Part 2

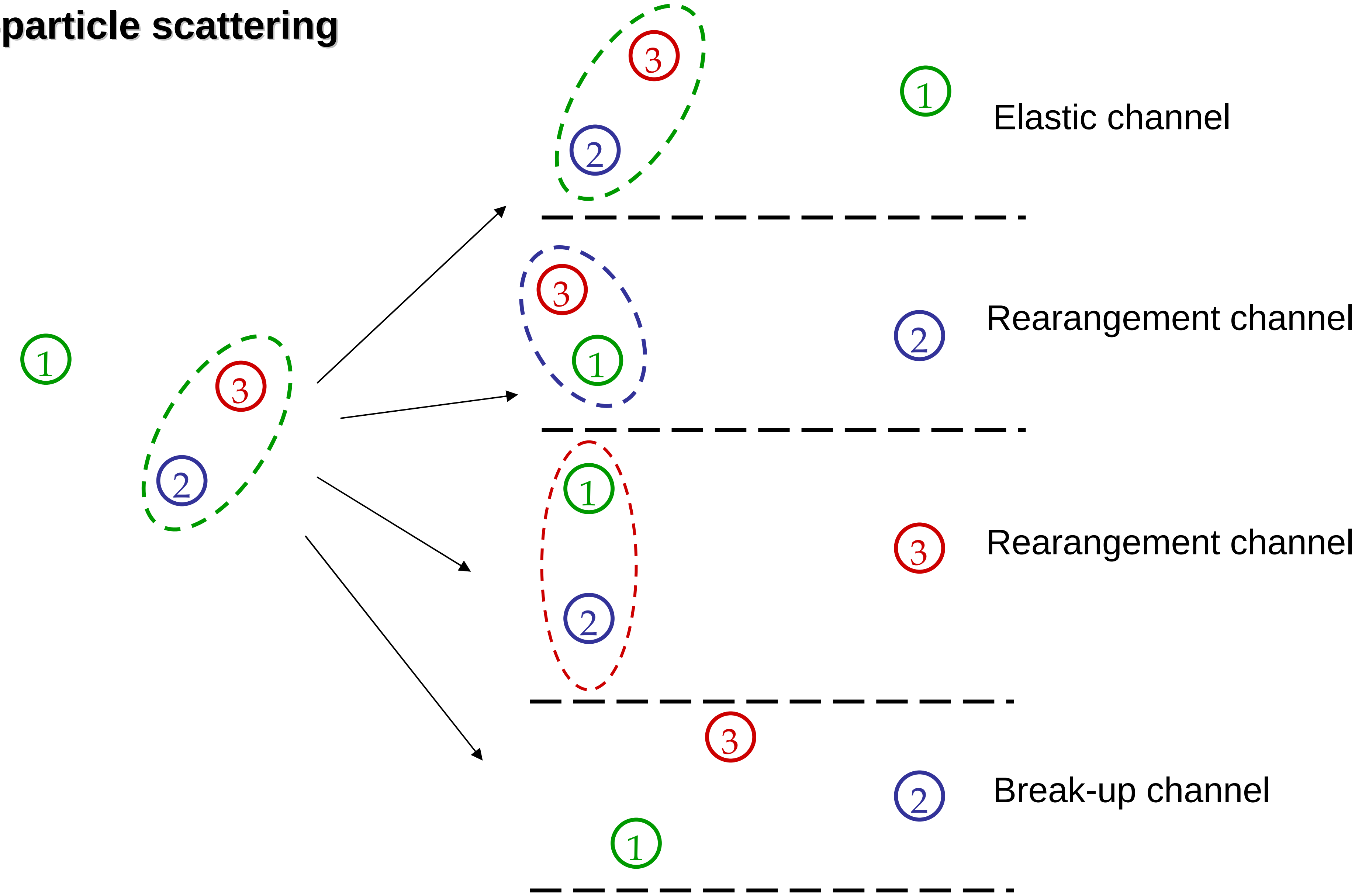
3-body problem (Faddeev eq.)

