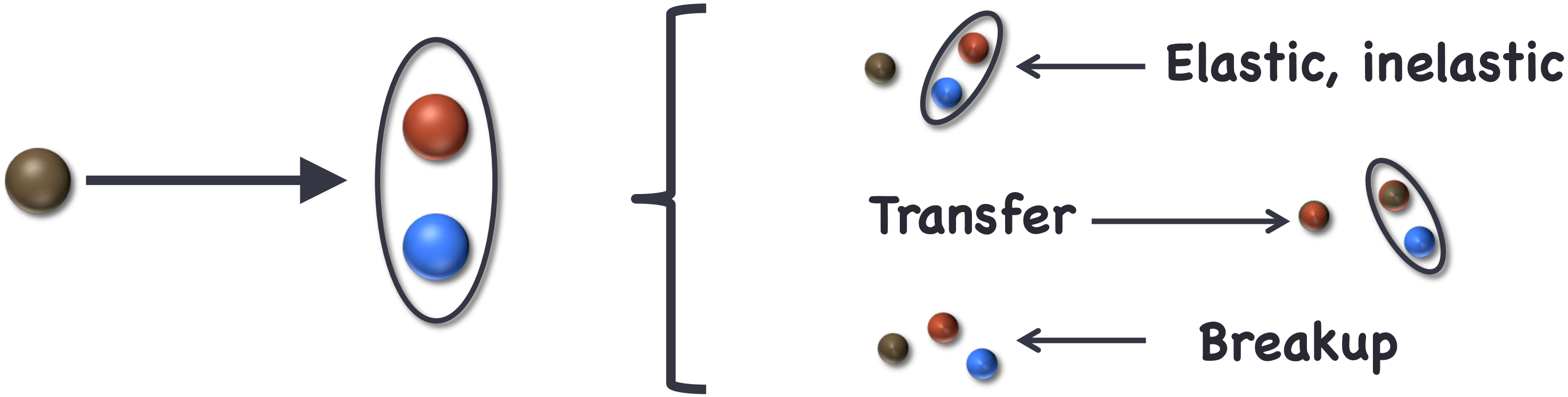

$$\hat{\mathcal{H}} = -\frac{\hbar^2}{2m}\hat{T}_\rho + \hat{\mathcal{H}}_\Omega$$

$$V_n(\rho) = \frac{\hbar^2}{2m}\left(\frac{\lambda_n(\rho) + \frac{15}{4}}{\rho^2} - Q_{nn}(\rho)\right)$$

Effective adiabatic potentials

$$\hat{\mathcal{H}}_\Omega \Phi_n(\rho,\Omega) = \frac{\hbar^2}{2m}\frac{1}{\rho^2}\lambda_n(\rho)\Phi_n(\rho,\Omega)$$

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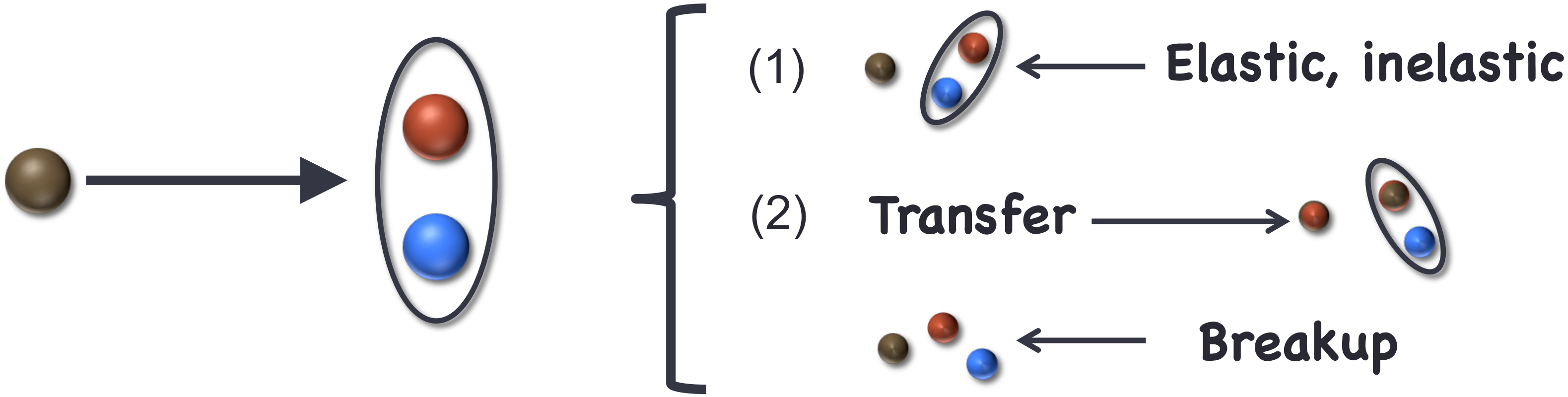
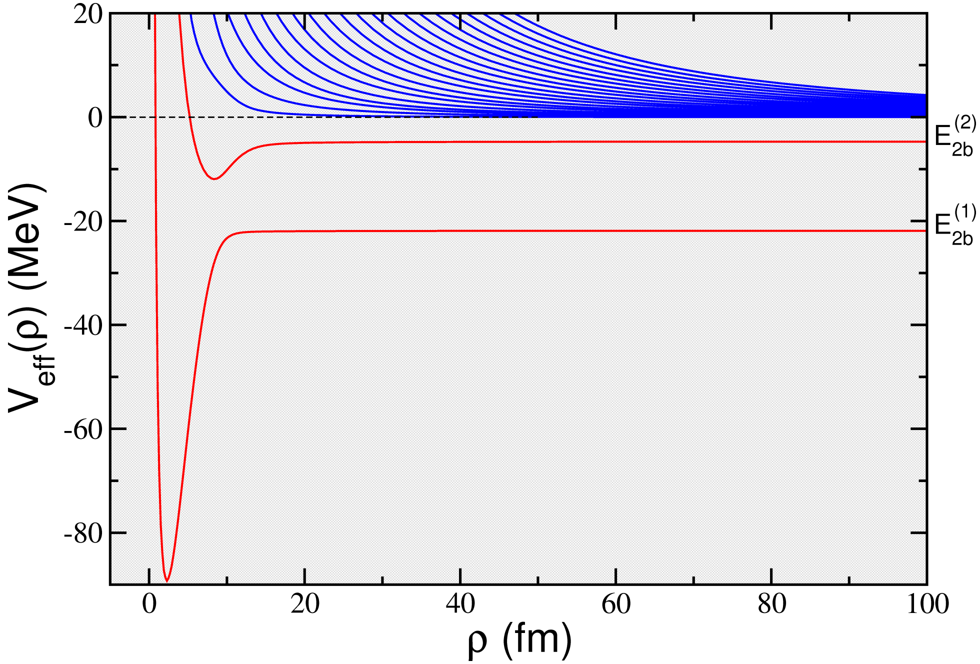
Results for 1+2 reactions with the adiabatic expansion method



If two bound two-body subsystems...



$$V_n(\rho) = \frac{\hbar^2}{2m}\left(\frac{\lambda_n(\rho) + \frac{15}{4}}{\rho^2} - Q_{nn}(\rho)\right)$$

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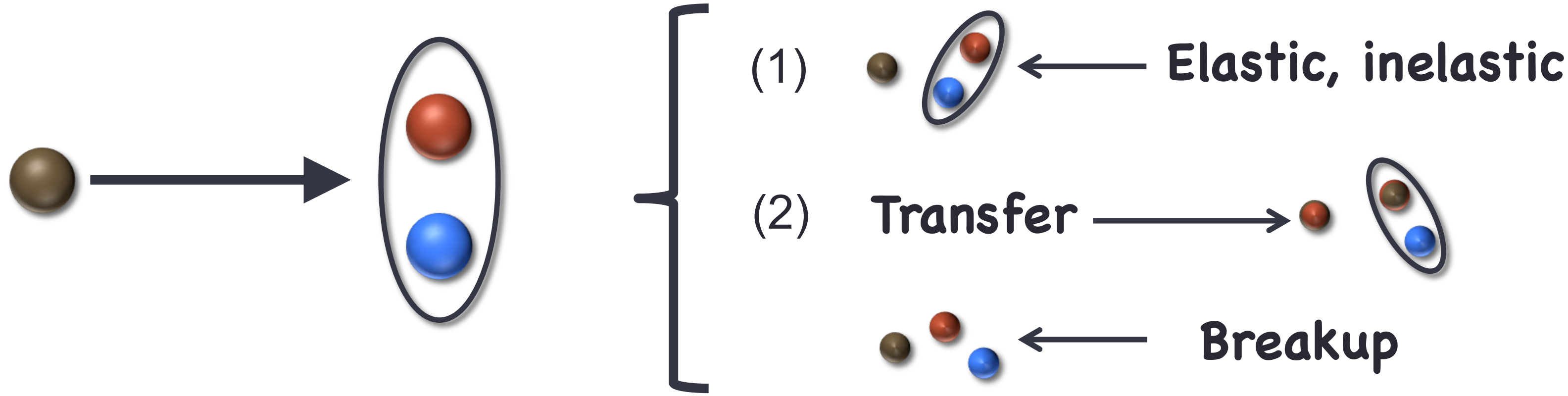

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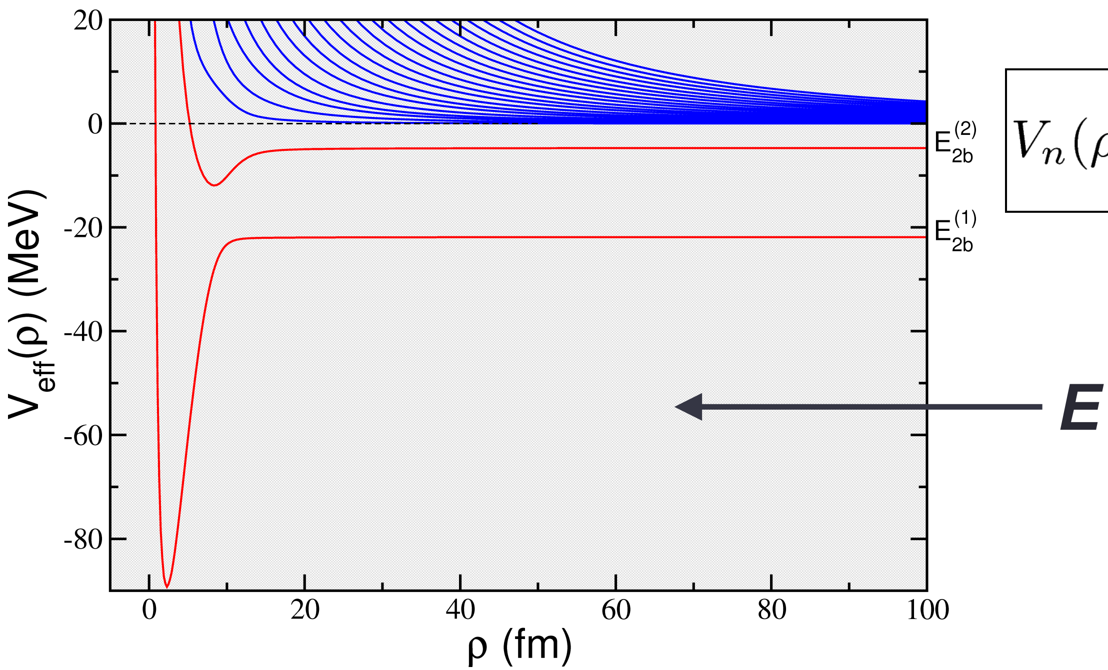
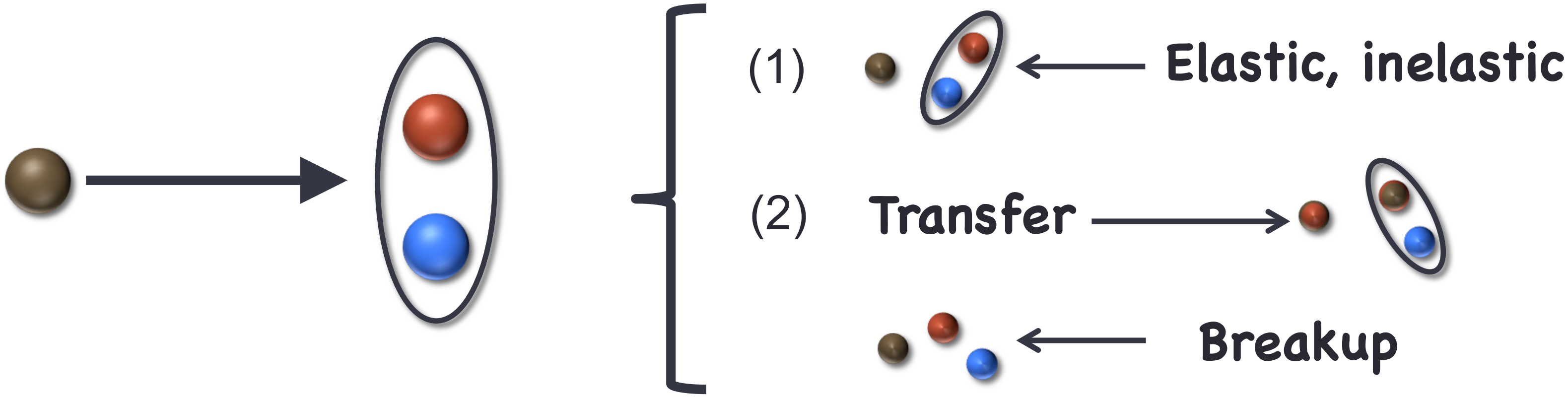


$$V_n(\rho) = \frac{\hbar^2}{2m}\left(\frac{\lambda_n(\rho) + \frac{15}{4}}{\rho^2} - Q_{nn}(\rho)\right)$$

Only bound three-body states are possible

Results for 1+2 reactions with the adiabatic expansion method



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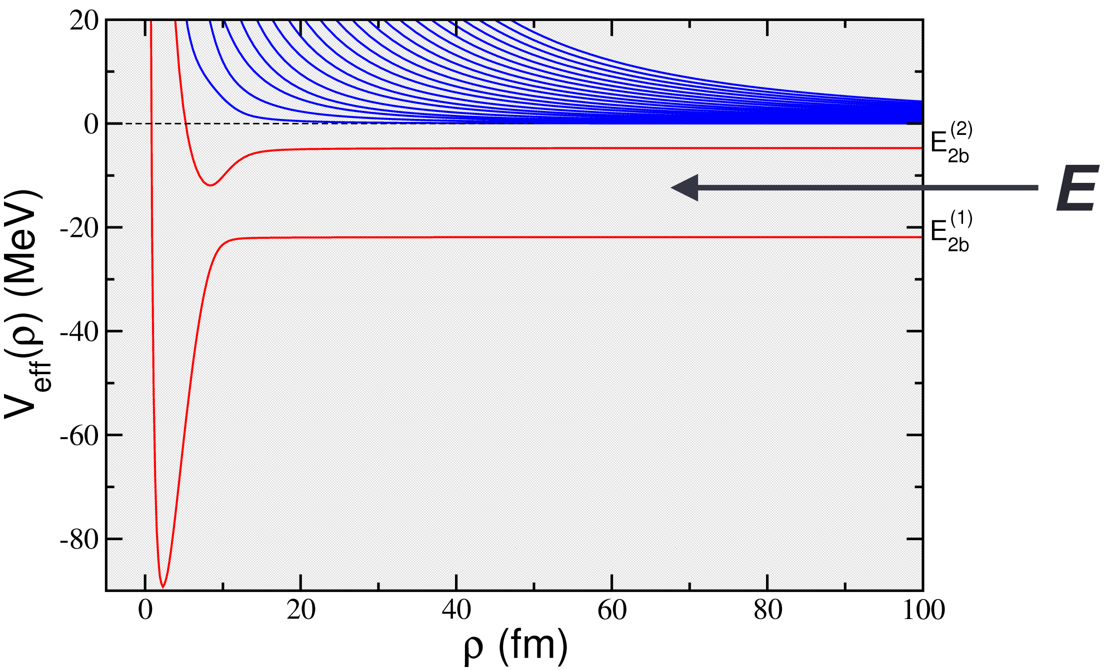
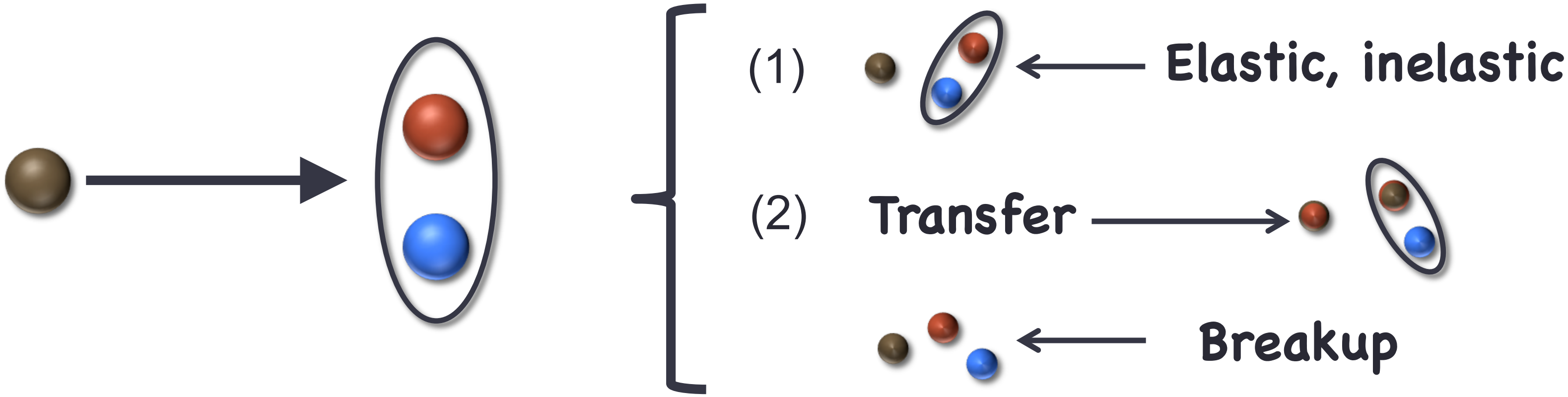


