Nuclear Theory in the Supercomputing Era

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# Computing Binary Scattering and Breakup in Three Body System

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  - The binary amplitude
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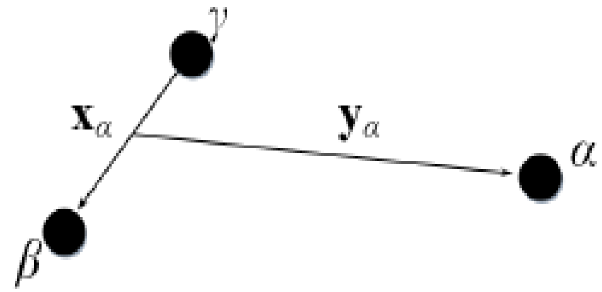
# Introduction

- <u>Three-body system</u>
- Hamiltonian in reduced Jacobi coordinates

$$\{\vec{x}_\alpha, \vec{y}_\alpha\}$$




$$\vec{x}_\alpha = \sqrt{\frac{2m_\beta m_\gamma}{m_\beta + m_\gamma}}\left(\vec{r}_\beta - \vec{r}_\gamma\right) \qquad \vec{y}_\alpha = \sqrt{\frac{2m_\alpha(m_\beta + m_\gamma)}{m_\alpha + m_\beta + m_\gamma}}\left(\vec{r}_\alpha - \frac{m_\beta \vec{r}_\beta + m_\gamma \vec{r}_\gamma}{m_\beta + m_\gamma}\right)$$

$$H = -\Delta_{\mathbf{x}_\alpha} - \Delta_{\mathbf{y}_\alpha} + V_\alpha(\mathbf{x}_\alpha) + V_\beta(\mathbf{x}_\beta) + V_\gamma(\mathbf{x}_\gamma)$$

Schrödinger equation for three-body system

$$H\Psi(\mathbf{x}_\alpha, \mathbf{y}_\alpha) = E\Psi(\mathbf{x}_\alpha, \mathbf{y}_\alpha)$$

- <u>Faddeev wave function components:</u> $U_\alpha$

$$\Psi(\vec{X}) = \sum_{\alpha=1}^{3} U_\alpha(\vec{X})$$

$$\vec{X} = \{\vec{x}_\alpha, \vec{y}_\alpha\}$$

- The system of Faddeev (FE) equations for components

$$\left(-\Delta + V_\alpha(\vec{x}_\alpha) - E\right) U_\alpha(\vec{X}) = -V_\alpha(\vec{x}_\alpha) \sum_{\beta \neq \alpha} U_\beta(\vec{X})$$

- <u>Identity of particles:</u> using cyclic permutation operators $P^{\pm}$ the wave function is represented as

$$\Psi(\vec{X}) = \left(I + P^{+} + P^{-}\right) U(\vec{X})$$

- FE is reduced to one equation for one component

$$U \equiv U_1$$

$$\left(-\Delta + V(\vec{x}) - E\right) U(\vec{X}) = -V(\vec{x}) \left(P^{+} + P^{-}\right) U(\vec{X})$$

# Scattering problem with the Faddeev equations

- For the zero total orbital momentum the equation

$$\left(-\Delta + V(\vec{x}) - E\right)U(\vec{X}) = -V(\vec{x})\left(P^{+} + P^{-}\right)U(\vec{X})$$

is reduced to the system of S-wave Faddeev equations

$$\left(-\frac{\partial^2}{\partial x^2} - \frac{\partial^2}{\partial y^2} + V^J(x) - E\right)U^J(x,y) = -V^J(x)\int_{-1}^{1} d\mu \frac{xy}{x'y'} B^J U^J(x',y')$$

- Together with boundary conditions

$$U_1^{\frac{1}{2}}(x,y) \sim \varphi(x)\left(\sin qy + a_0^{\frac{1}{2}}(q)\exp iqy\right) + A_1^{\frac{1}{2}}(\theta,E)\frac{\exp i\sqrt{E}\rho}{\sqrt{\rho}},$$

$$U_i^{\frac{1}{2}}(x,y) \sim A_i^{\frac{1}{2}}(\theta,E)\frac{\exp i\sqrt{E}\rho}{\sqrt{\rho}}, \quad i = 2,3$$

$$U^{\frac{3}{2}}(x,y) \sim \varphi(x)\left(\sin qy + a_0^{\frac{3}{2}}(q)\exp iqy\right) + A^{\frac{3}{2}}(\theta,E)\frac{\exp i\sqrt{E}\rho}{\sqrt{\rho}},$$

they form the n-d scattering problem above the breakup threshold.

$$\left(-\frac{\partial^2}{\partial x^2}-\frac{\partial^2}{\partial y^2}+V^J(x)-E\right)U^J(x,y)=-V^J(x)\int_{-1}^{1}d\mu\,\frac{xy}{x'y'}B^J U^J(x',y')$$