Bare particle-particle interaction with all its complexity

Faddeev eq.:

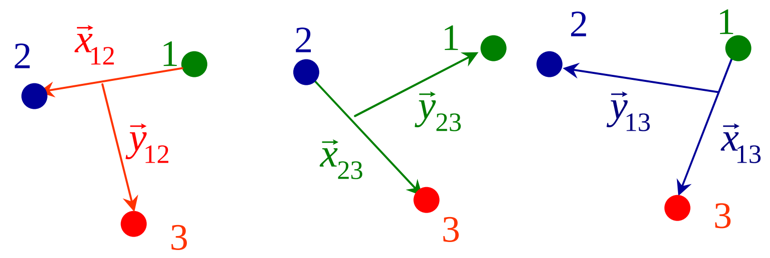
Bound states, scattering states, resonant states, capture (radiative, weak), …

3-particle scattering



• *Schrödinger eq. is not enough (problem to determine unique solution)*

Jacobi coordinates



Three equivalent sets of coordinates:

$$\begin{cases} \vec{x}_{ij} = \sqrt{2\frac{\mu_{ij}}{M}}\left(\vec{r}_j - \vec{r}_i\right) \\ \vec{y}_{ij} = \sqrt{2\frac{\mu_{ij,k}}{M}}\left(\vec{r}_k - \frac{\vec{r}_i m_i + \vec{r}_j m_j}{m_i + m_j}\right) \\ \vec{R} = \frac{\vec{r}_i m_i + \vec{r}_j m_j + \vec{r}_k m_k}{M} \end{cases}$$

with

$$\mu_{ij} = \frac{m_i m_j}{m_i + m_j}$$

$$\mu_{ij,k} = \frac{(m_i + m_j) m_k}{m_i + m_j + m_k}$$

Kinetic energy operator:

$$T = -\sum_{i=1}^{3} \frac{\hbar^2}{2m_i}\Delta_{\vec{r}_i} = \underbrace{-\frac{\hbar^2}{M}\left(\Delta_{\vec{x}_{ij}} + \Delta_{\vec{y}_{ij}}\right)}_{H_0} \underbrace{-\frac{\hbar^2}{M}\Delta_{\vec{R}}}_{H_{c.m.}}$$

Full Hamiltonian:

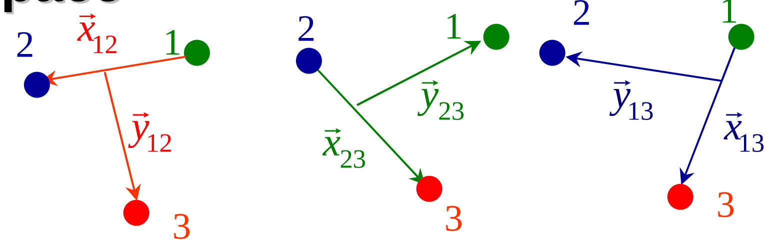
$$H = H_0 + V_{12}\left(\vec{x}_{12}\right) + V_{23}\left(\vec{x}_{23}\right) + V_{31}\left(\vec{x}_{31}\right) + \cancel{H_{c.m.}}$$

$$\left(H - E\right)\Psi\left(\vec{x}_{ij}, \vec{y}_{ij}\right) = 0$$

Faddeev equations in configuration space

$$(H-E)\Psi(\vec{x}_{ij},\vec{y}_{ij})=0$$

$$G_0=(H_0-E)^{-1}$$



✓ We consider three particle interacting via short-range pairvise forces

✓ We define Faddeev components: $F_{ij}=-G_0V_{ij}\Psi$

✓ We define equations for three Faddeev components (Faddeev equations)

$$\Psi(\vec{x},\vec{y})=\sum_{i<j=1}^{3}F_{ij}(\vec{x}_{ij},\vec{y}_{ij})$$

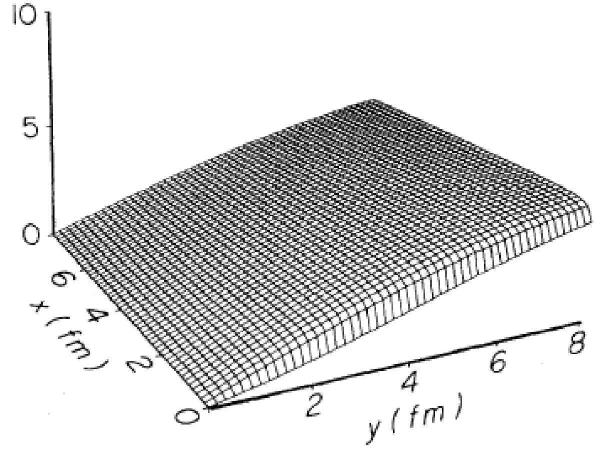
$$\begin{cases}(E-V_{12}-H_0)F_{12}=V_{12}(F_{23}+F_{13})\\(E-V_{23}-H_0)F_{23}=V_{23}(F_{12}+F_{23})\\(E-V_{13}-H_0)F_{13}=V_{13}(F_{23}+F_{12})\end{cases}$$

$$(F_{23}+F_{13})\xrightarrow[y_{12}\to\infty]{}0$$

• Sum of three Faddeev equations gives Schrödinger equation

• It permits to implement correct boundary conditions for the elastic & rearrangement channels