Only the elastic channel is open

1x1 S-matrix

$$\Psi_1 \rightarrow F_1 + S_{11} G_1$$

Results for 1+2 reactions with the adiabatic expansion method



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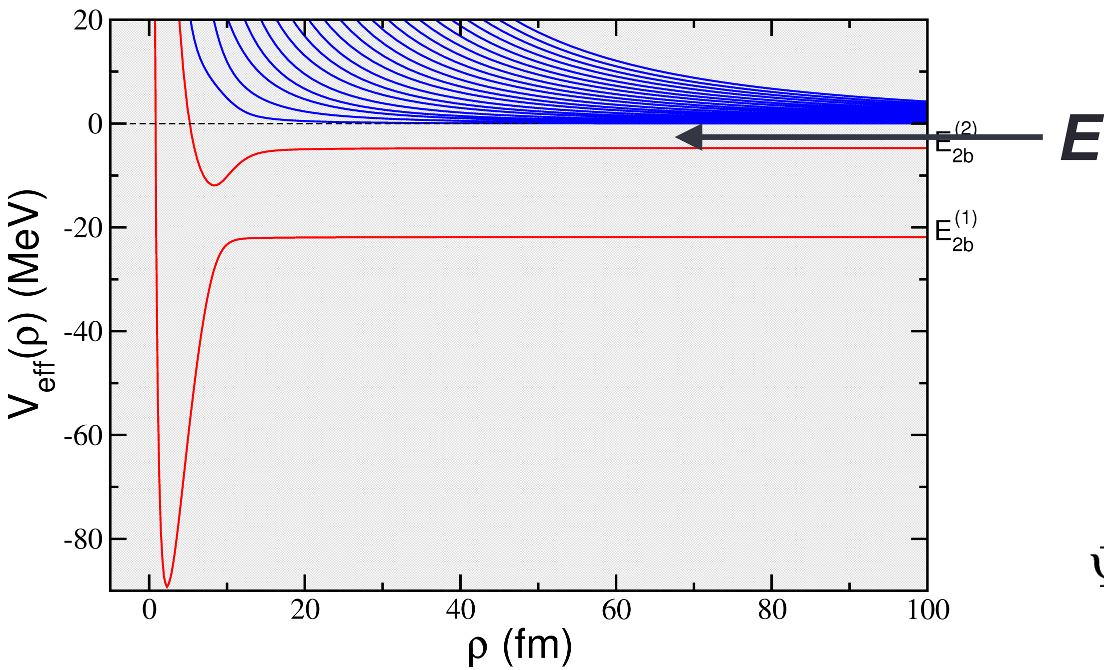
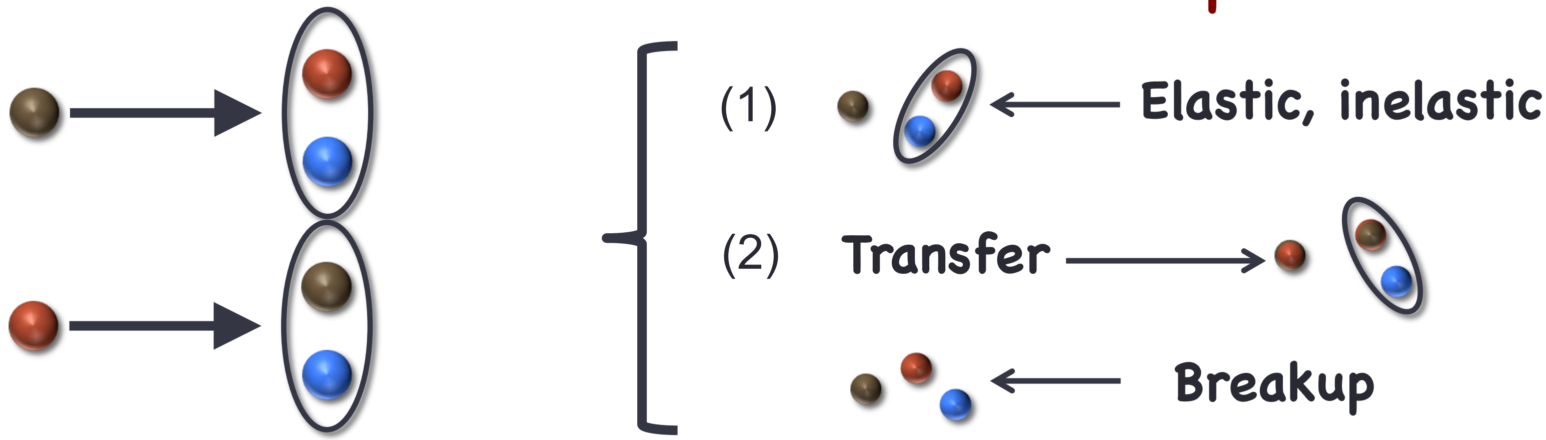


The elastic and the transfer (or inelastic) are open

2x2 S-matrix

$$\Psi_i \rightarrow \sum_{n=1}^{2} (F_n \delta_{in} + S_{in} G_n)$$

Results for 1+2 reactions with the adiabatic expansion method



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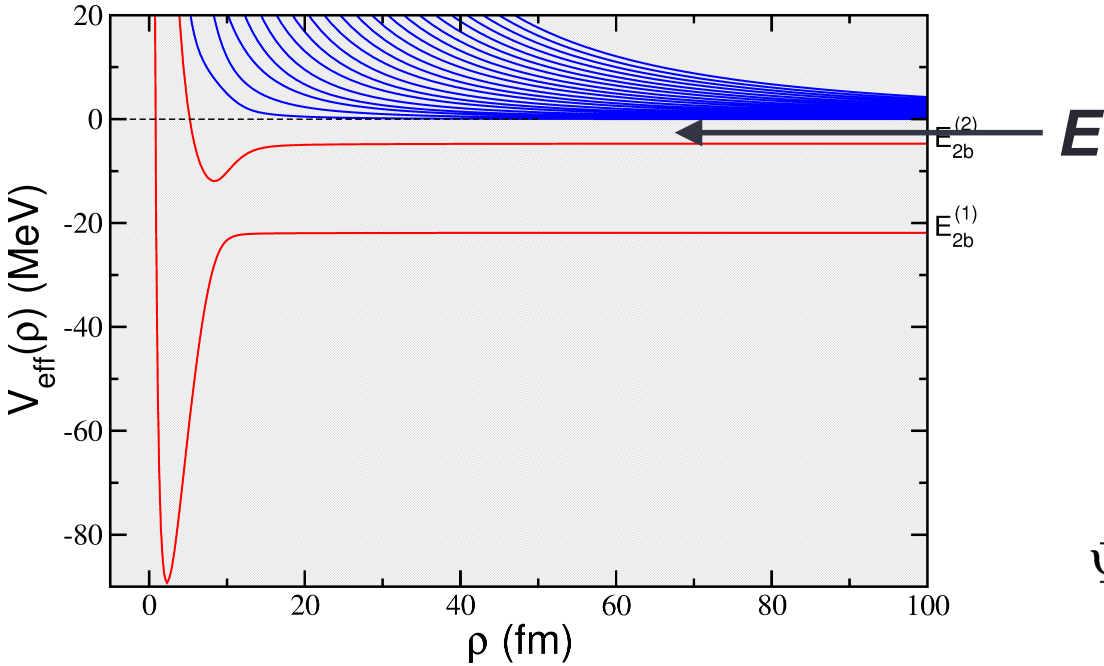

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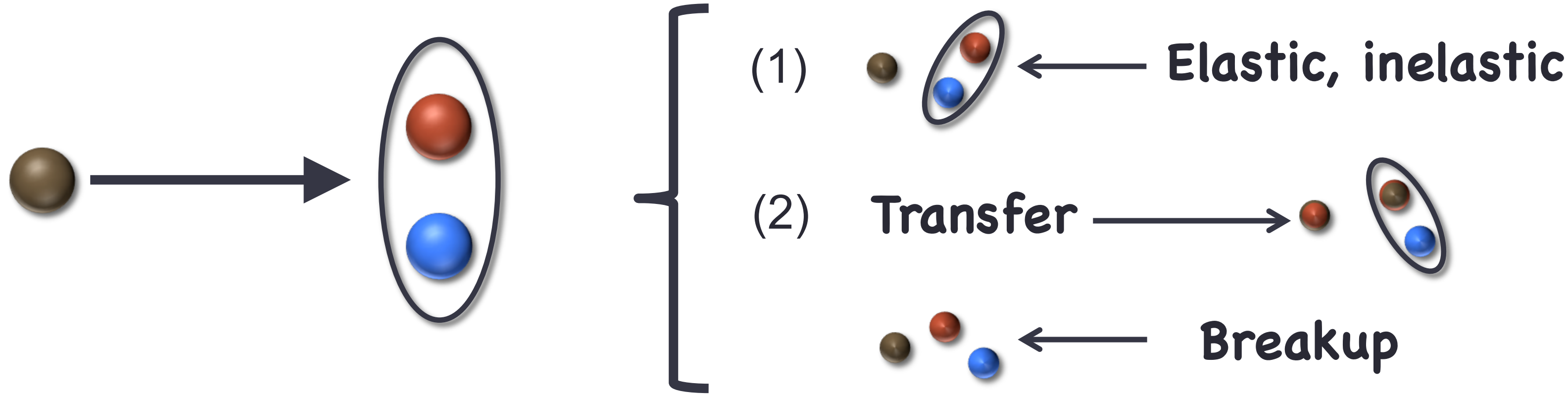

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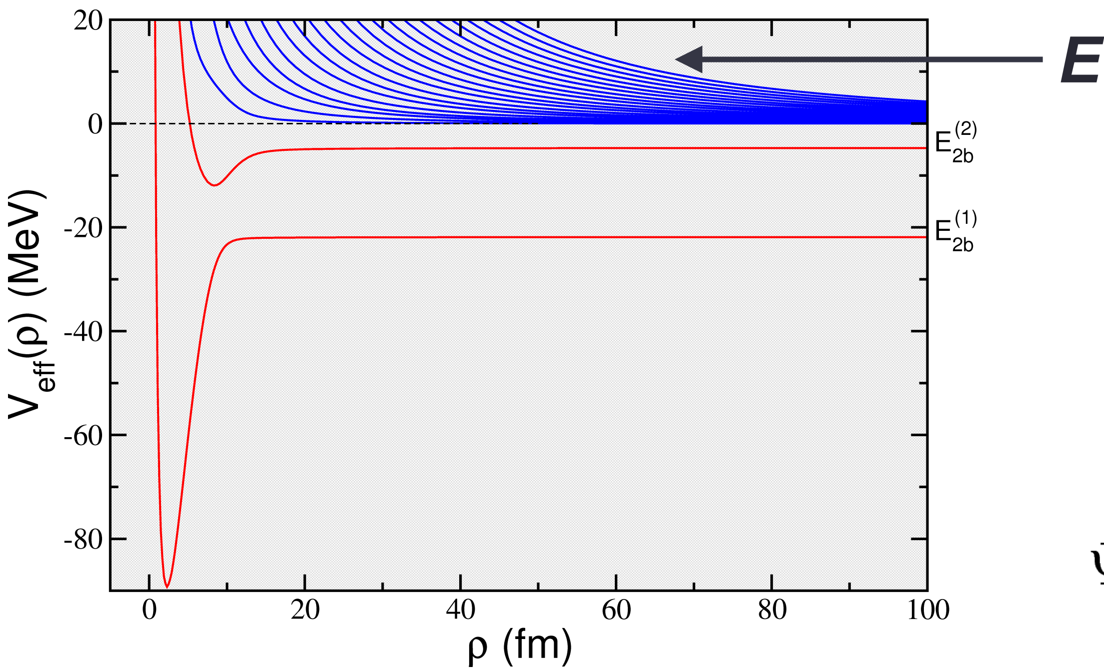
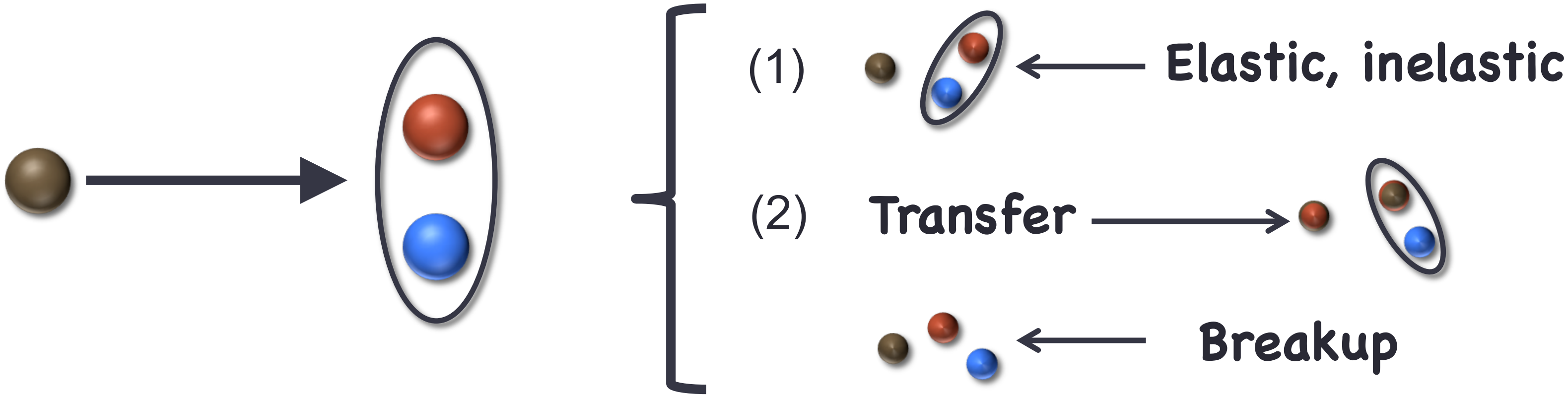


All the channels are open

NxN S-matrix

$$\Psi_i \to \sum_{n=1}^{\infty} (F_n \delta_{in} + S_{in} G_n)$$

Results for 1+2 reactions with the adiabatic expansion method



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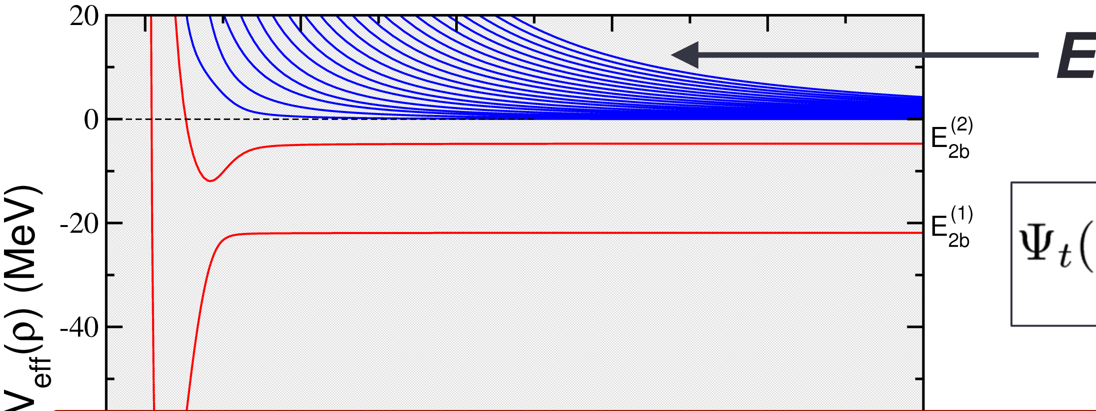