J stands for full momentum:

J=3/2 – quartet $U^{3/2}$ - scalar

J=1/2 – doublet $\left\{U_1^{1/2},U_2^{1/2},U_3^{1/2}\right\}$ - three component function

$$x'=\left(\frac{x^2}{4}-\frac{\sqrt{3}}{2}xy\mu+\frac{3y^2}{4}\right)^{\frac{1}{2}}\quad y'=\left(\frac{3x^2}{4}+\frac{\sqrt{3}}{2}xy\mu+\frac{y^2}{4}\right)^{\frac{1}{2}}\quad \mu=\cos(\hat{x},\hat{y})$$

$$B^{\frac{3}{2}}=-\frac{1}{2}\quad B^{\frac{1}{2}}=\begin{pmatrix}\frac{1}{4} & \frac{-3}{4} & 0\\ \frac{-3}{4} & \frac{1}{4} & 0\\ 0 & 0 & \frac{-1}{2}\end{pmatrix}$$

$$U_1^{\frac{1}{2}}(x,y)\sim\varphi(x)\left(\sin qy+a_0^{\frac{1}{2}}(q)\exp iqy\right)+A_1^{\frac{1}{2}}(\theta,E)\frac{\exp i\sqrt{E}\rho}{\sqrt{\rho}},$$

$$U_i^{\frac{1}{2}}(x,y)\sim A_i^{\frac{1}{2}}(\theta,E)\frac{\exp i\sqrt{E}\rho}{\sqrt{\rho}},\quad i=2,3$$

$$U^{\frac{3}{2}}(x,y)\sim\varphi(x)\left(\sin qy+a_0^{\frac{3}{2}}(q)\exp iqy\right)+A^{\frac{3}{2}}(\theta,E)\frac{\exp i\sqrt{E}\rho}{\sqrt{\rho}},$$

$a_0^J(q)$ - binary amplitude

$A_i^J(\theta,E)$ - breakup amplitude

$$U(x,0)=U(0,y)=0\qquad \theta=arctg(y/x)$$

$$\rho^2=x^2+y^2$$

$$\left(-\frac{\partial^2}{\partial x^2}+V(x)\right)\varphi(x)=\varepsilon\varphi(x)\qquad q^2=E-\varepsilon$$

# Integral representation for scattering amplitudes in configuration space

- The amplitude in the binary channel

$$a_0^{3/2}(q) = \int_0^\infty dy \sin qy \int_0^\infty dx\, \varphi(x) \left\{ \frac{1}{2} V(x) \int_{-1}^{1} d\mu \frac{xy}{x'y'} U^{3/2}(x', y') \right\}$$

- The amplitude in the breakup channel

$$A_0^{3/2}(\tilde{\theta}, E) = \frac{2}{\sqrt{3}} \sqrt{\frac{2}{\pi}} e^{i\pi/4} \int_0^\infty dy \sin qy \int_0^\infty dx\, \phi(\sqrt{E} \cos\tilde{\theta}, x) \left\{ \frac{1}{2} V(x) \int_{-1}^{1} d\mu \frac{xy}{x'y'} U^{3/2}(x', y') \right\}$$

where $\phi(k, x)$ is the scattering two-body wave function

$$\phi(k, x) \underset{x \to \infty}{\longrightarrow} e^{i\delta(k)} \sin(kx + \delta(k))$$

# Hyper spherical adiabatic expansion

- s-wave Faddeev equations in hyper-spherical coordinates:
  J=3/2

$$\left(-\frac{\partial^2}{\partial\rho^2}-\frac{1}{4\rho^2}-\frac{1}{\rho^2}\frac{\partial^2}{\partial\theta^2}+V(\rho\cos\theta)-E\right)U^{\frac{3}{2}}(\rho,\theta)=\frac{2}{\sqrt{3}}V(\rho\cos\theta)\int_{P(\theta)}^{Q(\theta)}U^{\frac{3}{2}}(\rho,\theta')d\theta'$$

- J=1/2

$$\left(-\frac{\partial^2}{\partial\rho^2}-\frac{1}{4\rho^2}-\frac{1}{\rho^2}\frac{\partial^2}{\partial\theta^2}+V^t(\rho\cos\theta)-E\right)U_1^{\frac{1}{2}}(\rho,\theta)=-\frac{1}{\sqrt{3}}V^t(\rho\cos\theta)\int_{P(\theta)}^{Q(\theta)}\left(U_1^{\frac{1}{2}}(\rho,\theta')-3U_2^{\frac{1}{2}}(\rho,\theta')\right)d\theta'$$

$$\left(-\frac{\partial^2}{\partial\rho^2}-\frac{1}{4\rho^2}-\frac{1}{\rho^2}\frac{\partial^2}{\partial\theta^2}+V^s(\rho\cos\theta)-E\right)U_2^{\frac{1}{2}}(\rho,\theta)=-\frac{1}{\sqrt{3}}V^s(\rho\cos\theta)\int_{P(\theta)}^{Q(\theta)}\left(-3U_1^{\frac{1}{2}}(\rho,\theta')+U_2^{\frac{1}{2}}(\rho,\theta')\right)d\theta'$$