F



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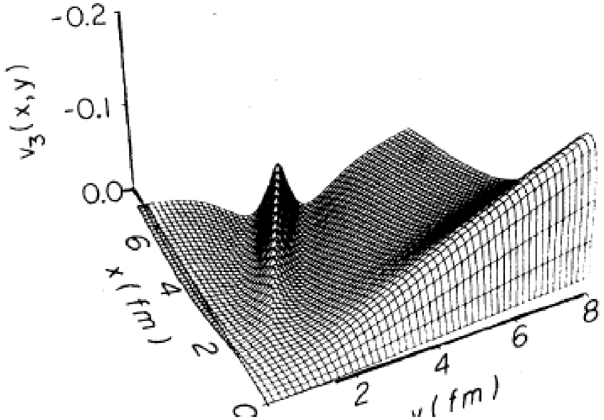
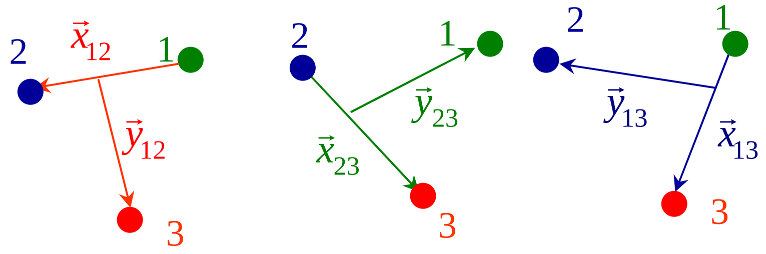


Solution of Faddeev equations

$$(H-E)\Psi(\vec{x}_{ij},\vec{y}_{ij})=0$$

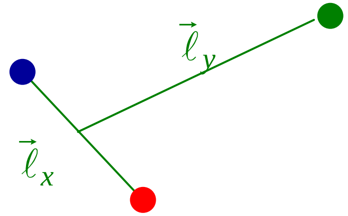
$$G_0=(H_0-E)^{-1}$$



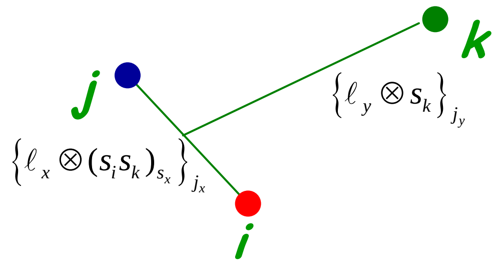
✓ Faddeev components are developed in bipolar harmonics basis

- spin-less particles

$$F_{ij}^{LM}(\vec{x}_{ij},\vec{y}_{ij})=\sum_{\alpha_{ij}=\ell_x,\ell_y}\frac{f_{ij,\alpha}(x_{ij},y_{ij})}{x_{ij}y_{ij}}\left[Y_{\ell_x}(\hat{x}_{ij})\otimes Y_{\ell_y}(\hat{y}_{ij})\right]_{LM}$$
$$=\sum_{\alpha_{ij}=\ell_x,\ell_y}\frac{f_{ij,\alpha}(x_{ij},y_{ij})}{x_{ij}y_{ij}}B_{\alpha_{ij}}^{JM}(\hat{x}_{ij},\hat{y}_{ij})$$