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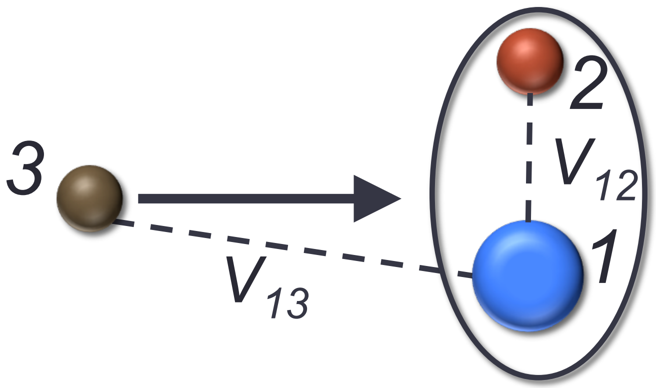
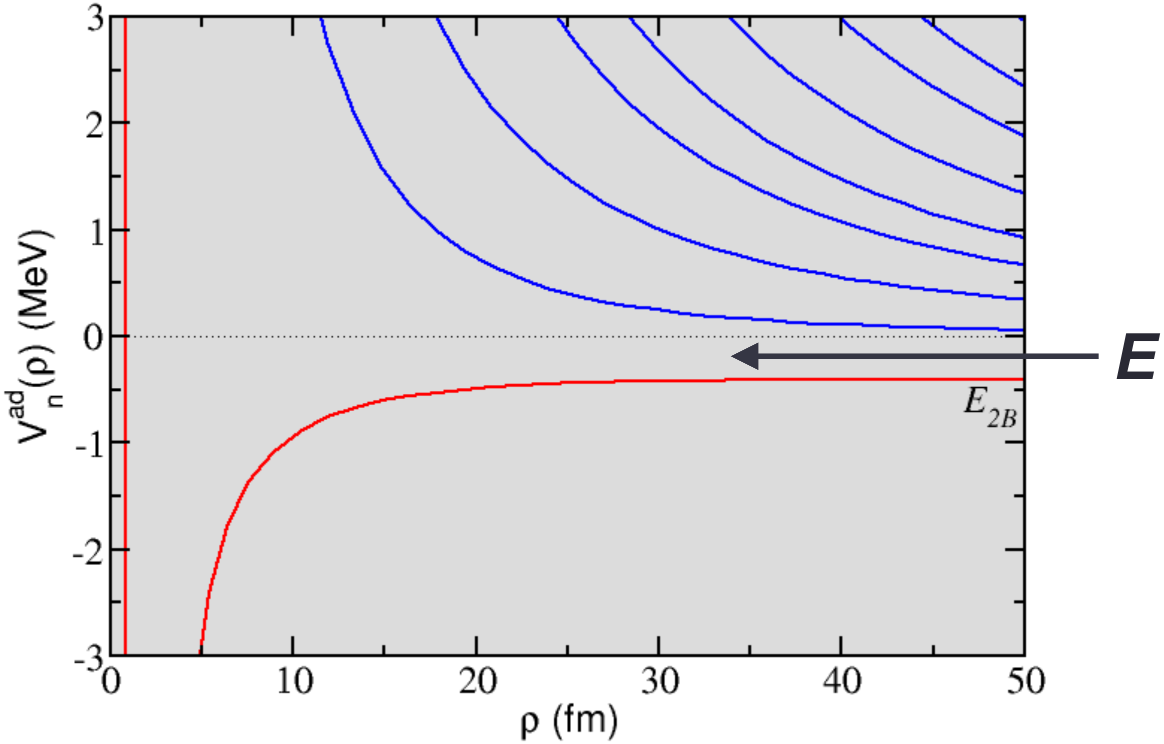
$$S = A^{-1}B$$

$$S \equiv (S_{nn'})$$

Results: A test case



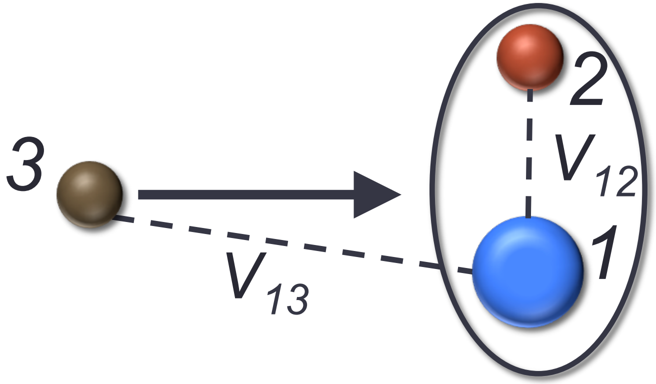
- Particles 2 and 3 do not interact
- Particle 1 with infinite mass
- Only 1 and 2 form a bound state



Only the elastic channel is open

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

Results: A test case



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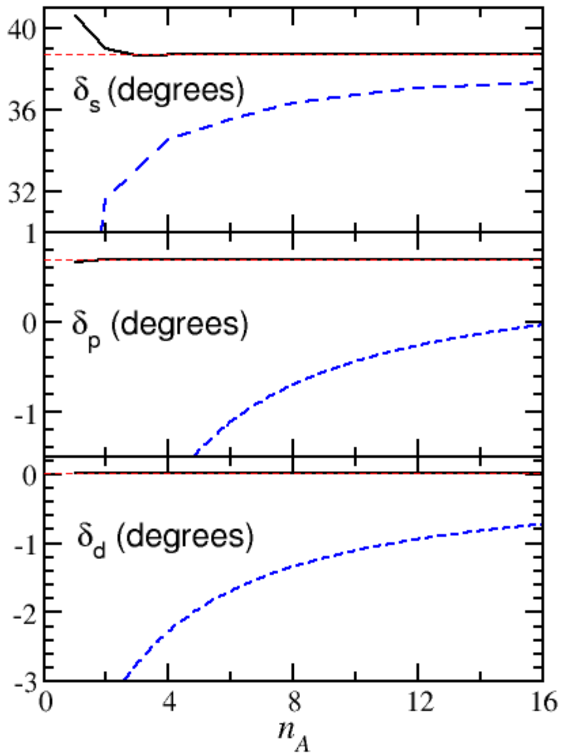

$$\Psi_t(\rho,\Omega) = \frac{1}{\rho^{5/2}} \sum_n f_n(\rho)\Phi_n(\rho,\Omega)$$

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**

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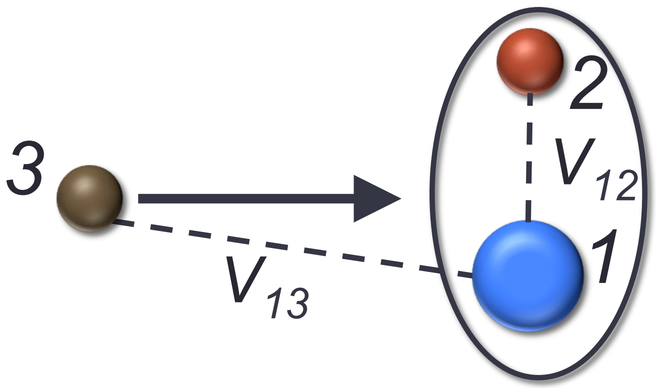

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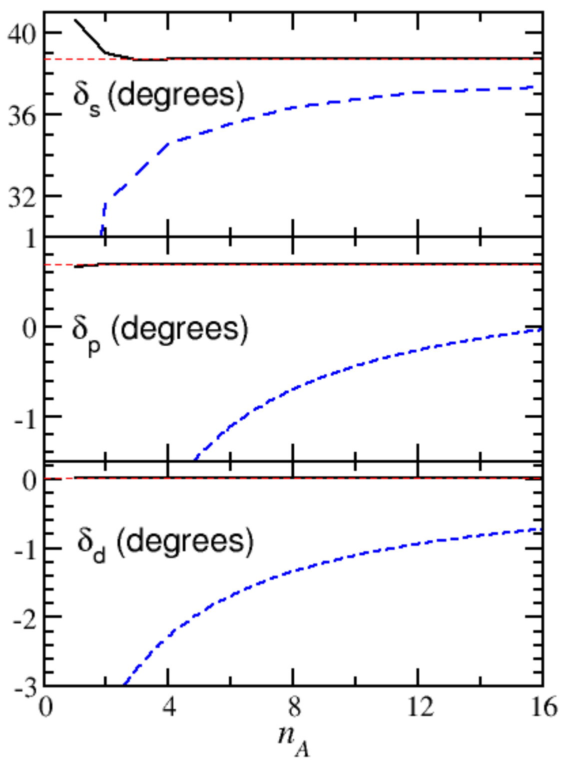
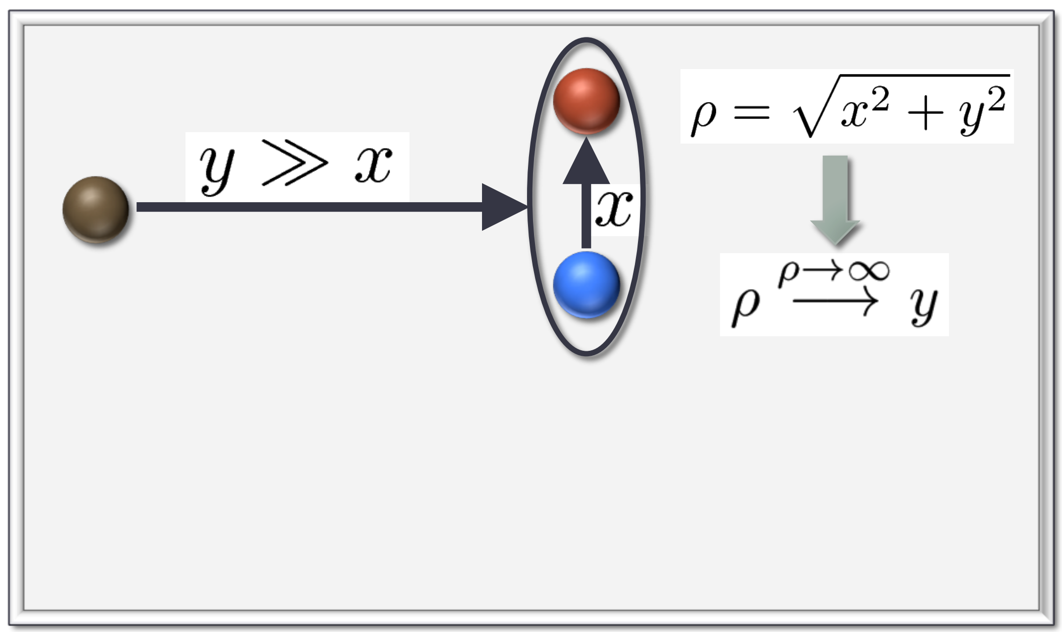
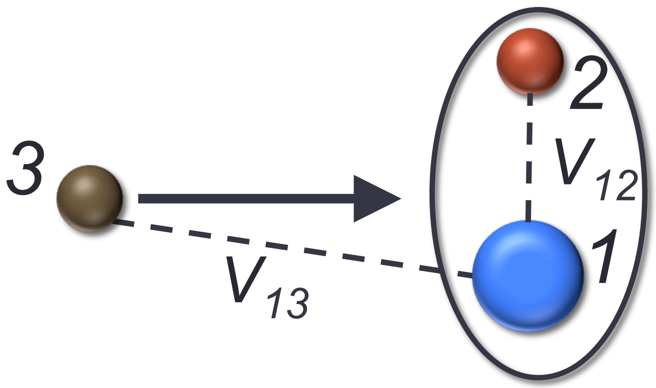
- Only 1 and 2 form a bound state



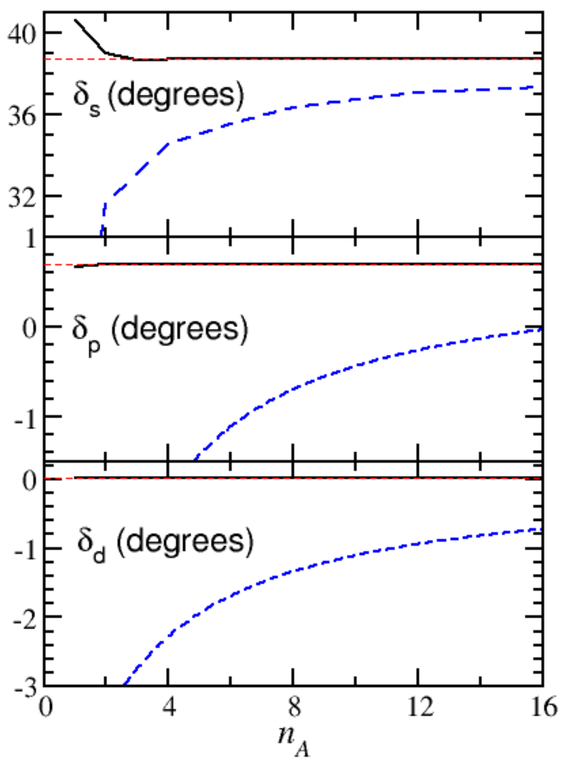
$$\Psi_t(\rho,\Omega) = \frac{1}{\rho^{5/2}} \sum_n f_n(\rho)\Phi_n(\rho,\Omega)$$



Results: A test case



- Particles 2 and 3 do not interact
- Particle 1 with infinite mass
- Only 1 and 2 form a bound state



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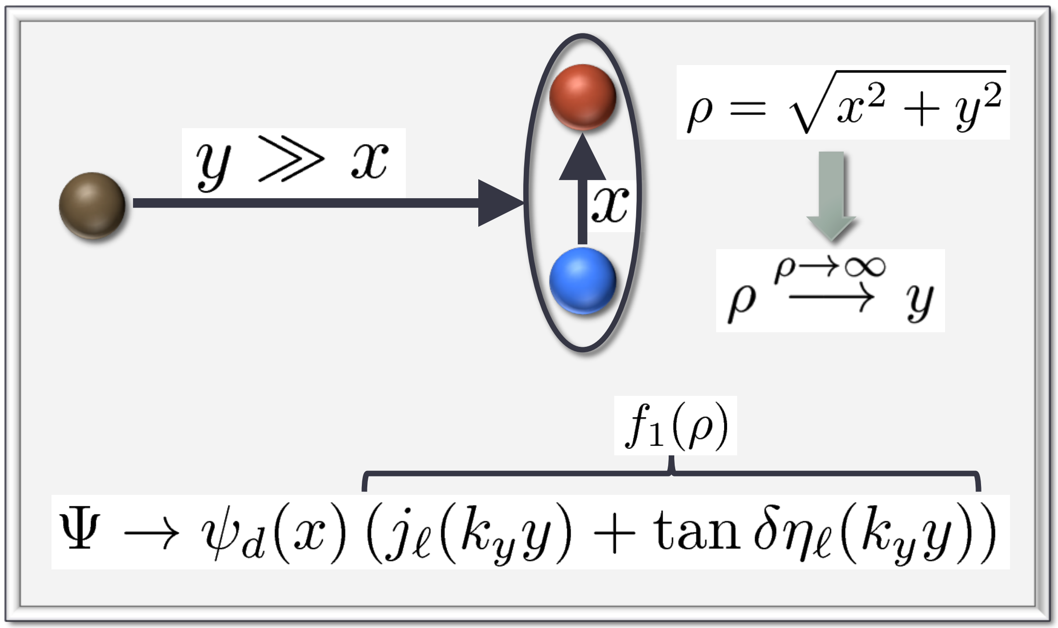
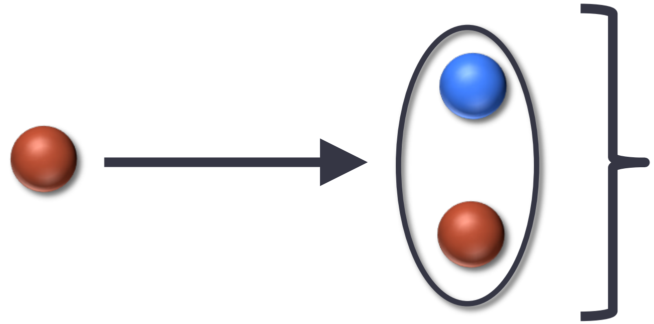


Results: n-deuteron breakup



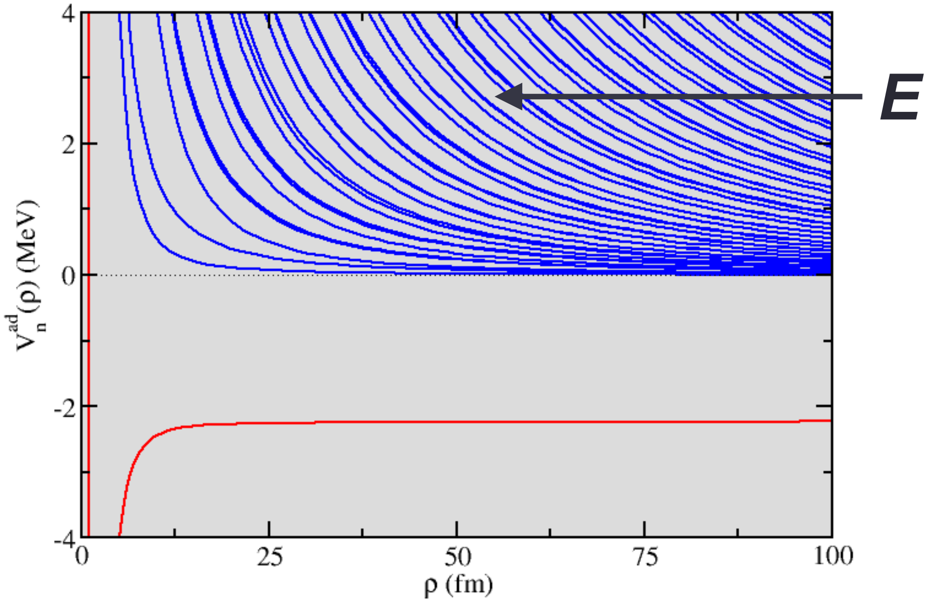
s-waves, J=1/2,3/2

$$V_s(r) = \left(-513.968e^{-1.55r} + 1438.72e^{-3.11r}\right)/r$$

$$V_t(r) = \left(-626.885e^{-1.55r} + 1438.72e^{-3.11r}\right)/r$$

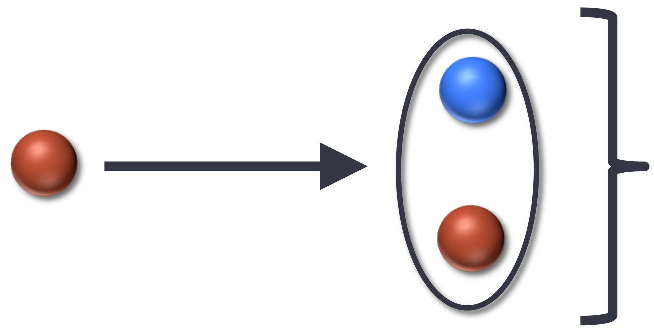
$$E_d = -2.2307 \text{ MeV}$$

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



The elastic and breakup channels are open

Results: n-deuteron breakup



s-waves, J=1/2

$$V_s(r) = \left(-513.968e^{-1.55r} + 1438.72e^{-3.11r}\right)/r$$

$$V_t(r) = \left(-626.885e^{-1.55r} + 1438.72e^{-3.11r}\right)/r$$

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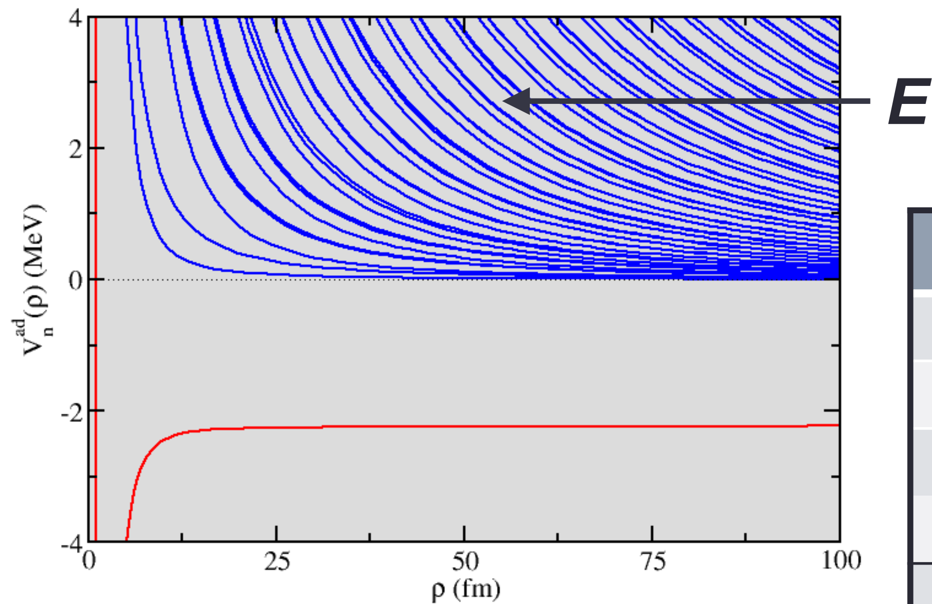
J.L. Friar et al., PRC 42 (1990) 1838, PRC 51 (1995) 2356