- here

$$U^J(\rho,\theta)\equiv\sqrt{\rho}\,U^J(x,y) \qquad P(\theta)=|\pi/3-\theta| \quad Q(\theta)=\pi/2-|\pi/6-\theta|$$

- The boundary conditions are also multiplied by $\sqrt{\rho}$

# Hyper spherical adiabatic expansion of boundary conditions

$$\left(-\frac{\partial^2}{\partial\rho^2}-\frac{1}{4\rho^2}-\frac{1}{\rho^2}\frac{\partial^2}{\partial\theta^2}+V(\rho\cos\theta)-E\right)U^{\frac{3}{2}}(\rho,\theta)=\frac{2}{\sqrt{3}}V(\rho\cos\theta)\int_{P(\theta)}^{Q(\theta)}U^{\frac{3}{2}}(\rho,\theta')d\theta'$$

- Take advantage of the expansion of the desired solution by the basis of eigenfunctions of the Sturm-Liouville problem

$$h(\rho)\phi_k(\rho\,|\,\theta)=\left(-\frac{1}{\rho^2}\frac{\partial^2}{\partial\theta^2}+V(\rho\cos\theta)\right)\phi_k(\rho\,|\,\theta)=\lambda_k(\rho)\phi_k(\rho\,|\,\theta),\quad \theta\in\left[0,\frac{\pi}{2}\right]$$

- Spectral properties of the problem are connected with the properties of the two-body problem

$$\left(-\frac{\partial^2}{\partial x^2}+V(x)\right)\varphi(x)=\varepsilon\varphi(x),\ x\in[0,\infty)$$

$$\lambda_0(\rho)\sim\varepsilon\qquad \phi_0(\rho\,|\,\theta)\sim\sqrt{\rho}\varphi(\rho\cos\theta)\left(1+O(\rho^{-\mu})\right)$$

$$\rho\to\infty$$

$$\lambda_k\sim\left(\frac{2k}{\rho}\right)^2\qquad \phi_k(\rho\,|\,\theta)\sim\frac{2}{\sqrt{\pi}}\sin 2k\theta$$

$$\left(-\frac{\partial^2}{\partial\rho^2}-\frac{1}{4\rho^2}-\frac{1}{\rho^2}\frac{\partial^2}{\partial\theta^2}+V(\rho\cos\theta)-E\right)U^{\frac{3}{2}}(\rho,\theta)=\frac{2}{\sqrt{3}}V(\rho\cos\theta)\int_{P(\theta)}^{Q(\theta)}U^{\frac{3}{2}}(\rho,\theta')d\theta'$$

- Use the expansion of the desired solution

$$U(\rho,\theta)=\phi_0(\rho\,|\,\theta)F_0(\rho)+\sum_{i=1}^{\infty}\phi_i(\rho\,|\,\theta)F_i(\rho)$$

after projection to the basis function $F_k(\rho)$, we get the system of coupled equations

$$\boxed{\left(-\frac{\partial^2}{\partial\rho^2}-\frac{1}{4\rho^2}+\lambda_k(\rho)-E\right)F_k(\rho)=\sum_{i=0}^{\infty}\left(2A_{ki}(\rho)\frac{\partial}{\partial\rho}+B_{ki}(\rho)-W_{ki}(\rho)\right)F_i(\rho)}$$

$$A_{ki}(\rho)=\left\langle\phi_k(\rho\,|\,\cdot),\frac{\partial}{\partial\rho}\phi_i(\rho\,|\,\cdot)\right\rangle=\int_0^{\pi/2}d\theta\,\phi_k(\rho\,|\,\theta)\frac{\partial\phi_i(\rho\,|\,\theta)}{\partial\rho}$$

$$B_{ki}(\rho)=\int_0^{\pi/2}d\theta\,\phi_k(\rho\,|\,\theta)\frac{\partial^2\phi_i(\rho\,|\,\theta)}{\partial^2\rho}$$

$$W_{ki}(\rho)=\frac{2}{\sqrt{3}}\int_0^{\pi/2}d\theta\,\phi_k(\rho\,|\,\theta)\,V(\rho\cos\theta)\int_{P(\theta)}^{Q(\theta)}d\theta'\phi_i(\rho\,|\,\theta')$$