- particles with spin



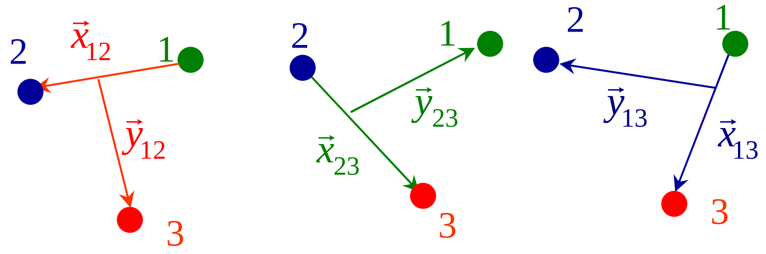
$$F_{ij}^{JM}(\vec{x}_{ij},\vec{y}_{ij})=\sum_{\alpha_{ij}=\ell_x,\ell_y,s_x,j_x,j_y}\frac{f_{ij,\alpha}(x_{ij},y_{ij})}{x_{ij}y_{ij}}\left[\left\{Y_{\ell_x}(\hat{x}_{ij})\otimes s_x\right\}_{j_x}\otimes\left\{Y_{\ell_y}(\hat{y}_{ij})\otimes s_k\right\}_{j_y}\right]_{JM}$$
$$=\sum_{\alpha_{ij}=\ell_x,\ell_y,s_x,j_x,j_y}\frac{f_{ij,\alpha}(x_{ij},y_{ij})}{x_{ij}y_{ij}}B_{\alpha_{ij}}^{JM}(\hat{x}_{ij},\hat{y}_{ij},s_i,s_j,s_k)$$

$$\left[\left\{\ell_x\otimes(s_is_k)_{s_x}\right\}_{j_x}\otimes\left\{\ell_y\otimes s_k\right\}_{j_y}\right]_{JM}$$

Solution of Faddeev equations

$$\left(H-E\right)\Psi\left(\vec{x}_{ij},\vec{y}_{ij}\right)=0$$

$$G_0=(H_0-E)^{-1}$$



✓ Faddeev equations are projected onto bipolar harmonics basis

$$\left(E-V_{ij}-H_0\right)F_{ij}=V_{ij}\left(F_{jk}+F_{ik}\right)$$

$$\Downarrow$$

$$\left[E+\frac{\hbar^2}{M}\frac{d^2}{dx_{ij}^2}-\frac{\hbar^2}{M}\frac{\ell_x(\ell_x+1)}{x_{ij}^2}+\frac{\hbar^2}{M}\frac{d^2}{dy_{ij}^2}-\frac{\hbar^2}{M}\frac{\ell_y(\ell_y+1)}{y_{ij}^2})-V_{ij}(x_{ij})\right]f_{ij,\alpha_{ij}}(x_{ij},y_{ij})=$$

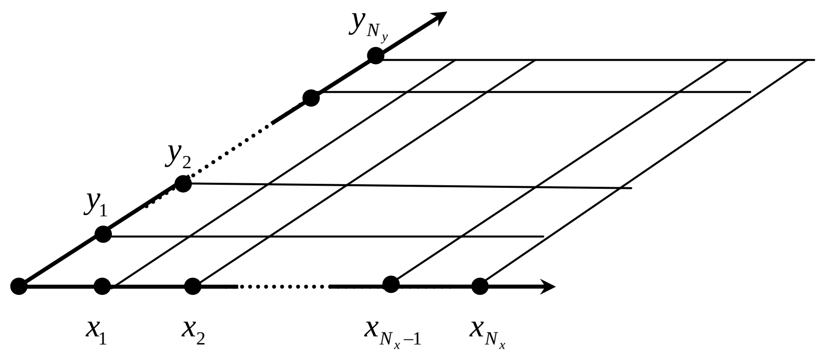
$$=\sum_{\alpha'_{jk}}V_{ij}(x_{ij})\int\int d\hat{x}_{ij}d\hat{y}_{ij}\frac{x_{ij}y_{ij}}{x_{jk}y_{jk}}f_{jk,\alpha'_{jk}}(x_{jk},y_{jk})B^{JM*}_{\alpha_{ij}}(\hat{x}_{ij},\hat{y}_{ij},\cdots)B^{JM}_{\alpha'_{jk}}(\hat{x}_{jk},\hat{y}_{jk},\cdots)+$$

$$+\sum_{\alpha'_{ik}}V_{ij}(x_{ij})\int\int d\hat{x}_{ij}d\hat{y}_{ij}\frac{x_{ij}y_{ij}}{x_{ik}y_{ik}}f_{jk,\alpha'_{ik}}(x_{ik},y_{ik})B^{JM*}_{\alpha_{ij}}(\hat{x}_{ij},\hat{y}_{ij},\cdots)B^{JM}_{\alpha'_{ik}}(\hat{x}_{ik},\hat{y}_{ik},\cdots)$$

Numerical Solution

✓ Partial-wave Faddeev amplitudes are developped on the 2D collocation basis

$$f_{ij,\alpha_{ij}}(x_{ij},y_{ij}) = \sum_{k_x=0}^{n_{col}(N_x+1)-1} \sum_{k_y=0}^{n_{col}(N_y+1)-1} c_{\alpha_{ij},k_x,k_y} S_{k_y}(y_{ij}) S_{k_x}(x_{ij})$$