The elastic and breakup channels are open

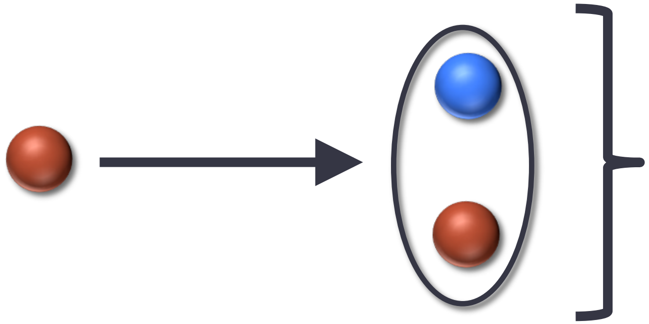
E_{lab}=14.1 MeV	$\vert S_{11}\vert$	Re(δ_{11})
8 adiabs.	0.464	105.57
12 adiabs.	0.464	105.53
16 adiabs.	0.464	105.53
20 adiabs.	0.465	105.53
Benchmark	0.465	105.51

$$B_{ij} = \frac{2m}{\hbar^2}\int d\tau \Psi_t^i(\tau)(H-E)F_j(\tau)$$

$$S = A^{-1}B$$

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

Results: n-deuteron breakup

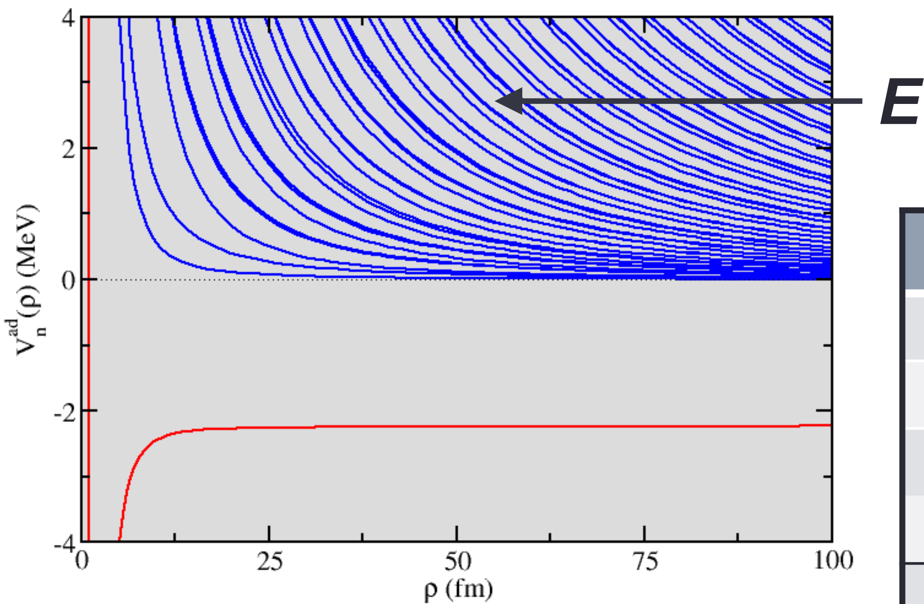


s-waves, J=3/2

$$V_t(r) = \left(-626.885 e^{-1.55r} + 1438.72 e^{-3.11r}\right)/r$$

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

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



The elastic and breakup channels are open

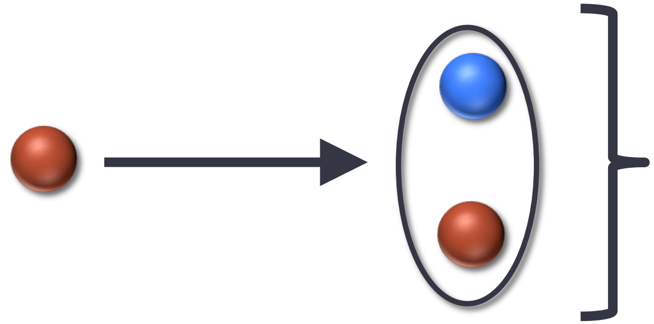
E_{lab}=14.1 MeV	$\lvert S_{11} \rvert$	Re(δ_{11})
8 adiabs.	0.979	68.99
12 adiabs.	0.978	68.98
16 adiabs.	0.978	68.96
20 adiabs.	0.978	68.86
Benchmark	0.978	68.96

$$B_{ij} = \frac{2m}{\hbar^2} \int d\tau \Psi_t^i(\tau)(H-E)F_j(\tau)$$

$$S = A^{-1}B$$

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

Results: n-deuteron breakup



s-waves, J=3/2

$$V_t(r) = \left(-626.885e^{-1.55r} + 1438.72e^{-3.11r}\right)/r$$

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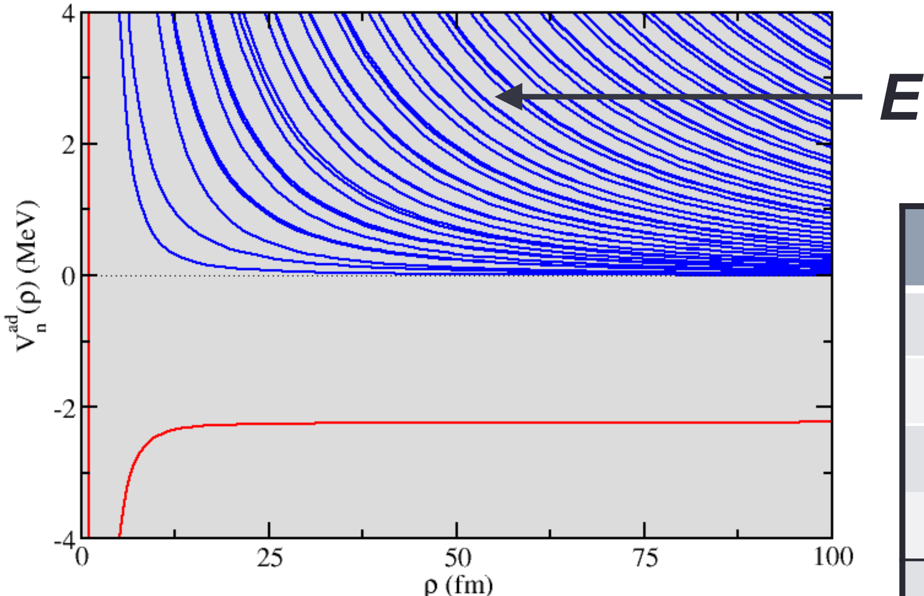
J.L. Friar et al., PRC 42 (1990) 1838, PRC 51 (1995) 2356



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16 adiabs.	0.978	68.96
20 adiabs.	0.978	68.86
Benchmark	0.978	68.96

$$\sum_{n=2}^{\infty} |S_{1n}|^2 = 1 - |S_{11}|^2$$

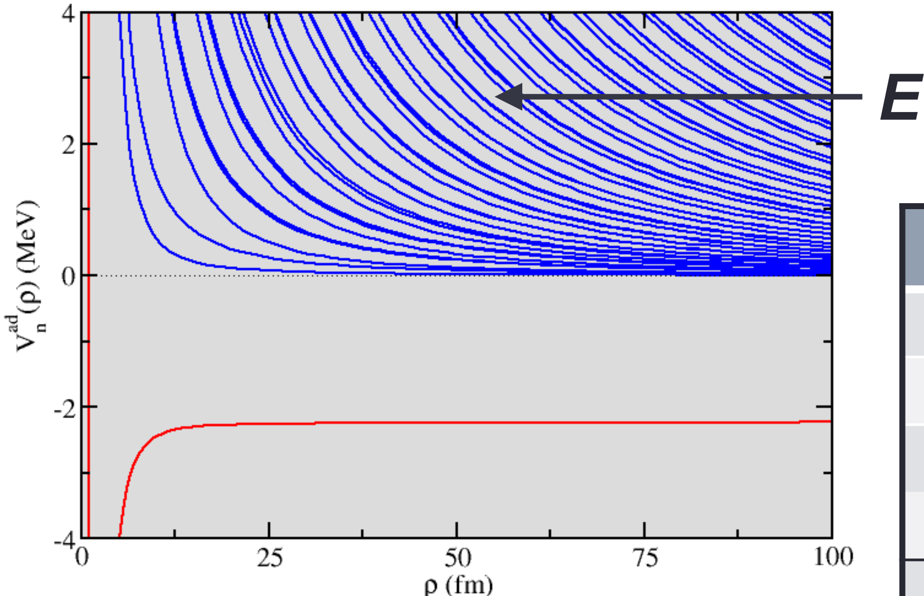
$$\sigma_{bk} = \frac{\pi}{p_y^2} \frac{(2J+1)}{(2s_p+1)(s_t+1)} (1 - |S_{11}|^2)$$

Results: n-deuteron breakup

s-waves, J=3/2

Transition amplitude

$$A^{\sigma_1,\sigma_2,\sigma_3}_{\sigma_d\sigma_n} \propto \sum_{JM} \langle s_d s_n \sigma_d \sigma_n | JM \rangle \sum_{n>1} i^{-K} S_{1n} \langle \sigma_1\sigma_2\sigma_3 | \Phi^{JM}_n(\Omega_\kappa)\rangle$$



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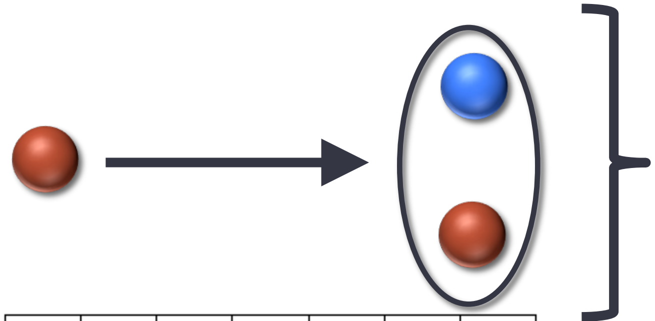
Results: n-deuteron breakup



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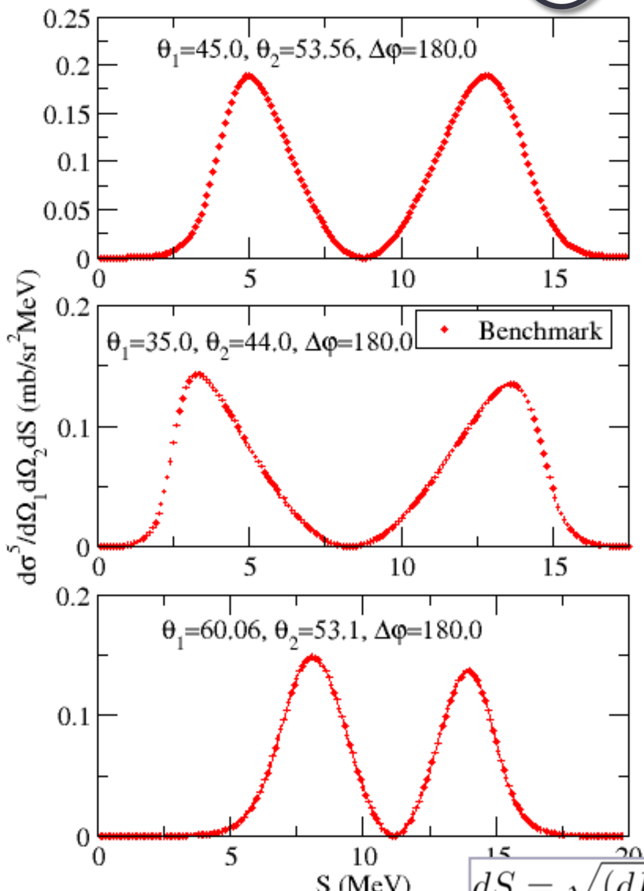
J.L. Friar et al., PRC 42 (1990) 1838, PRC 51 (1995) 2356



$$dS = \sqrt{(dE_1)^2 + (dE_2)^2}$$

The elastic and breakup channels are open

E_{lab}=14.1 MeV	$\lvert S_{11}\rvert$	Re(δ_{11})
8 adiabs.	0.979	68.99
12 adiabs.	0.978	68.98
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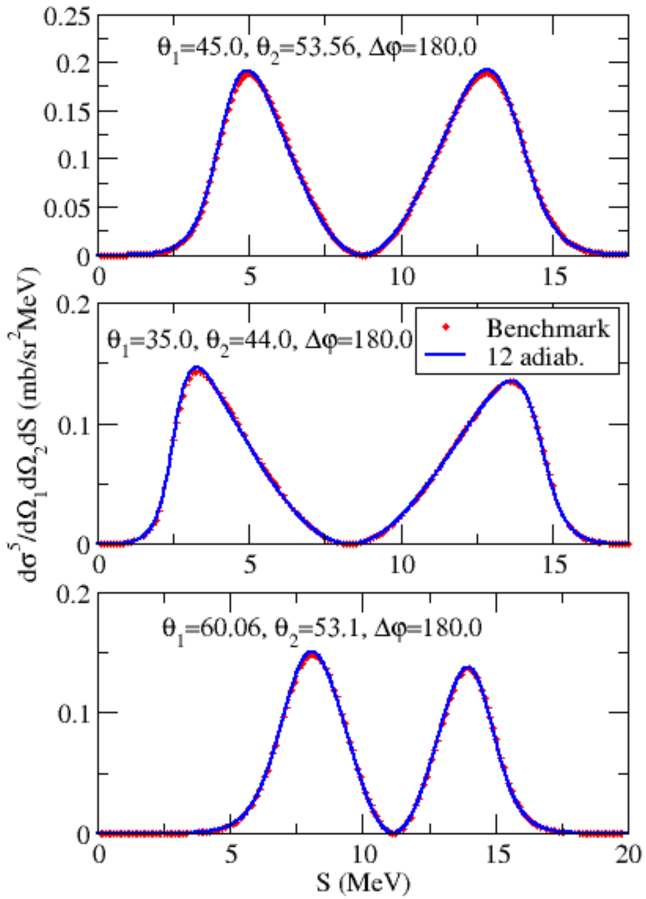
$$\sigma_{bk} = \frac{\pi}{p_y^2} \frac{(2J+1)}{(2s_p+1)(s_t+1)} (1 - |S_{11}|^2)$$

Results: n-deuteron breakup

s-waves, J=3/2

Transition amplitude

$$A^{\sigma_1,\sigma_2,\sigma_3}_{\sigma_d\sigma_n} \propto \sum_{JM} \langle s_d s_n \sigma_d \sigma_n | JM \rangle \sum_{n>1} i^{-K} S_{1n} \langle \sigma_1\sigma_2\sigma_3 | \Phi_n^{JM}(\Omega_\kappa)\rangle$$



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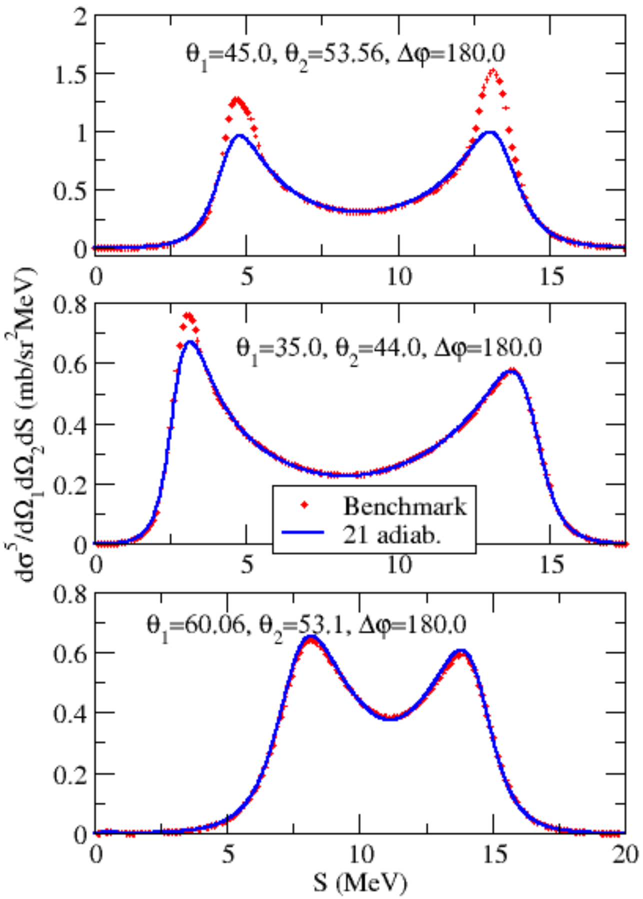
$$\sigma_{bk} = \frac{\pi}{p_y^2}\frac{(2J+1)}{(2s_p+1)(s_t+1)}(1-|S_{11}|^2)$$