# Geometric Connections

$$A_{ki}(\rho) = \left\langle \phi_k(\rho\,|\,\cdot), \frac{\partial}{\partial\rho}\phi_i(\rho\,|\,\cdot)\right\rangle = \int_0^{\pi/2} d\theta\, \phi_k(\rho\,|\,\theta)\frac{\partial\phi_i(\rho\,|\,\theta)}{\partial\rho}$$

$$h(\rho)\phi_k(\rho\,|\,\theta) = \left(-\frac{1}{\rho^2}\frac{\partial^2}{\partial\theta^2} + V(\rho\cos\theta)\right)\phi_k(\rho\,|\,\theta) = \lambda_k(\rho)\phi_k(\rho\,|\,\theta), \quad \theta\in\left[0,\frac{\pi}{2}\right]$$

Geometric Connections are the most slowly decreasing terms in the right side of the system of coupled equations.

$$A_{ki} = \frac{\left\langle \varphi_k \,|\, \partial_\rho \left(V(\rho\cos\theta)\right) |\, \varphi_i \right\rangle}{\rho^2(\lambda_i - \lambda_k)}$$

The asymptotic of geometric connections

$$A_{ki} \approx \rho^{-5/2}, k = 0 \;\; or \;\; i = 0$$

$$A_{ki} \approx \rho^{-2}, k, i \neq 0$$

In the limit $\rho \to \infty$ the equations

$$\left(-\frac{\partial^2}{\partial\rho^2} - \frac{1}{4\rho^2} + \lambda_k(\rho) - E\right)F_k(\rho) = \sum_{i=0}^{\infty}\left(2A_{ki}(\rho)\frac{\partial}{\partial\rho} + B_{ki}(\rho) - W_{ki}(\rho)\right)F_i(\rho)$$

$$\rho \to \infty$$

become uncoupled

$$\left(-\frac{\partial^2}{\partial\rho^2}-\frac{1}{4\rho^2}+\lambda_k^{as}(\rho)-E\right)F_k(\rho)=0$$

$$\lambda_0^{as} = \varepsilon$$

$$\lambda_k^{as}=\left(2k/\rho\right)^2 \; k=1,2,\ldots$$

Solution in terms of Bessel $J_0, Y_0$ and Hankel $H_0^{(1)}$ functions

$$F_0^{as}(\rho)=\sqrt{\frac{\pi q\rho}{2}}\frac{Y_0(q\rho)+J_0(q\rho)}{\sqrt{2}}+a_0^{\frac{3}{2}}(q)\sqrt{\frac{\pi q\rho}{2}}H_0^{(1)}(q\rho)\exp\left(i\pi/4\right)$$

$$F_k^{as}(\rho)=a_k^{\frac{3}{2}}(E)\sqrt{\frac{\pi\sqrt{E}\rho}{2}}H_{2k}^{(1)}(\sqrt{E}\rho)\exp\left(i\pi/4+ik\pi\right)$$

- Equivalent boundary conditions

$$U(\rho,\theta)=\phi_0(\rho\,|\,\theta)F_0(\rho)+\sum_{i=1}^{\infty}\phi_i(\rho\,|\,\theta)F_i(\rho)$$

$$U^{\frac{3}{2}}(\rho,\theta)\sim\phi_0(\rho\,|\,\theta)\left(\sqrt{\frac{\pi q\rho}{2}}\frac{Y_0(q\rho)+J_0(q\rho)}{\sqrt{2}}+a_0^{\frac{3}{2}}(q)\sqrt{\frac{\pi q\rho}{2}}H_0^{(1)}(q\rho)\exp\left(i\pi/4\right)\right)+$$

$$+\sum_{k=1}^{N_\phi}a_k^{\frac{3}{2}}(E)\,\phi_k(\rho\,|\,\theta)\sqrt{\frac{\pi\sqrt{E}\rho}{2}}H_{2k}^{(1)}(\sqrt{E}\rho)\exp\left(i\pi/4+ik\pi\right)$$

# Equivalent boundary conditions

- J=3/2

$$U^{\frac{3}{2}}(\rho,\theta) \sim \phi_0(\rho\,|\,\theta)\left(\sqrt{\frac{\pi q\rho}{2}}\,\frac{Y_0(q\rho)+J_0(q\rho)}{\sqrt{2}} + a_0^{\frac{3}{2}}(q)\sqrt{\frac{\pi q\rho}{2}}H_0^{(1)}(q\rho)\exp\left(i\pi/4\right)\right)+$$

$$+\sum_{k=1}^{N_\phi} a_k^{\frac{3}{2}}(E)\,\phi_k(\rho\,|\,\theta)\,\sqrt{\frac{\pi\sqrt{E}\rho}{2}}H_{2k}^{(1)}(\sqrt{E}\rho)\exp\left(i\pi/4+ik\pi\right)$$

$$A^{\frac{3}{2}}\left(\theta,E\right)=\lim_{\rho\to\infty} A^{\frac{3}{2}}\left(\theta,E,\rho\right)=\lim_{\rho\to\infty}\sum_{k=1}^{N_\phi} a_k^{\frac{3}{2}}(E)\phi_k(\rho\,|\,\theta)=\sum_{k=1}^{N_\phi} a_k^{\frac{3}{2}}(E)\frac{2}{\sqrt{\pi}}\sin 2k\theta$$