✓ Numerical solution is found by requiring set of equations to be valid on the $(N_x{*}n_{col}){*}(N_y{*}n_{col})$ Gauss quadrature points of 2D grid + boundary conditions

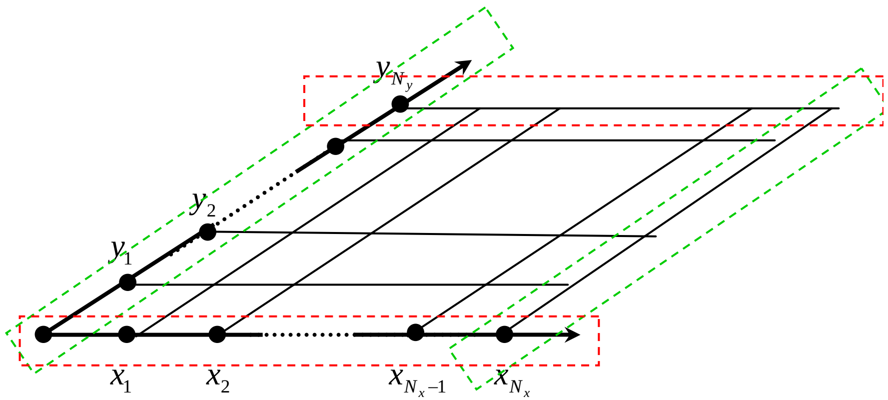
Boundary conditions

- Bound state problem

$$\begin{cases} f_{ij,\alpha_{ij}}(x_{ij},0)=0; \quad f_{ij,\alpha_{ij}}(0,y_{ij})=0 \\ f_{ij,\alpha_{ij}}(x_{N_x},y_{ij})=0; \quad f_{ij,\alpha_{ij}}(x_{ij},y_{N_y})=0 \end{cases}$$

- Scattering problem
  a) If α_{ij} channel is closed

$$\begin{cases} f_{ij,\alpha_{ij}}(x_{ij},0)=0; \quad f_{ij,\alpha_{ij}}(0,y_{ij})=0 \\ f_{ij,\alpha_{ij}}(x_{N_x},y_{ij})=0; \quad f_{ij,\alpha_{ij}}(x_{ij},y_{N_y})=0 \end{cases}$$



  b) If α_{ij} channel is open

$$\begin{cases} f_{ij,\alpha_{ij}}(x_{ij},0)=0; \quad f_{ij,\alpha_{ij}}(0,y_{ij})=0 \\ f_{ij,\alpha_{ij}}(x_{N_x},y_{ij})=0 \\ f_{ij,\alpha_{ij}}(x_{ij},y_{N_y})=\phi_{BS}(E_{\alpha_{ij}},x_{ij})*\chi_{sc\_wave}(E-E_{\alpha_{ij}},y_{N_y}) \end{cases}$$

Numerical costs

One should find $D_{IMEN} = \underbrace{\left(N_{\alpha_{ij}} + N_{\alpha_{ik}} + N_{\alpha_{jk}}\right)}_{N_\alpha}\underbrace{\left(N_x \cdot n_{col}\right)}_{DIM_x}\underbrace{\left(N_y \cdot n_{col}\right)}_{DIM_y}$ coefficients C_{α_{ij},k_x,k_y}

- For bound states eigenvalue-eigenvector problem for matrices of size D_{IMEN}* D_{IMEN}