Results: n-deuteron breakup

***s*-waves, *J*=1/2+*J*=3/2**

Transition amplitude

$$A^{\sigma_1,\sigma_2,\sigma_3}_{\sigma_d\sigma_n} \propto \sum_{JM} \langle s_d s_n \sigma_d \sigma_n | JM \rangle \sum_{n>1} i^{-K} S_{1n} \langle \sigma_1\sigma_2\sigma_3 | \Phi^{JM}_n(\Omega_\kappa) \rangle$$



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E_{lab}=14.1 MeV	$\lvert S_{11}\rvert$	Re(δ_{11})
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Benchmark	0.465	105.51

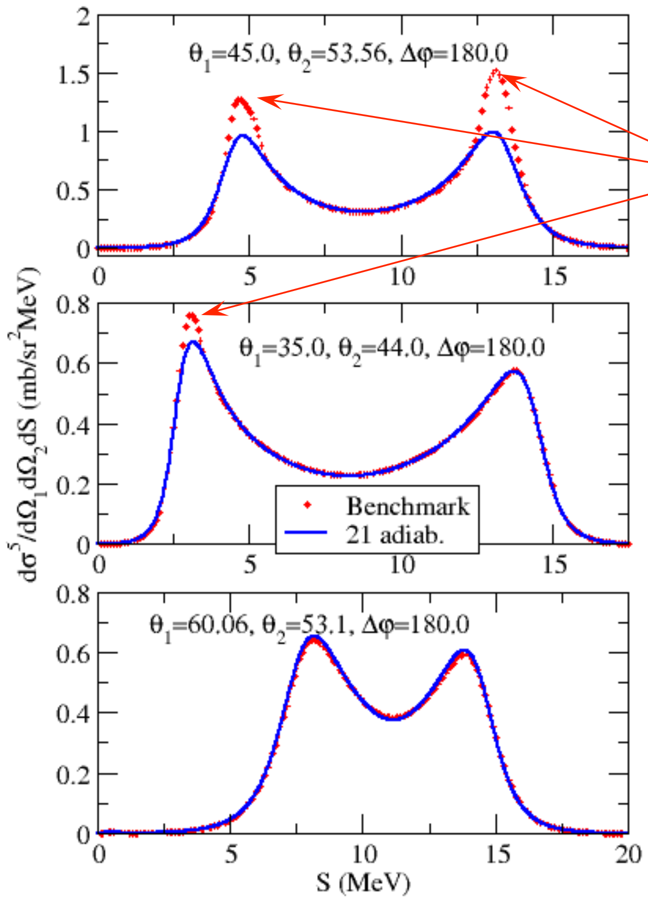
$$\sigma_{bk} = \frac{\pi}{p_y^2} \frac{(2J+1)}{(2s_p+1)(s_t+1)} (1 - |S_{11}|^2)$$

Results: n-deuteron breakup

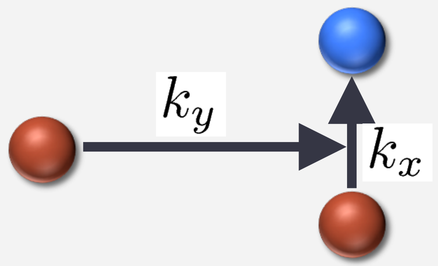
s-waves, J=1/2+J=3/2

Transition amplitude

$$A^{\sigma_1,\sigma_2,\sigma_3}_{\sigma_d\sigma_n} \propto \sum_{JM} \langle s_d s_n \sigma_d \sigma_n | JM \rangle \sum_{n>1} i^{-K} S_{1n} \langle \sigma_1\sigma_2\sigma_3 | \Phi_n^{JM}(\Omega_\kappa) \rangle$$



$$\tan\alpha_\kappa = k_x/k_y \approx 0$$



The proton and one neutron fly together with zero relative energy.

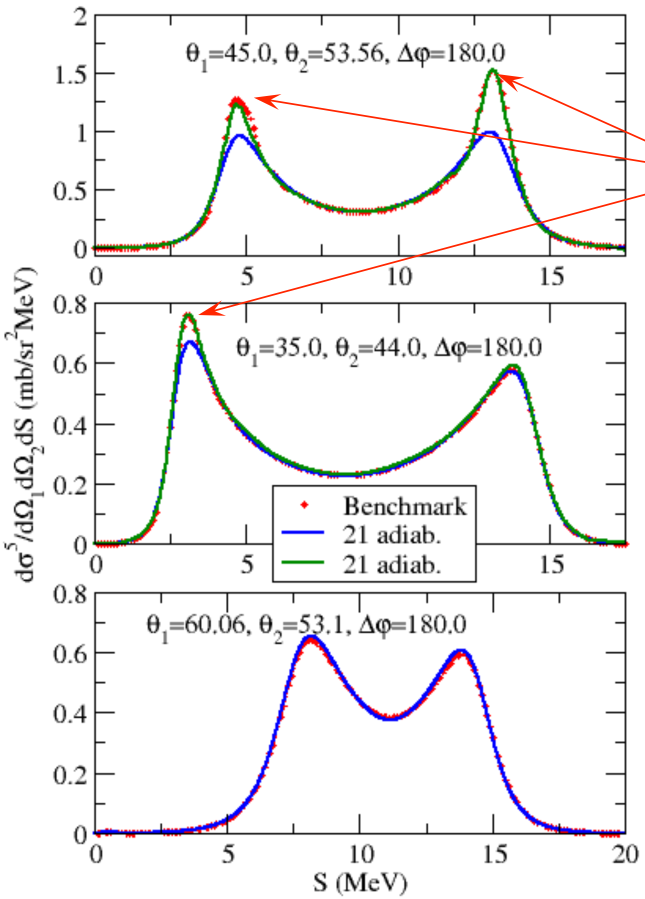
- ✓ Similar to the elastic channel (two-body bound state)
- ✓ A large amount of adiabatic terms required.

Results: n-deuteron breakup

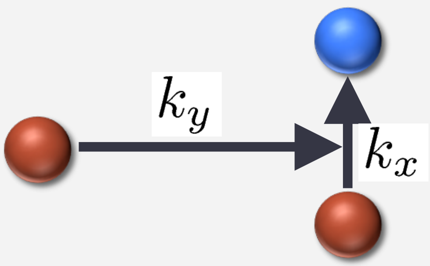
s-waves, J=1/2+J=3/2

Transition amplitude

$$A^{\sigma_1,\sigma_2,\sigma_3}_{\sigma_d\sigma_n} \propto \sum_{JM} \langle s_d s_n \sigma_d \sigma_n | JM \rangle \sum_{n>1} i^{-K} S_{1n} \langle \sigma_1\sigma_2\sigma_3 | \Phi_n^{JM}(\Omega_\kappa) \rangle$$



$$\tan\alpha_\kappa = k_x/k_y \approx 0$$

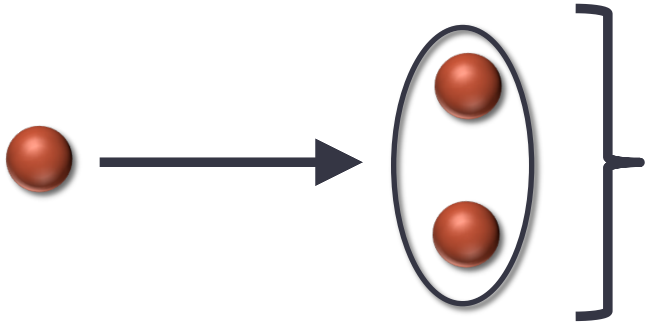


The proton and one neutron fly together with zero relative energy.

- ✓ Similar to the elastic channel (two-body bound state)
- ✓ A large amount of adiabatic terms required.

$$\langle \Psi_1^{JM} | H - E | e^{i(\boldsymbol{k}_x\cdot\boldsymbol{x}+\boldsymbol{k}_y\cdot\boldsymbol{y})} | \sigma_1\sigma_2\sigma_3 \rangle\rangle \propto \sum_{n>1} i^{-K} S_{1n} \langle \sigma_1\sigma_2\sigma_3 | \Phi_n^{JM}(\Omega_\kappa) \rangle$$

Results: ^{4}He-(^{4}He)$_2$ collision



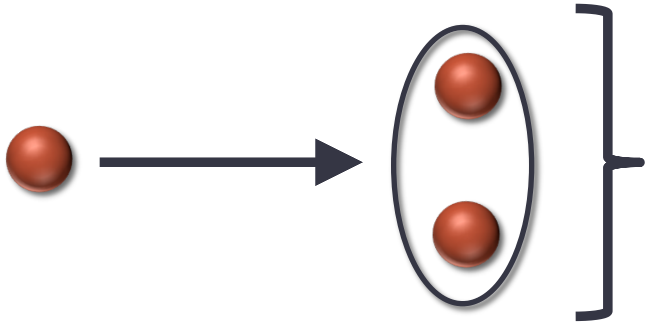
$$V_{2b}(r) = -1.227 e^{-r^2/10.03^2} \mathrm{K}$$

$$E_{2b} = -1.2959 \text{ mK}$$
$$a = 189.95 \text{ a.u.}$$
$$r_e = 13.846 \text{ a.u.}$$

LM2M2 potential

$$E_{2b} = -1.3017 \text{ mK}$$
$$a = 189.05 \text{ a.u.}$$
$$r_e = 13.843 \text{ a.u.}$$

Results: ^{4}He-(^{4}He)$_2$ collision



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E. Nielsen et al., JPB 31 (1998) 4085

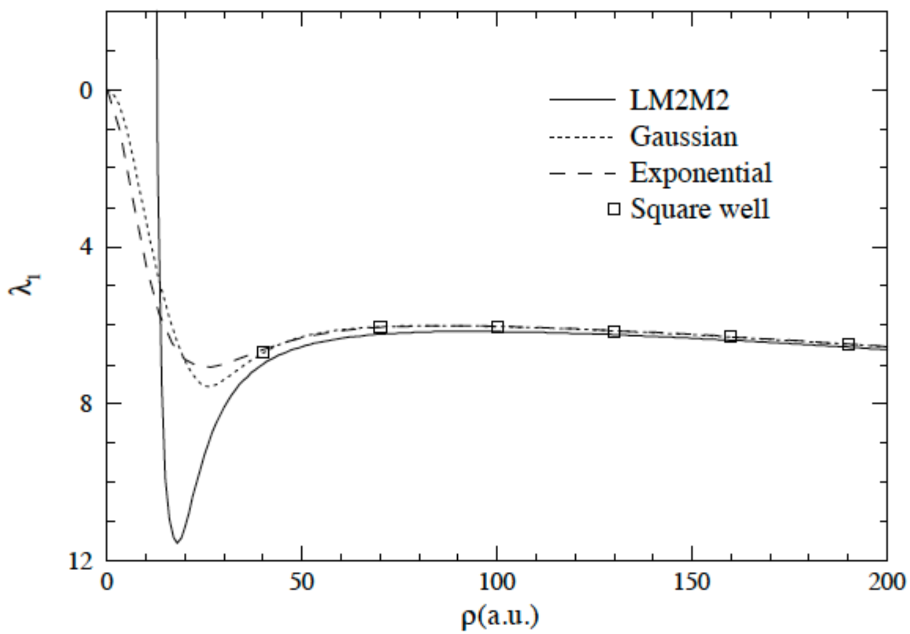


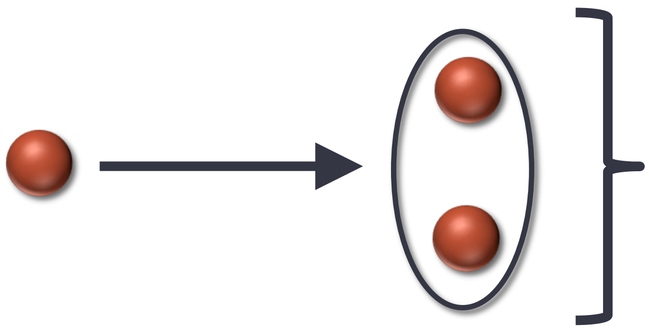
Figure 4. The lowest angular eigenvalue as a function of ρ for the ^{4}He-trimer for the realistic LM2M2 [26] potential and the three schematic potentials defined in table 1. The square well results are obtained from equation (15).

LM2M2 potential

$$E_{2b} = -1.3017 \text{ mK}$$
$$a = 189.05 \text{ a.u.}$$
$$r_e = 13.843 \text{ a.u.}$$

$$V_n(\rho) = \frac{\hbar^2}{2m}\left(\frac{\lambda_n(\rho) + \frac{15}{4}}{\rho^2} - Q_{nn}(\rho)\right)$$

Results: ^{4}He-(^{4}He)$_2$ collision



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$$E_{2b} = -1.2959 \text{ mK}$$
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E. Nielsen et al., PR 347 (2001) 373

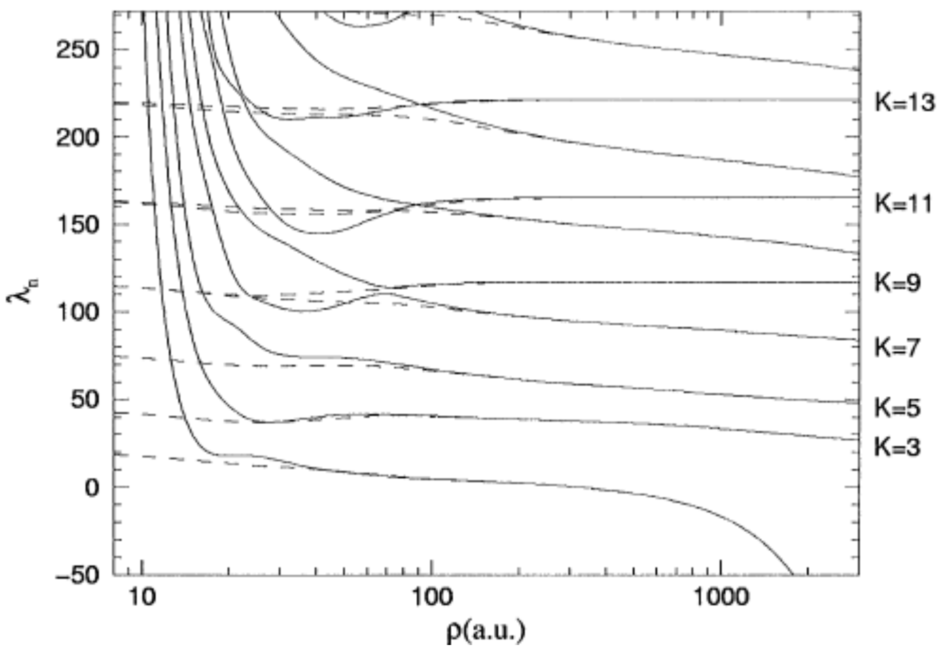


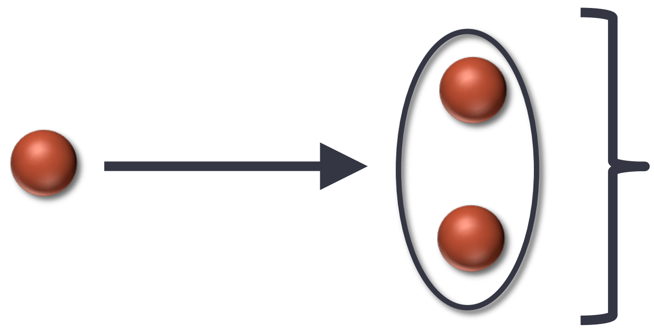
Fig. 10. The angular eigenvalues as function of hyperradius for the $^4He_3$-trimer calculated with the LM2M2 potential (solid curves) and the Gaussian model potentials (dashed curves) for angular momentum and parity $L^\pi = 1^-$.