- J=1/2

$$U_1^{\frac{1}{2}}(\rho,\theta) \sim \phi_0(\rho\,|\,\theta)\left(\sqrt{\frac{\pi q\rho}{2}}\,\frac{Y_0(q\rho)+J_0(q\rho)}{\sqrt{2}} + a_0^{\frac{1}{2}}(q)\sqrt{\frac{\pi q\rho}{2}}H_0^{(1)}(q\rho)\exp\left(i\pi/4\right)\right)+$$

$$+\sum_{k=1}^{N_\phi} a_{1,k}^{\frac{1}{2}}(E)\,\phi_k(\rho\,|\,\theta)\,\sqrt{\frac{\pi\sqrt{E}\rho}{2}}H_{2k}^{(1)}(\sqrt{E}\rho)\exp\left(i\pi/4+ik\pi\right),$$

$$U_2^{\frac{1}{2}}(\rho,\theta) \sim \sum_{k=1}^{N_\phi} a_{2,k}^{\frac{1}{2}}(E)\,\phi_k(\rho\,|\,\theta)\,\sqrt{\frac{\pi\sqrt{E}\rho}{2}}H_{2k}^{(1)}(\sqrt{E}\rho)\exp\left(i\pi/4+ik\pi\right),$$

# Calculating amplitudes from asymptotics

The solution of the system
(we cut the infinite system of equation assuming the applying of the asymptotic boundary conditions at some $\rho_{\max}$)

$$\left(H - h^2 E\right)\Psi = \Phi_0 + a_0 \Phi_0^1 + \sum_{k=1}^{N_\phi} a_k \Phi_k$$

makes it possible to obtain the coefficients $a_0$ $a_k$

from comparison of this solution

$$\Psi = \Psi_0 + a_0 \Psi_0^1 + \sum_{k=1}^{N_\phi} a_k \Psi_k$$

and asymptotic

$$\Phi = \Phi_0 + a_0 \Phi_0^1 + \sum_{k=1}^{N_\phi} a_k \Phi_k$$

for

$$\rho = \rho_{\max} - h$$

The system for obtaining the coefficients is

$$a_0\left[\left\langle \phi_l \mid \Psi_0^1 \right\rangle - \left\langle \phi_l \mid \Phi_0^1 \right\rangle\right] + \sum_{k=1}^{N_\phi} a_k \left[\left\langle \phi_l \mid \Psi_k \right\rangle - \left\langle \phi_l \mid \Phi_k \right\rangle\right] = -\left\langle \phi_l \mid \Psi_0 \right\rangle + \left\langle \phi_l \mid \Phi_0 \right\rangle$$

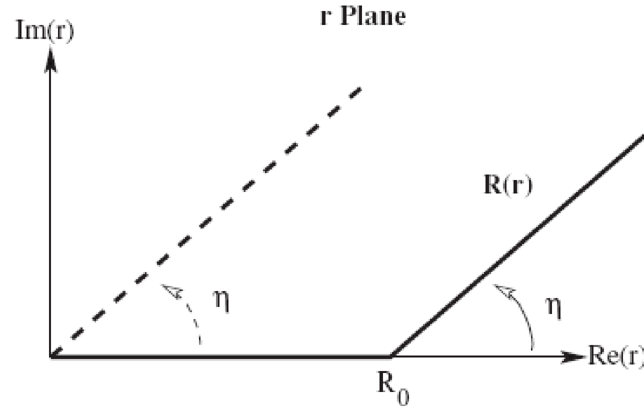
# Exterior complex scaling

$$\left(-\frac{\partial^2}{\partial\rho^2}-\frac{1}{4\rho^2}-\frac{1}{\rho^2}\frac{\partial^2}{\partial\theta^2}+V(\rho\cos\theta)-E\right)U^{\frac{3}{2}}(\rho,\theta)=\frac{2}{\sqrt{3}}V(\rho\cos\theta)\int_{P(\theta)}^{Q(\theta)}U^{\frac{3}{2}}(\rho,\theta')d\theta'$$