$$[A]c^{(i)} = E^{(i)}c^{(i)}$$

- For the scattering problem system of D_{IMEN} linear equations must be solved

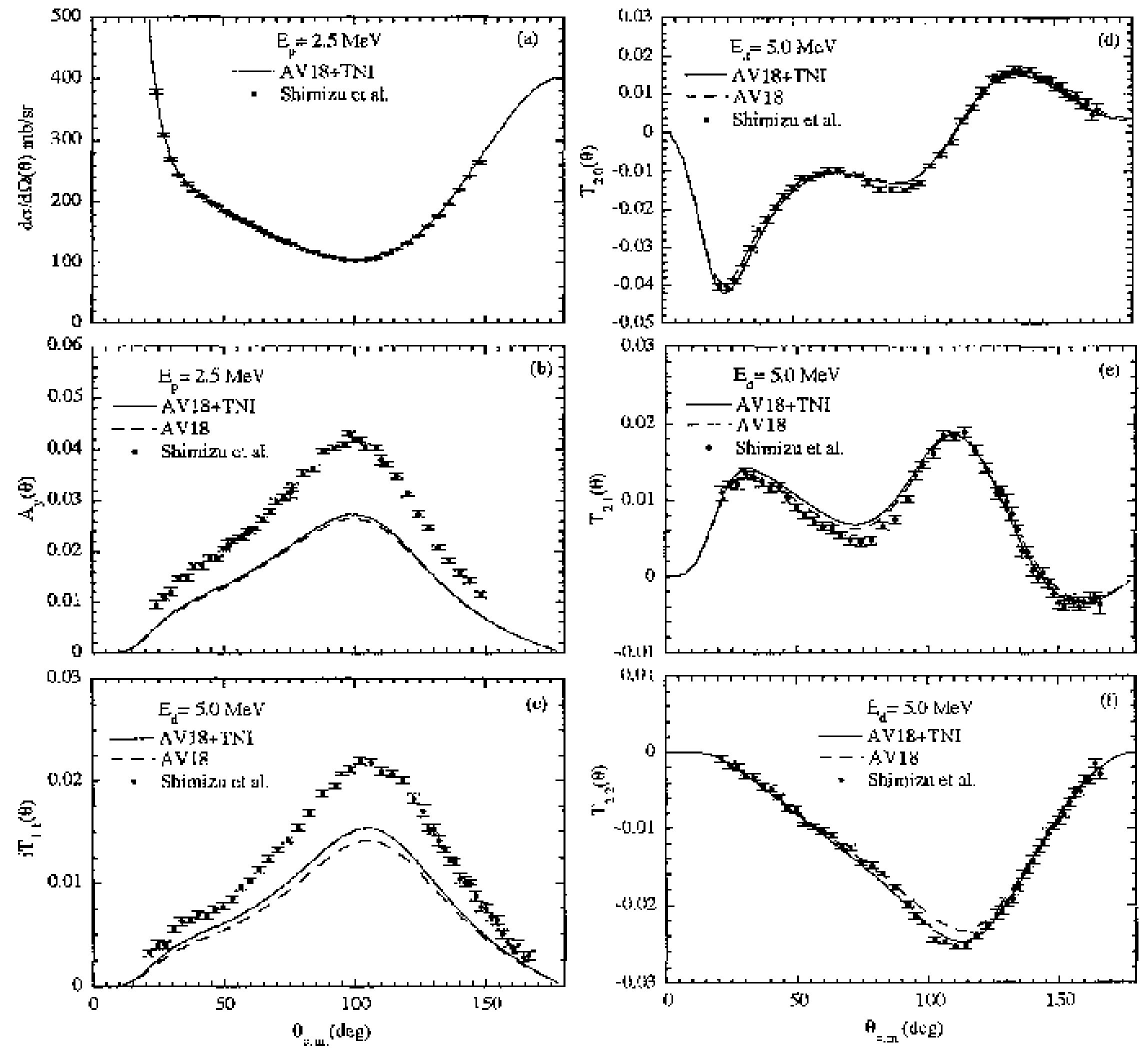
$$[A]c = X$$

For the realistic 3-Body problem

$$D_{IMEN} \sim (50-150)\cdot 30\cdot 30 \sim 10^5$$

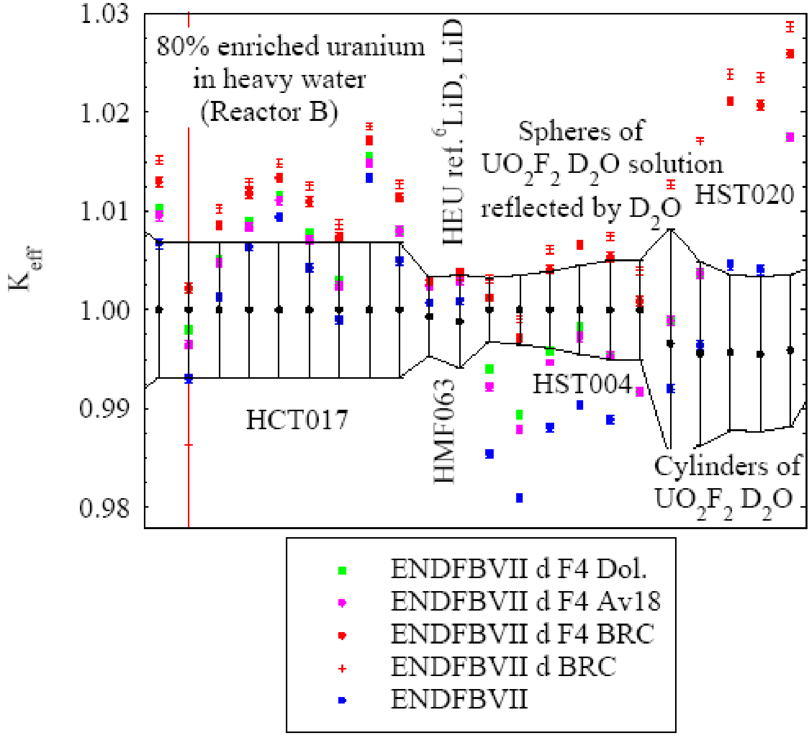
$\sum l_i$	N_α (^{3}H)
0	2
2	11
4	20
6	29
8	38
10	47
12	**56**
14	65
16	74