LM2M2 potential

$$E_{2b} = -1.3017 \text{ mK}$$
$$a = 189.05 \text{ a.u.}$$
$$r_e = 13.843 \text{ a.u.}$$

$$V_n(\rho) = \frac{\hbar^2}{2m}\left(\frac{\lambda_n(\rho) + \frac{15}{4}}{\rho^2} - Q_{nn}(\rho) \right)$$

Results: ^{4}He-(^{4}He)$_2$ collision



$$V_{2b}(r) = -1.227e^{-r^2/10.03^2}\text{K}$$

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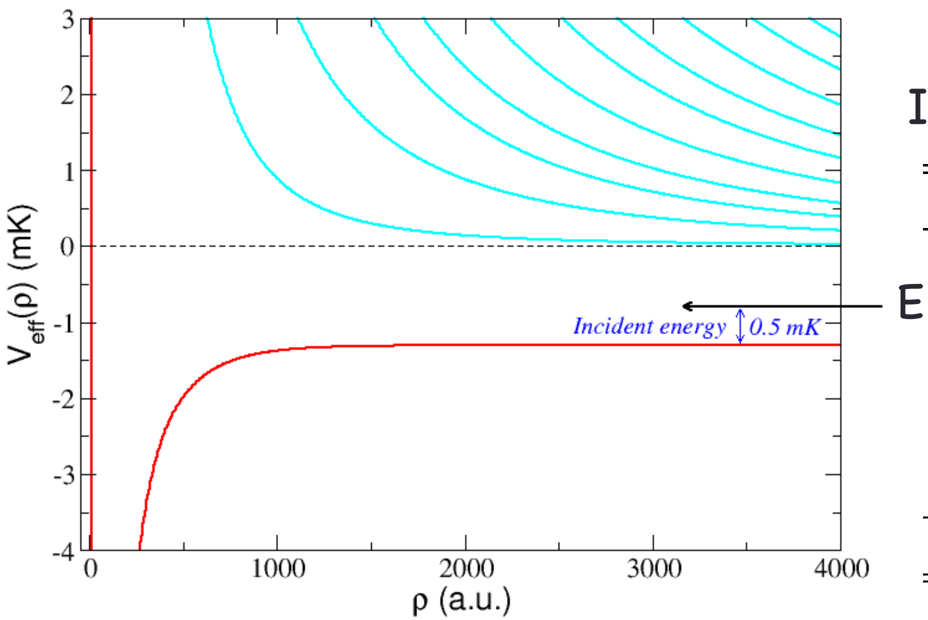
As the LM2M2 potential

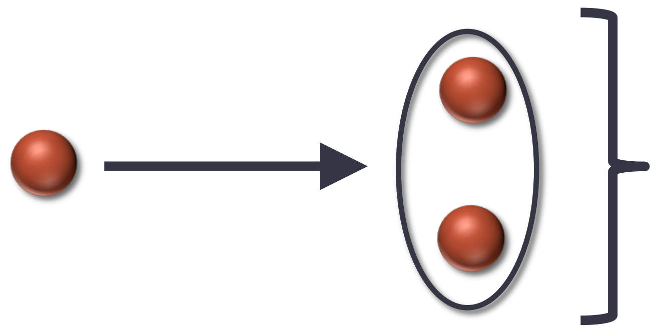


Incident energy: 0.5 mK (E=-0.7959 mK)

n_A	δ_s	δ_p	δ_d	δ_f
1	-39.72	-13.19	2.01	-0.27
2	-40.30	-13.13	2.11	-0.28
4	-40.43	-13.11	2.13	-0.28
8	-40.50	-13.11	2.14	-0.28
18	-40.54	-13.11	2.14	-0.28
22	-40.54	-13.11	2.14	-0.28
HH-calculation	**−40.55**	—	—	—

$$B_{ij} = \frac{2m}{\hbar^2}\int d\tau \Psi_t^i(\tau)(H-E)F_j(\tau)$$

Results: ^{4}He-(^{4}He)$_2$ collision



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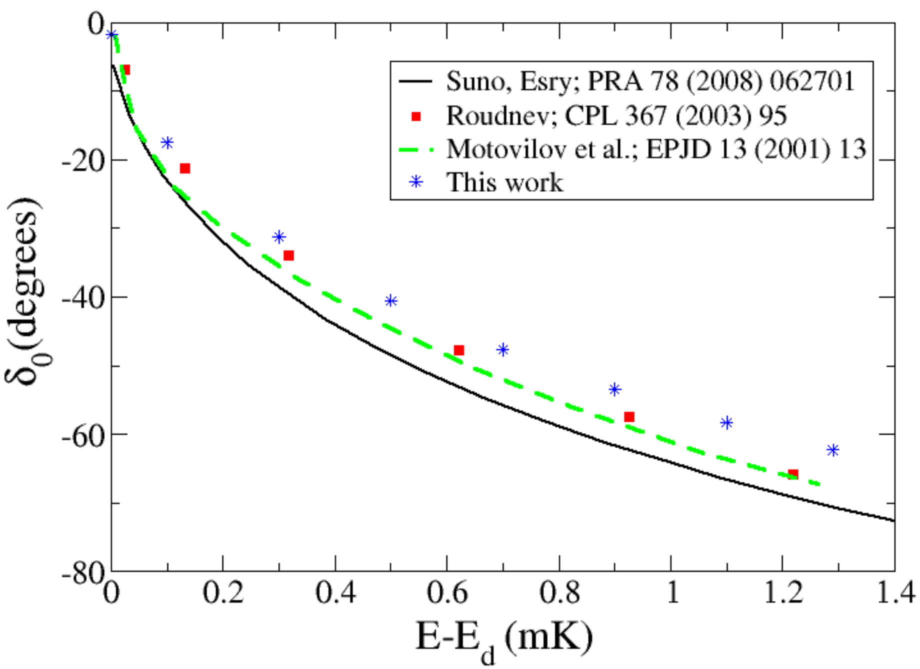
As the LM2M2 potential



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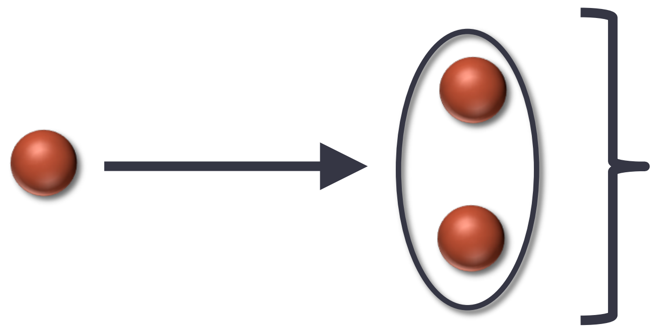
HH-calculation	**−40.55**	—	—	—

E. Garrido, C. Romero-Redondo, A. Kievsky, M. Viviani, PRA 86 (2012) 052709

Results: ^{4}He-(^{4}He)$_2$ collision



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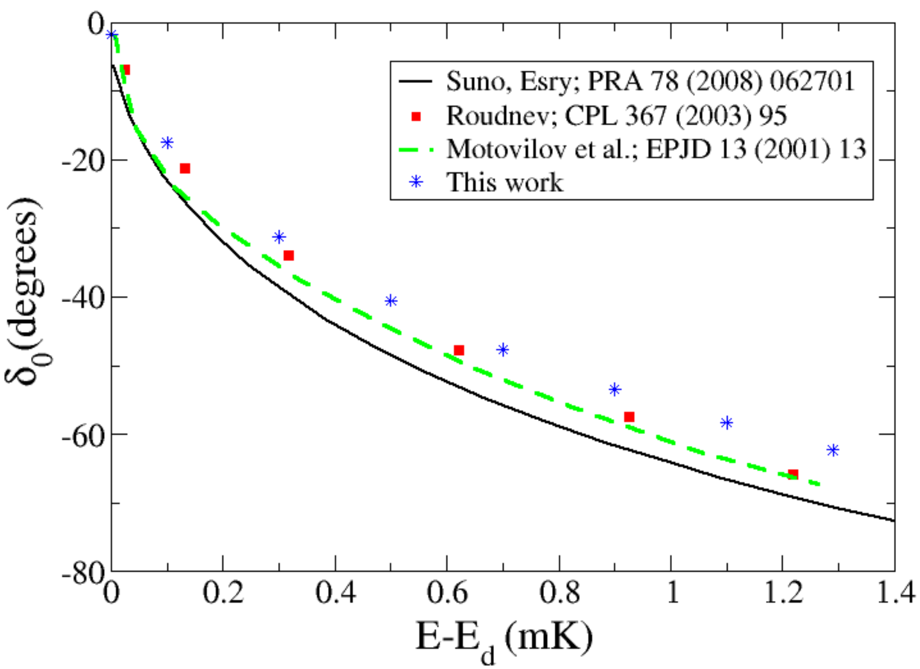
As the LM2M2 potential

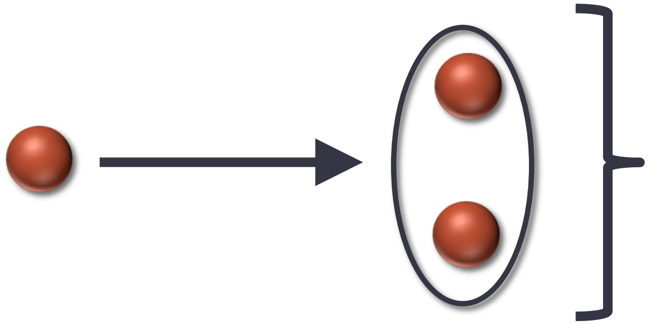


potential	E_0 [mK]	E_1 [mK]	a_0 [a.u.]
LM2M2	−126.4	−2.265	217.3
gaussian	−150.0	−2.467	165.9
(W_0 [K], ρ_0 [a.u.])			
(306.9, 4)	−126.4	−2.283	211.7
(18.314, 6)	−126.4	−2.287	210.6
(4.0114, 8)	−126.4	−2.289	210.0
(1.4742, 10)	−126.4	−2.292	209.2

$$V_n(\rho) \rightarrow V_n(\rho) + W_{3b}(\rho)$$

$$W_{3b}(\rho) = W_0 e^{-\rho^2/\rho_0^2}$$

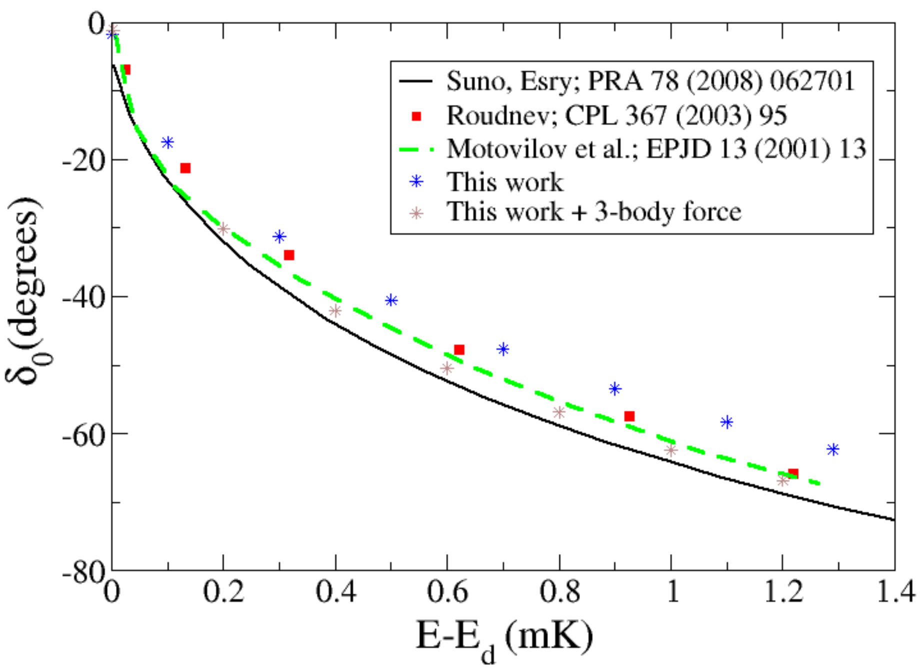
Results: ^{4}He-(^{4}He)$_2$ collision



$$V_{2b}(r) = -1.227 e^{-r^2/10.03^2} \mathrm{K}$$

$$E_{2b} = -1.2959 \text{ mK}$$
$$a = 189.95 \text{ a.u.}$$
$$r_e = 13.846 \text{ a.u.}$$

As the LM2M2 potential



potential	E_0 [mK]	E_1 [mK]	a_0 [a.u.]
LM2M2	−126.4	−2.265	217.3
gaussian	−150.0	−2.467	165.9
(W_0 [K], ρ_0 [a.u.])			
(306.9, 4)	−126.4	−2.283	211.7
(18.314, 6)	−126.4	−2.287	210.6
(4.0114, 8)	−126.4	−2.289	210.0
(1.4742, 10)	−126.4	−2.292	209.2

$$V_n(\rho) \rightarrow V_n(\rho) + W_{3b}(\rho)$$

$$W_{3b}(\rho) = W_0 e^{-\rho^2/\rho_0^2}$$

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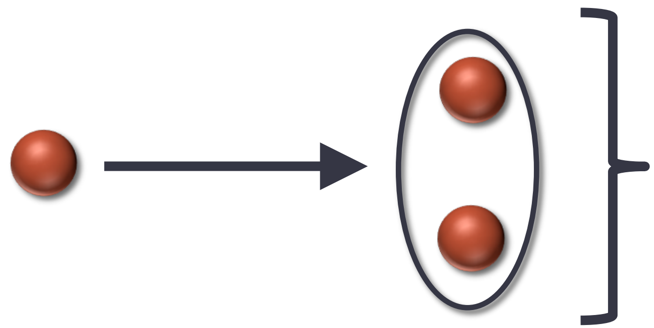

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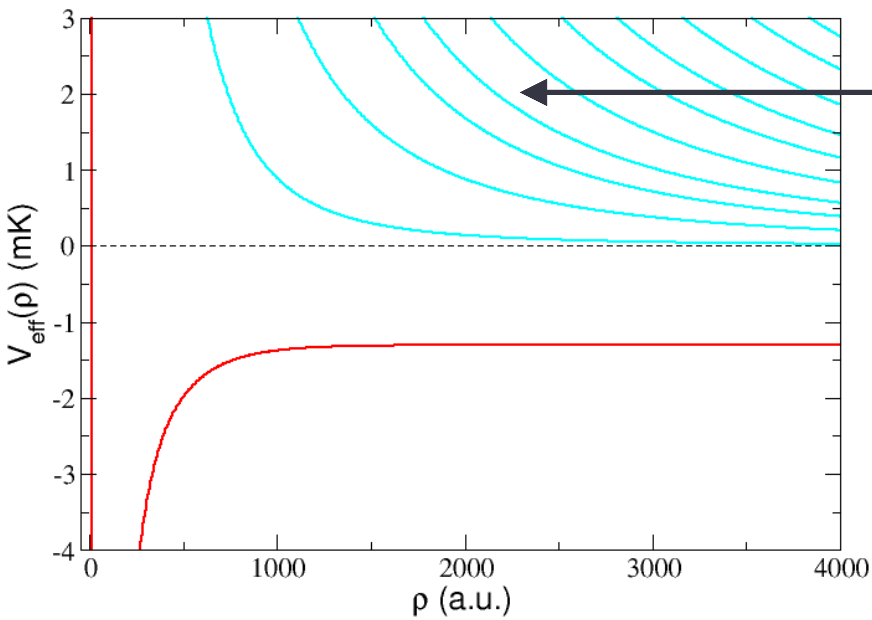
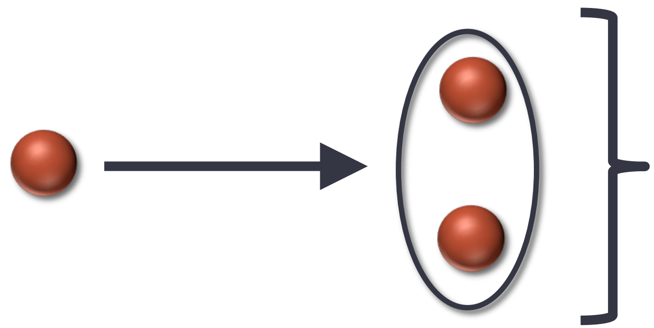


E

The elastic and breakup channels are open

Results: ^4He-$(^4He)_2$ collision



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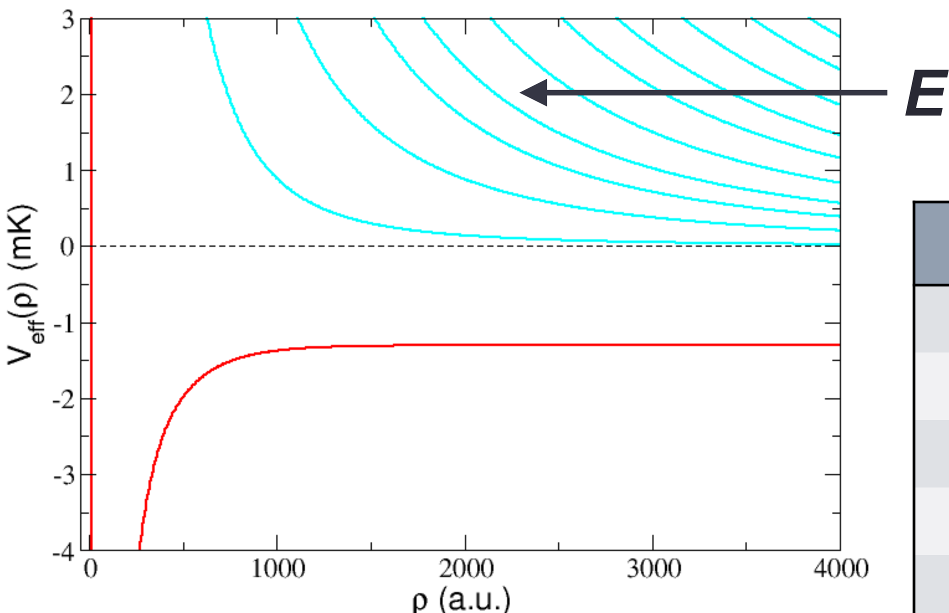

The elastic and breakup channels are open

E_{lab}=25 mK	$\lvert S_{11}\rvert$	Re(δ_{11})
n=4	0.913	35.06
n=6	0.911	34.69
n=8	0.910	34.61
n=10	0.911	34.59
n=12	0.911	34.59

$$\sum_{n=2}^{\infty} |S_{1n}|^2 = 1 - |S_{11}|^2$$

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

Results: ^{4}He-(^{4}He)$_2$ collision

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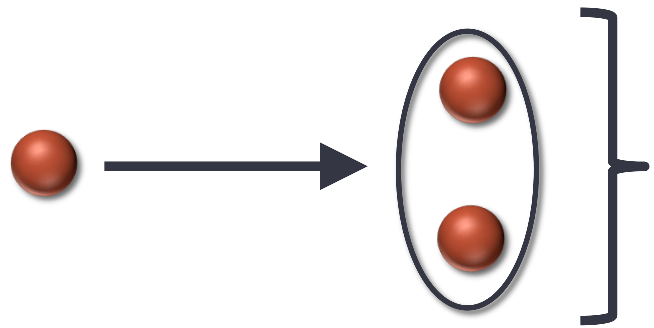