- Exterior rotation of the hyper radius into the upper complex half plane

$$\rho \to R = R(\rho)$$

$$-\frac{\partial^2}{\partial R^2} \to -\frac{1}{(R'_\rho)^2}\frac{\partial^2}{\partial\rho^2}+\frac{R''_\rho}{(R'_\rho)^3}\frac{\partial}{\partial\rho}$$




$$R(\rho)=\begin{cases}\rho, & \rho<\rho_0\\ \rho+(\rho-\rho_0)\exp(i\eta), & \rho>\rho_0\end{cases}$$

$$U^{\frac{3}{2}}(x,y)\sim\varphi(x)\left(\sin qy+a_0^{\frac{3}{2}}(q)\exp iqy\right)+A^{\frac{3}{2}}(\theta,E)\frac{\exp i\sqrt{E}\rho}{\sqrt{\rho}},$$

$$U^{3/2}(\rho|\theta)\sim\phi_0(\rho|\theta)(\sin qy+a_0^{3/2}\exp iqy)+A^{3/2}(\theta,E)\exp i\sqrt{E}\rho$$

$$\boxed{\exp iqy=\exp^{(iq(\rho_0+(\rho-\rho_0)\cos\eta)\sin\theta)}\exp^{(-q(\rho-\rho_0)\sin\eta\sin\theta)}\underset{\rho\to\infty}{\longrightarrow}0}$$

- Incoming wave $\sin qy$ does not vanish after the complex scaling.

We subtract $\sqrt{R}\varphi(R\cos\theta)\sin qy$ from the solution in order to get homogeneous boundary conditions.

$$U^{3/2}(\theta,R)=\sqrt{R}\varphi(R\cos\theta)\sin qy+\tilde{U}^{3/2}(\theta,R)$$

We obtain the inhomogeneous equation

$$\left(-\frac{\partial^2}{\partial R^2}-\frac{1}{4R^2}-\frac{1}{R^2}\frac{\partial^2}{\partial\theta^2}+V(R\cos\theta)-E\right)\tilde{U}^{3/2}(\theta,R)-\frac{2}{\sqrt{3}}V(R\cos\theta)\int_{P(\theta)}^{Q(\theta)}d\theta'\tilde{U}^{3/2}(\theta',R)=$$
$$\frac{2}{\sqrt{3}}V(R\cos\theta)\int_{P(\theta)}^{Q(\theta)}\sqrt{R}\varphi(R\cos\theta')\sin(qR\sin\theta')d\theta'$$

with homogeneous zero boundary conditions for the solution

$$\tilde{U}^{3/2}(R,\theta)\underset{\rho=0}{=}0$$
$$\tilde{U}^{3/2}(R,\theta)\underset{\rho\to\infty}{\to}0$$

Decreasing as $\rho\to\infty$ is exponential !

The same equations will be in case of J=1/2 (doublet).

# Integral representation for the amplitudes in hyper spherical coordinates

- The amplitude in the binary channel is defined as

$$a_0^{3/2}(q) = \int_0^\infty d\rho \int_0^{\pi/2} d\theta \sqrt{\rho} \sin(q\rho \sin\theta) \varphi(\rho\cos\theta) \left\{ \frac{2}{\sqrt{3}} V(\rho\cos\theta) \int_{P(\theta)}^{Q(\theta)} U^{3/2}(\rho, \theta') d\theta' \right\}$$

The amplitude in the breakup channel is defined as

$$A_0^{3/2}(\tilde{\theta}, E) = \sqrt{\frac{2}{\pi\sqrt{E}}} e^{i\pi/4} \int_0^\infty \sqrt{\rho} d\rho \times$$

$$\times \int_0^{\pi/2} d\theta \sin(y\sqrt{E}\sin\tilde{\theta}) \phi(\sqrt{E}\cos\tilde{\theta}, \rho\cos\theta) \left\{ \frac{2}{\sqrt{3}} V(\rho\cos\theta) \int_{P(\theta)}^{Q(\theta)} U^{3/2}(\rho, \theta') d\theta' \right\}$$

where $\phi(\sqrt{E}\cos\tilde{\theta}, \rho\cos\theta)$ is the two-body scattering wave function.

The amplitudes are calculated using the solution

$$U^{3/2}(\theta, R) = \sqrt{R}\varphi(R\cos\theta)\sin qy + \tilde{U}^{3/2}(\theta, R)$$

obtained by solving the homogeneous boundary value problem for real R.

# Two-body potential

$$\left(-\frac{\partial^2}{\partial x^2}-\frac{\partial^2}{\partial y^2}+V^J(x)-E\right)U^J(x,y)=-V^J(x)\int_{-1}^{1}d\mu\,\frac{xy}{x'y'}B^J U^J(x',y')$$