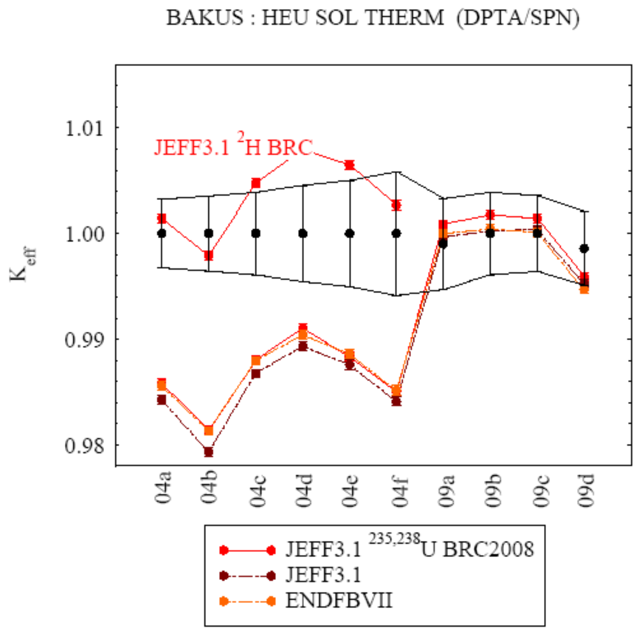
Proton-deutron scattering



Neutron-deutron scattering

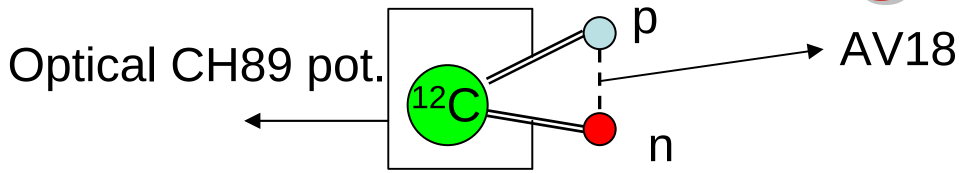
in the fuel-elements for heavy-water reactors