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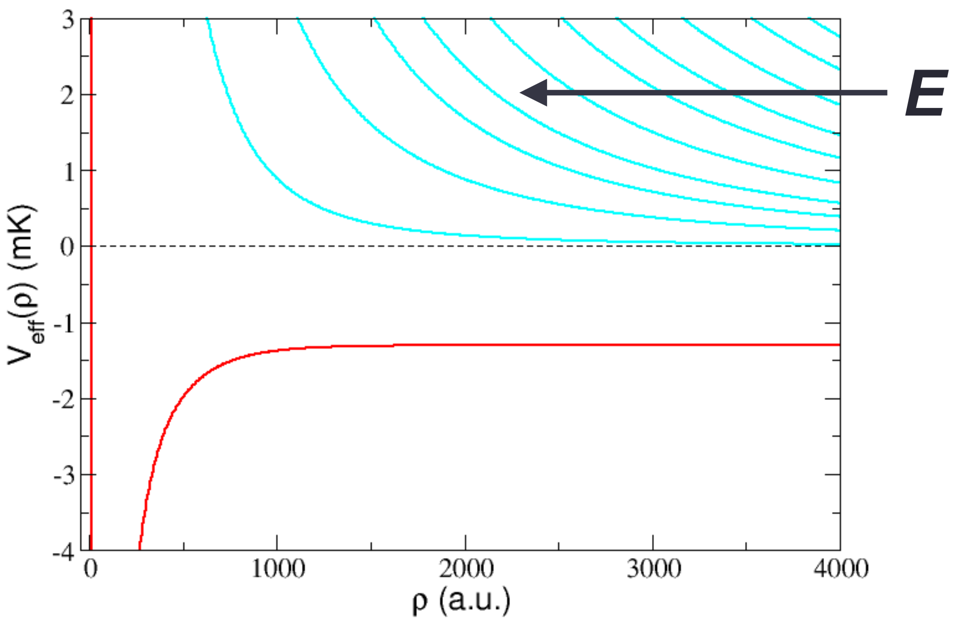


$$\sum_{n=2}^{\infty} |S_{1n}|^2 = 1 - |S_{11}|^2$$

Recombination Rate

$$^4\mathrm{He} + {}^4\mathrm{He} + {}^4\mathrm{He} \rightarrow {}^4\mathrm{He} + ({}^4\mathrm{He})_2$$

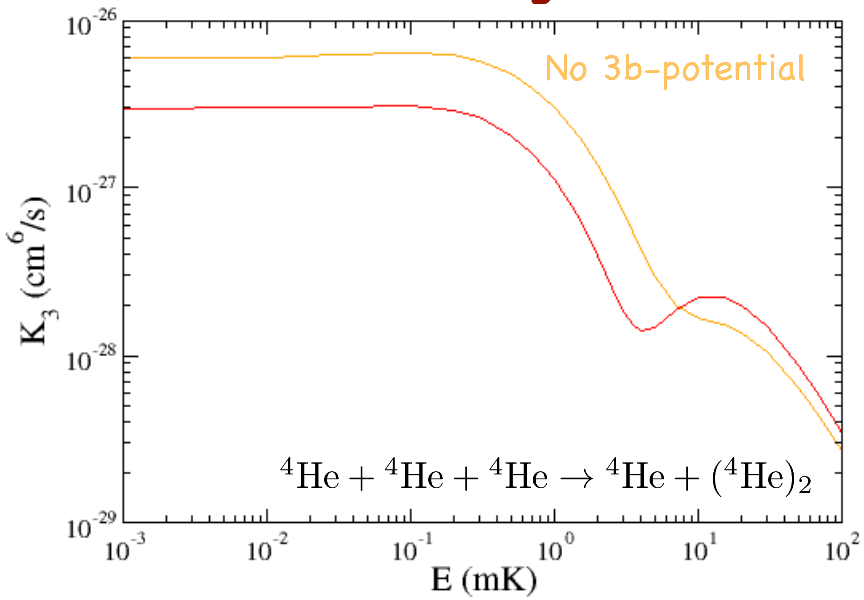
$$K_3 = 3! \sum_J \sum_{n=2}^{\infty} \frac{32(2J+1)\pi^2}{\mu k^4} |S_{1n}|^2$$

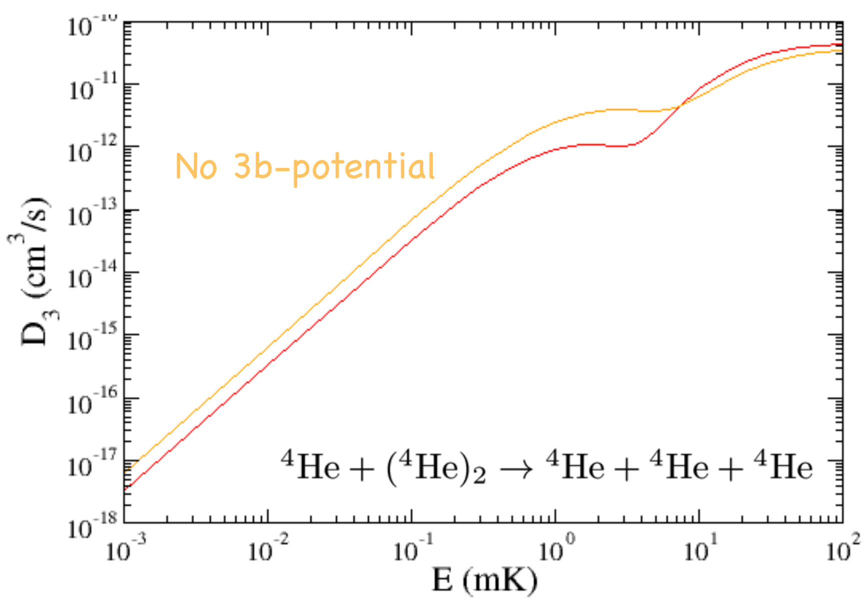
Dissociation Rate

$$^4\mathrm{He} + ({}^4\mathrm{He})_2 \rightarrow {}^4\mathrm{He} + {}^4\mathrm{He} + {}^4\mathrm{He}$$

$$D_3 = 2! \sum_J \sum_{n=2}^{\infty} \frac{32(2J+1)\pi^2}{\mu_{1,23} k_{1,23}} |S_{1n}|^2$$

Results: ^4He-$(^4He)_2$ collision





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Recombination Rate

$$^4He + {^4He} + {^4He} \to {^4He} + (^4He)_2$$

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Dissociation Rate

$$^4He + (^4He)_2 \to {^4He} + {^4He} + {^4He}$$

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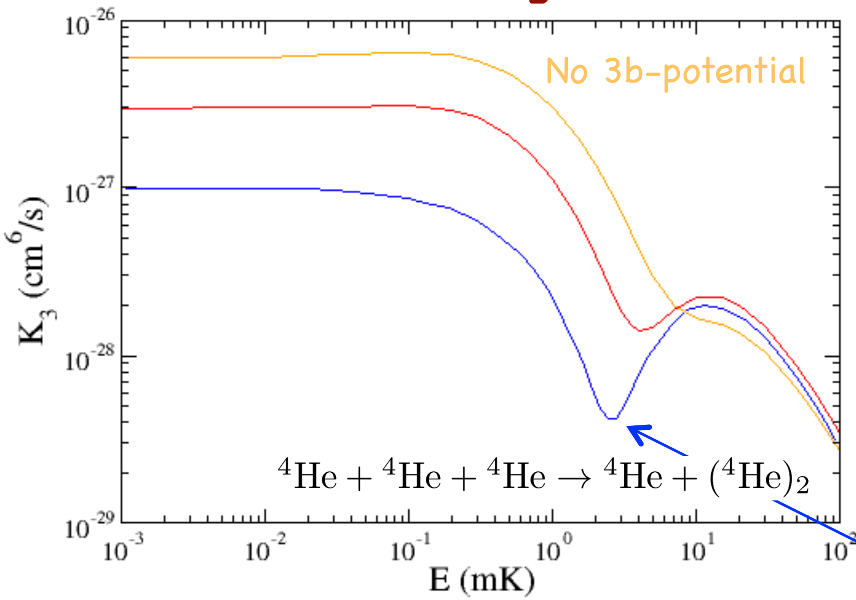

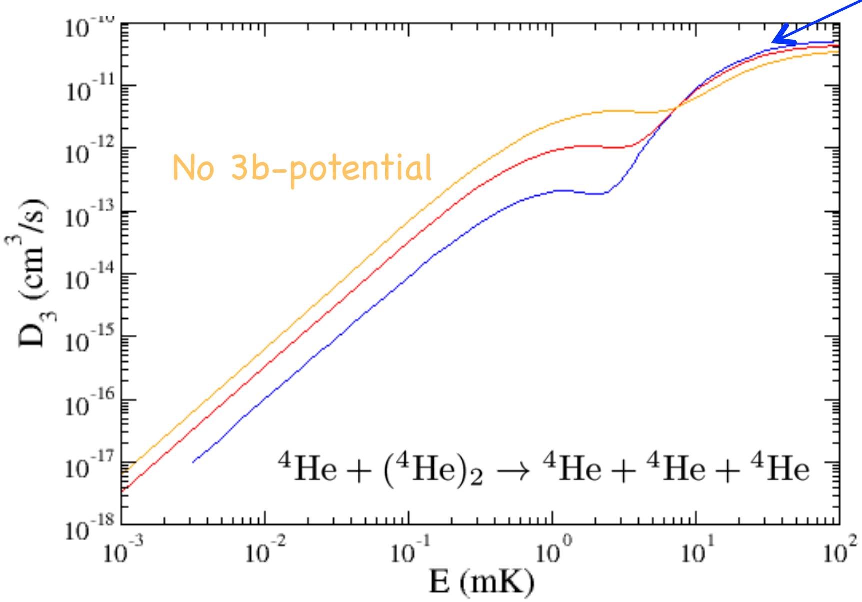

H. Suno and B.D. Esry, PRA 78 (2008) 062701

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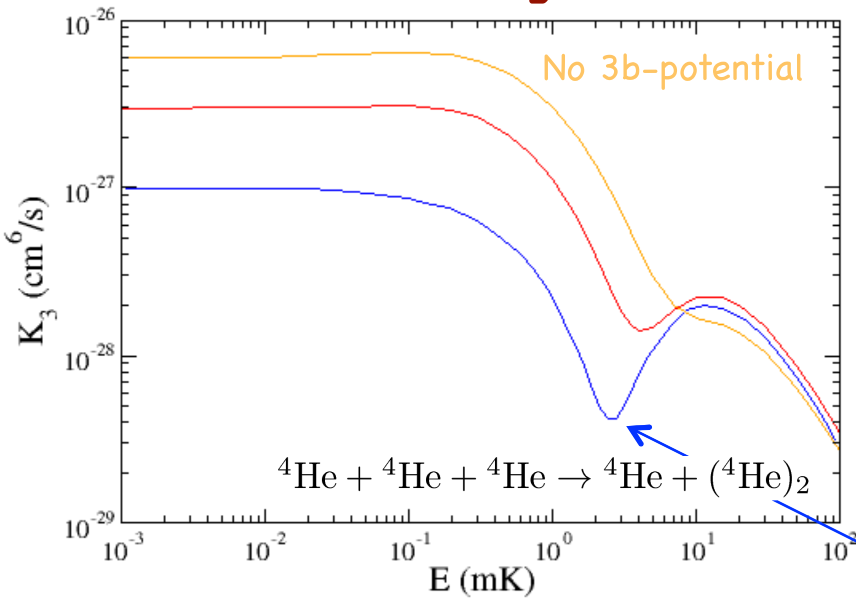
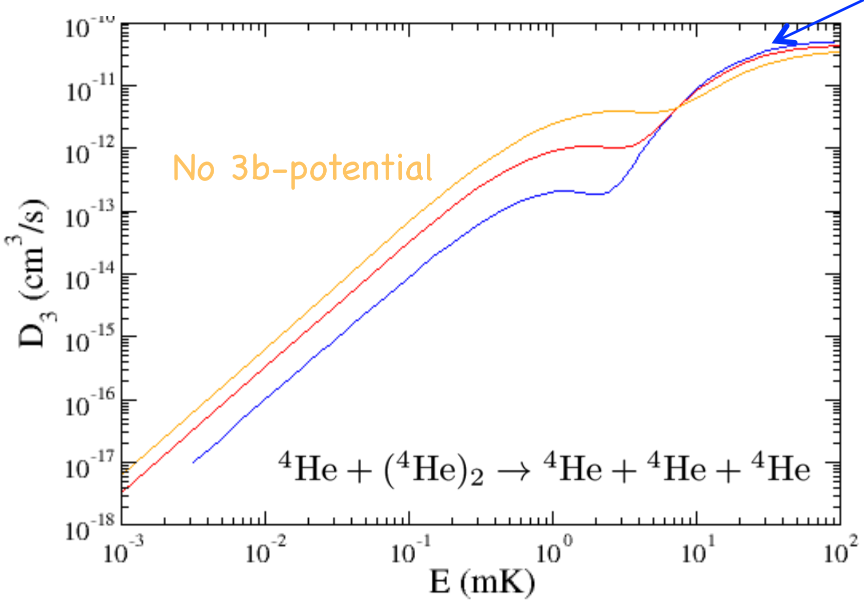


H. Suno and B.D. Esry, PRA 78 (2008) 062701



SAPT potential

$$E_{2b} = -1.564\ \mathrm{mK}$$
$$a = 173.50\ \mathrm{a.u.}$$
$$r_e = 13.79\ \mathrm{a.u.}$$
$$\langle r \rangle = 90.3\ \mathrm{a.u.}$$

M. Jeziorska et al., JCP 127 (2007) 124303

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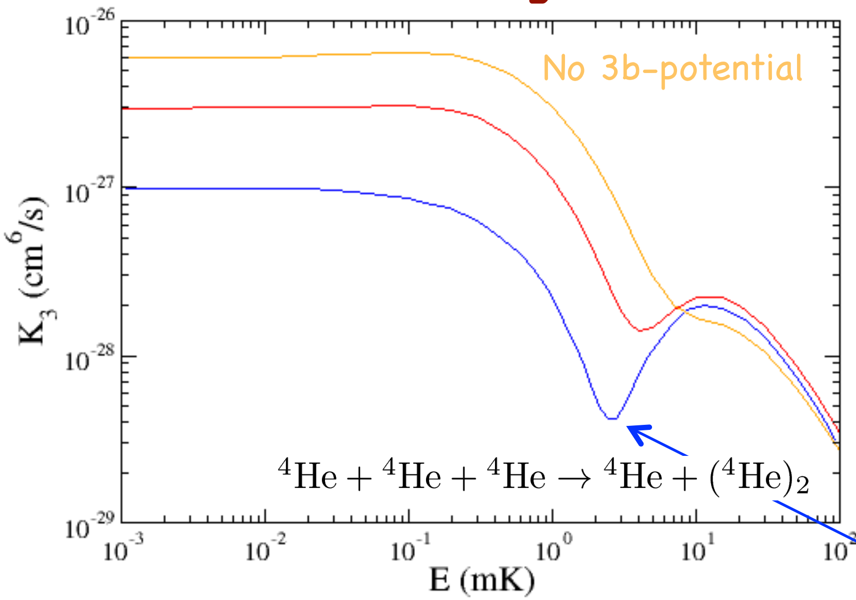

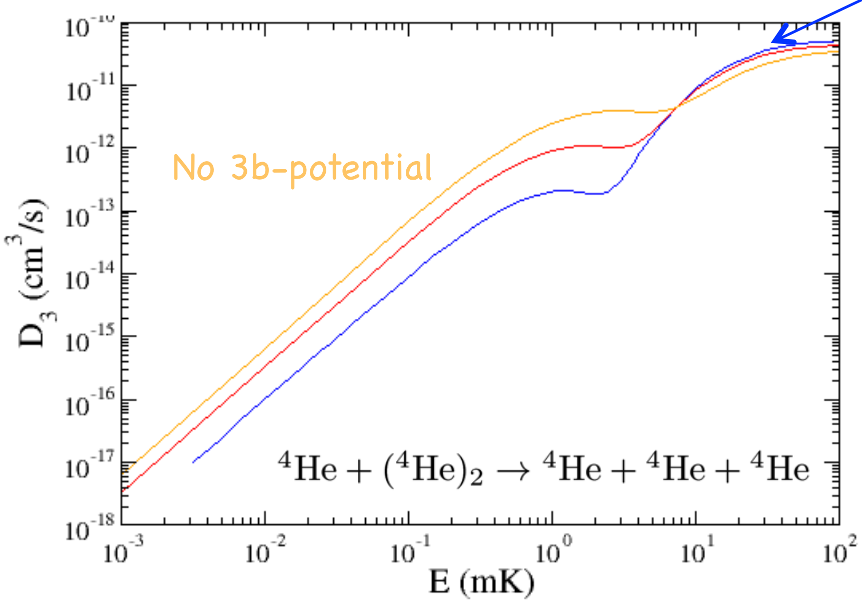

H. Suno and B.D. Esry, PRA 78 (2008) 062701

$$V_{2b}(r) = -1.234 e^{-r^2/10.03^2} \mathrm{K}$$

$$E_{2b} = -1.554 \text{ mK}$$
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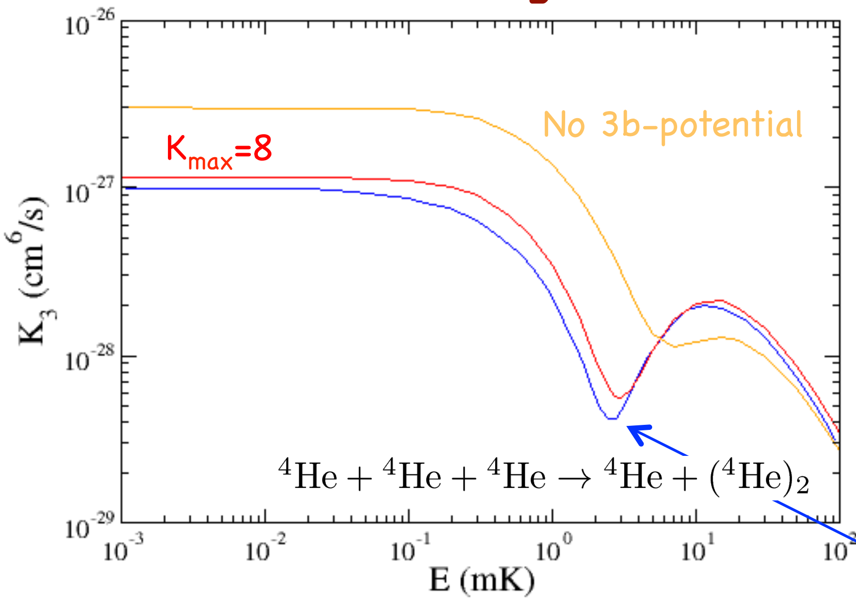