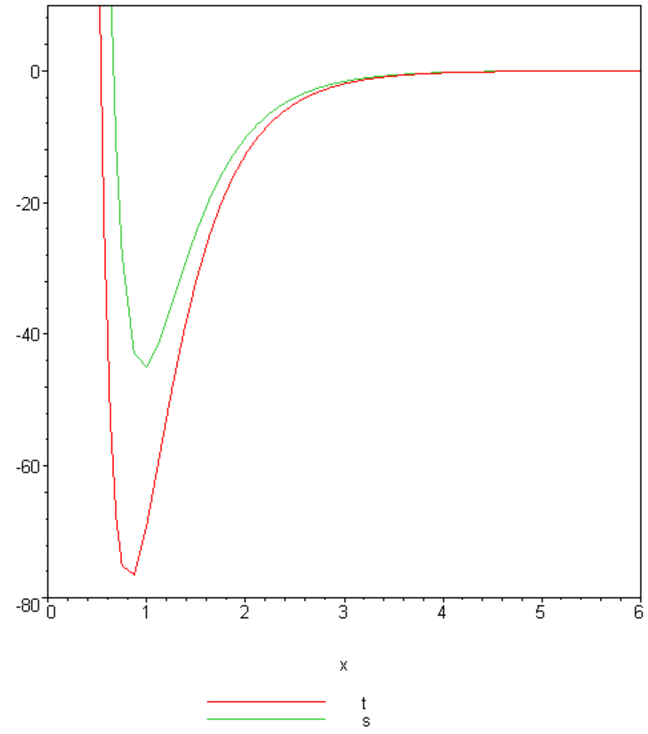
$$V^{3/2}=V^t$$

$$V^{1/2}=diag\{V^t,V^s,V^s\}$$

**Malfliet-Tjon 1-3**

$$V^t(x)=\frac{1}{x}\left(-626.885e^{-1.55x}+1438.72e^{-3.11x}\right)$$

$$V^s(x)=\frac{1}{x}\left(-513.968e^{-1.55x}+1438.72e^{-3.11x}\right)$$




A deuteron binding energy: $E_d=-2.2307\ MeV$

# Computational scheme

$$\left(-\frac{\partial^2}{\partial\rho^2}-\frac{1}{4\rho^2}-\frac{1}{\rho^2}\frac{\partial^2}{\partial\theta^2}+V(\rho\cos\theta)-E\right)U^{\frac{3}{2}}(\rho,\theta)=\frac{2}{\sqrt{3}}V(\rho\cos\theta)\int_{P(\theta)}^{Q(\theta)}U^{\frac{3}{2}}(\rho,\theta')d\theta'$$

The method of numerical solution for
the 2D boundary value problem includes:

1) an expansion of the solution in a basis of the Hermitian cubic splines on the nonuniform $\theta$-grid

$$U^{3/2}(\rho,\theta)=\sum_{j=1}^{N_\theta}S_j(\theta)\,c_j(\rho)$$

There are 4 spline-functions
at the interval [0,1]:

$$S_{00}(t)=2t^3-3t^2+1$$

$$S_{10}(t)=t^3-2t^2+t$$

$$S_{01}(t)=-2t^3+3t^2$$

$$S_{11}(t)=t^3-t^2$$

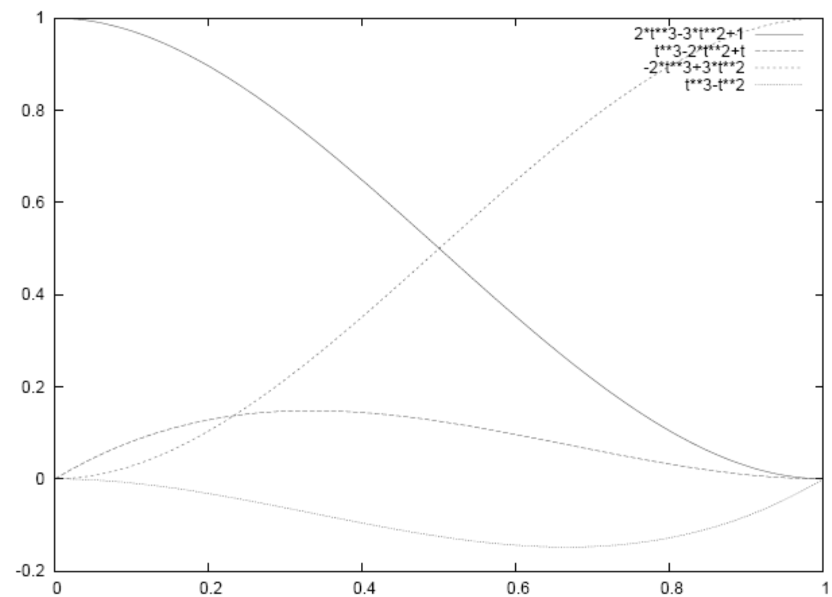



Рис. 9: Эрмитовые базисные сплайны на интервале [0, 1].