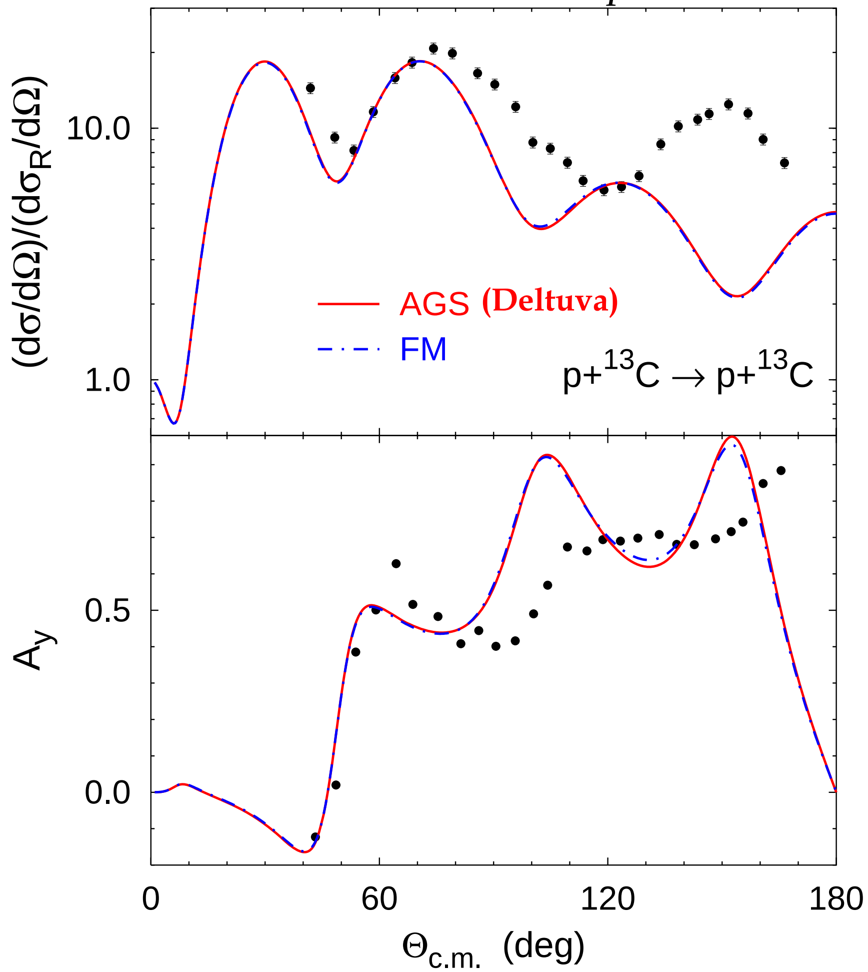


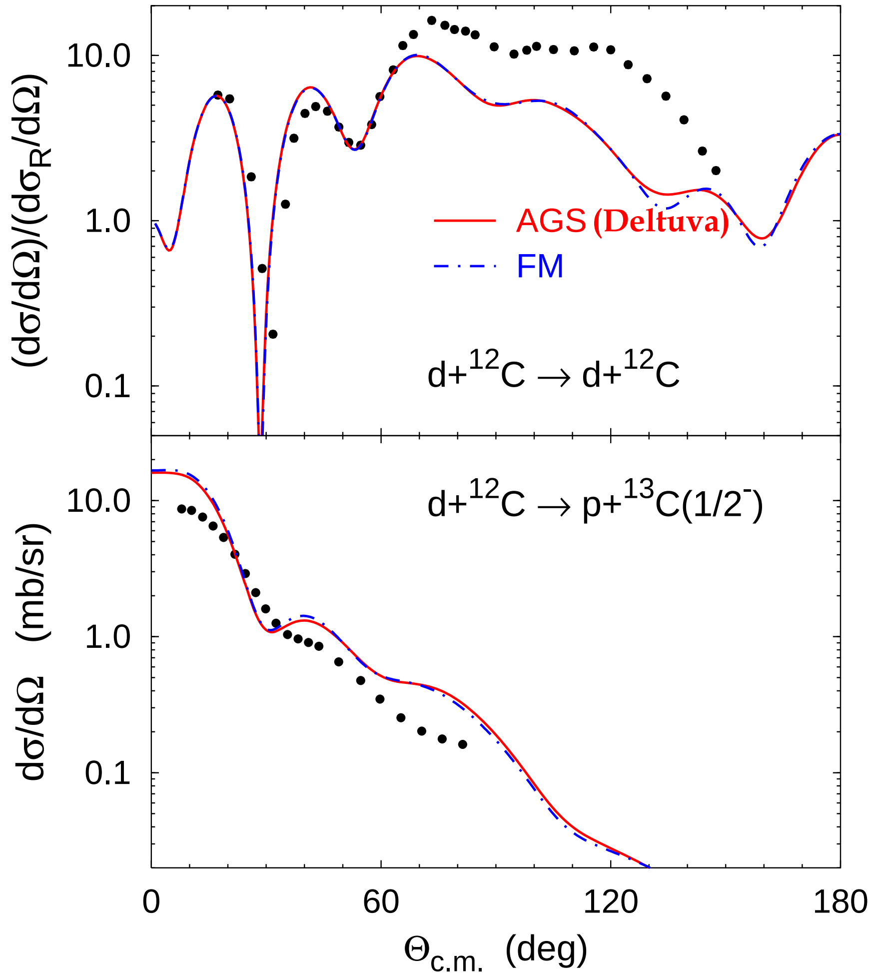


Deutron-carbon scattering

$$^{13}C + p \Leftrightarrow \begin{cases} ^{12}C + d \\ ^{13}C + p \\ ^{12}C + n + p \end{cases}$$







Atomic system: e-H scattering