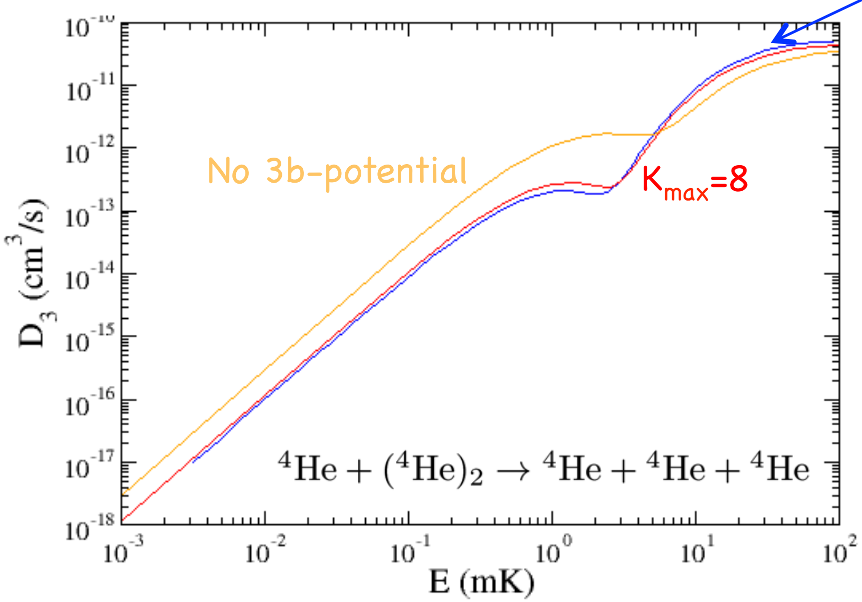

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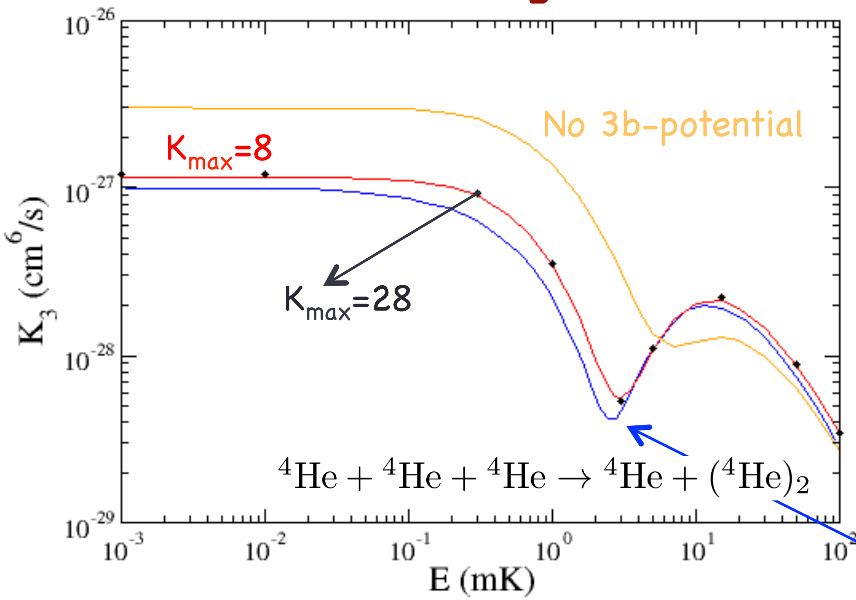

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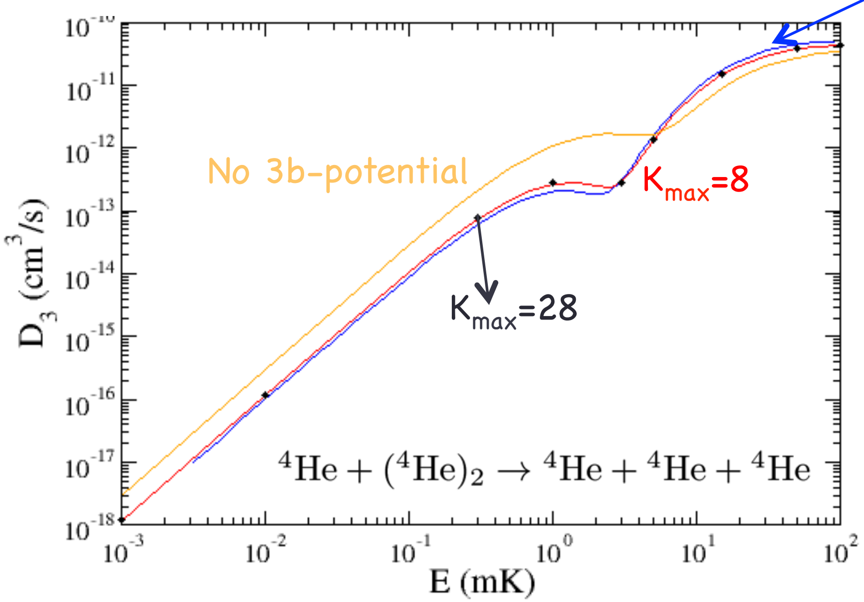

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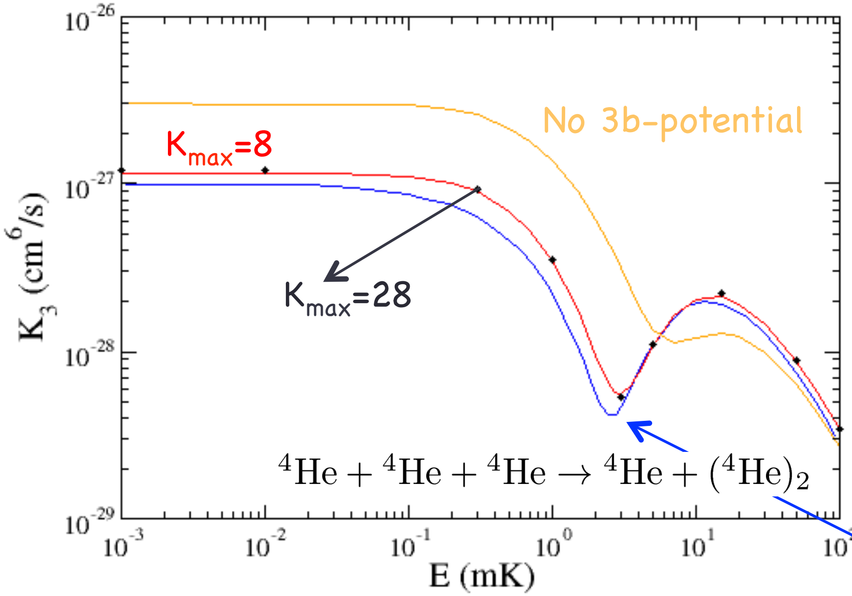

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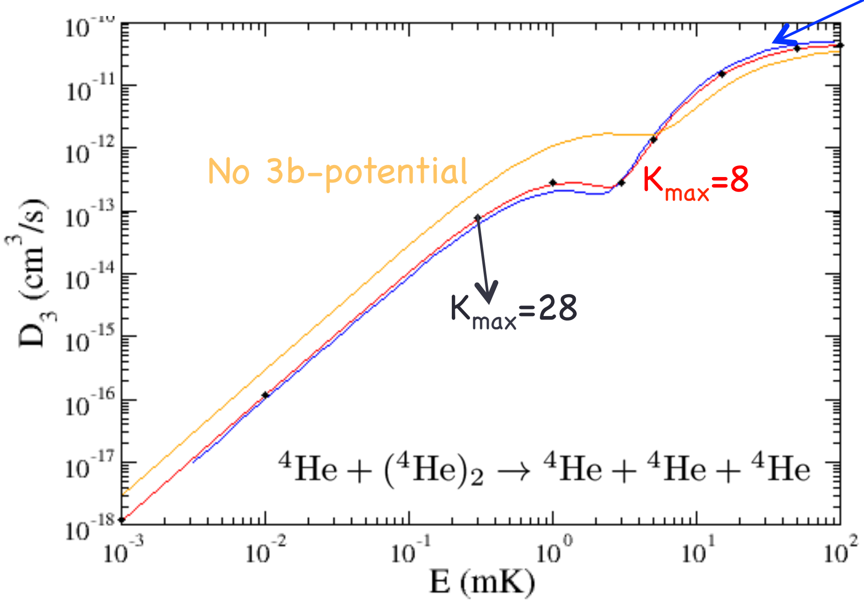
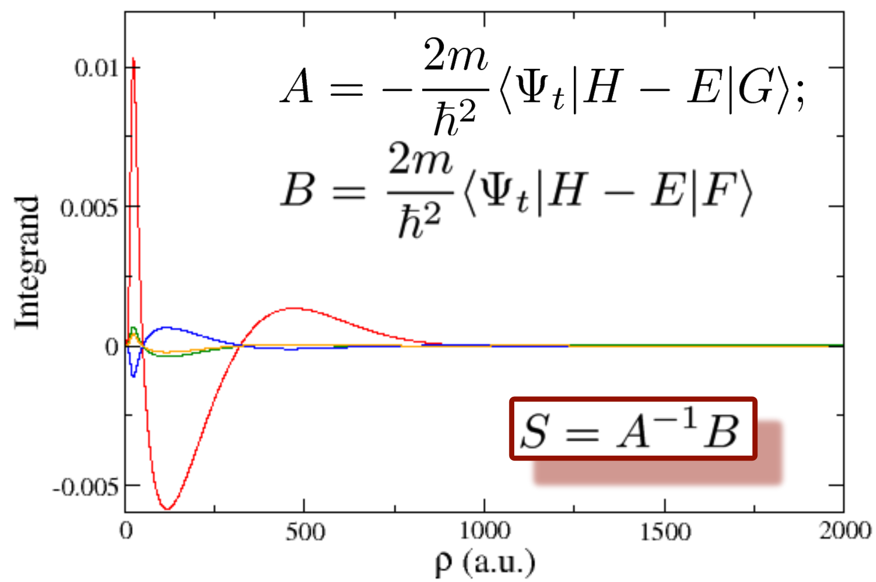
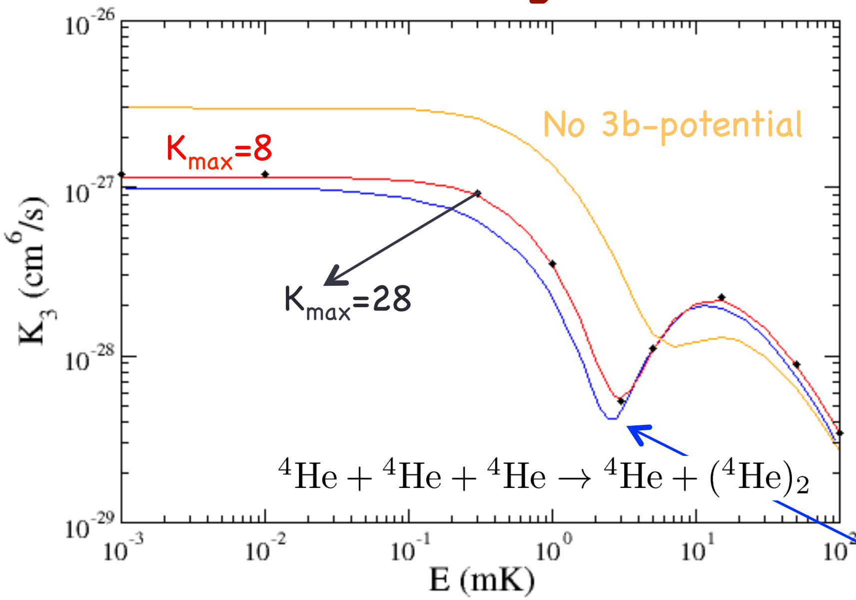




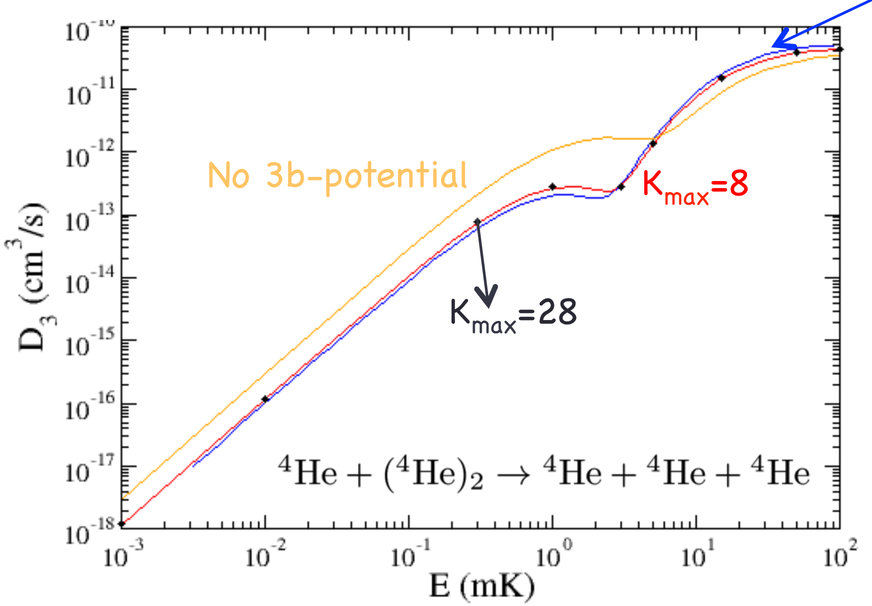
$$A = -\frac{2m}{\hbar^2} \langle \Psi_t | H - E | G \rangle;$$
$$B = \frac{2m}{\hbar^2} \langle \Psi_t | H - E | F \rangle$$
$$S = A^{-1} B$$

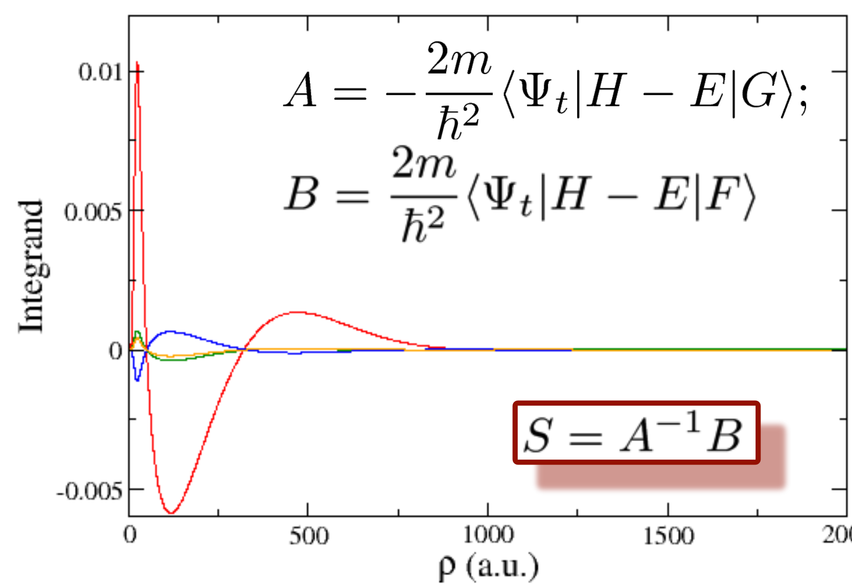
Results: ^4He-$(^4He)_2$ collision



The scattering observables were obtained by solving the coupled equations (14) using a combination of the finite element method (FEM) [50] and the R-matrix method [41]. Typically, about 12 adiabatic channels (thus $\nu_{max}=11$) are used, and 10^4 elements, in each of which fifth order polynomials are used to expand the radial wave function, extend from $R=5$ to 5×10^5 a.u. The scattering S matrix is then extracted using the R-matrix method. Each energy took less than 1 minute of wall clock time using one 1.6 GHz Itanium2 processor on an SGI Altix 4700 supercomputer. We have checked the stability of the S matrix with respect to the final matching distance, number of FEM sectors, and the number of coupled channels, and have found our results accurate to two significant digits.

H. Suno and B.D. Esry, PRA 78 (2008) 062701





Summary and conclusions:

✓ When investigating **1+N** reactions, extraction of the S-matrix from the asymptotic part of the (1+N)-body cross section is a very hard task:

- We need the wave function at very large distances.
- Even when done, the result can be inaccurate.

✓ We have developed a method, based on the **Kohn variational principle**, that leads to **two integral relations** the permit to obtain the S-matrix from the **internal part** of the wave function.

- They can be used to describe elastic, inelastic, transfer, **and breakup** reactions.

✓ The method reproduces available benchmark calculations for neutron-deuteron scattering below and above the breakup threshold.

- Not only the S-matrix is reproduced, but also the differential cross sections.

✓ We have applied the method to ^{4}He-(^{4}He)$_2$, (^{4}He-^{4}He-^{6}Li) reactions together with the adiabatic expansion method: Soft-core potentials are a good alternative to the hard-core potentials **when used together with an effective three-body force**.

- Elastic scattering phase-shifts well reproduced.
- Dissociation and recombination rates are sensitive to the details of the two-body interaction.

THANK YOU !!!

C. Romero-Redondo, *TRIUMF, Vancouver, Canada*

A. Kievsky, M. Viviani, *INFN, Pisa, Italy*

E. Garrido, *IEM-CSIC, Madrid, Spain*

Vancouver, February 2014