- The nonuniform $\theta$-grid is chosen using the appropriate non uniform x-grid for two-body value problem

$$\left(-\frac{d^2}{dx^2}+V(x)\right)\varphi(x)=\varepsilon\varphi(x) \quad x\in[0,R(\rho)]$$

which allows getting the binding energy for potential MT1-3 $E_d = 2.23069\ MeV$

The knots $x_i$ are transformed from the x-grid into $\theta$ grid according to the formula

$$\theta_i = \arccos\frac{x_i}{R(\rho)}$$

In such a way, the non uniform $\theta$ grid is obtained for the “two body” part of the Faddeev equation

$$\left(-\frac{1}{\rho^2}\frac{\partial^2}{\partial\theta^2}+V(\rho\cos\theta)\right)\phi_k(\rho\,|\,\theta)=\lambda_k\phi_k(\rho\,|\,\theta)$$

2) Using the finite-difference approximation on the uniform $\rho$ grid

$$\frac{U^{3/2}(\rho_{m-1},\theta)-2U^{3/2}(\rho_m,\theta)+U^{3/2}(\rho_{m+1},\theta)}{h^2},\quad h=\rho_m-\rho_{m-1}$$

Approximations 1) and 2) guarantee the accuracy of the solution $\sim O(h^2)$
and the system of linear equations for the coefficients
of splines $c_i(\rho_m)$

$$\sum_{i=1}^{N_\theta}\left[\frac{S_i^{\rho_{m-1}}(\theta_j)c_i(\rho_{m-1})-2S_i^{\rho_m}(\theta_j)c_i(\rho_m)+S_i^{\rho_{m+1}}(\theta_j)c_i(\rho_{m+1})}{h^2}-\frac{1}{\rho_m^2}\frac{\partial^2 S_i^{\rho_m}}{\partial^2\theta}(\theta_j)c_i(\rho_m)+D_i^{\rho_m}(\theta_j)c_i(\rho_m)\right]=0$$

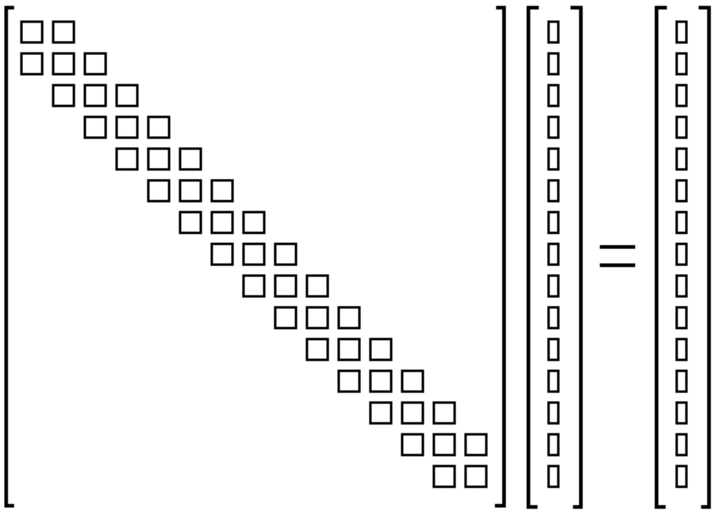
where

$$D_i^{\rho_m}(\theta_j)=\left(V(\rho_m\cos\theta_j)-\frac{1}{4\rho_m^2}-E\right)S_i^{\rho_m}(\theta_j)-V(\rho_m\cos\theta_j)\frac{2}{\sqrt{3}}\int_{P(\theta_j)}^{Q(\theta_j)}S_i^{\rho_m}(\theta')d\theta'$$

The boundary value problem is formed from this system by applying the asymptotic boundary conditions to the last equation

# Sweeping algorithm

The linear system has a block three diagonal form
Sweeping algorithm is used for solving



$A_i$ – low diagonal block

$B_i$ – upper diagonal block

$C_i$ – diagonal block

$F_i$ – right hand block

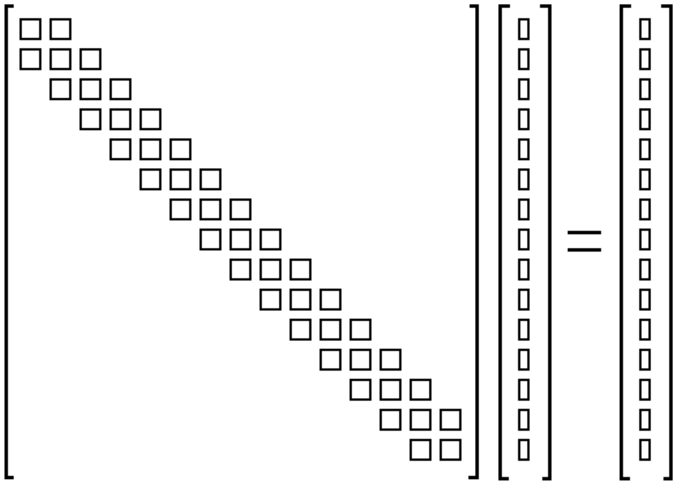
$$\begin{cases} B_1 X_1 + C_1 X_2 = F_1, \\ A_i X_{i-1} + B_i X_i + C_i X_{i+1} = F_i, i = 2, \dots, N-1, \\ A_N X_{N-1} + B_N X_N = F_N, \end{cases}$$

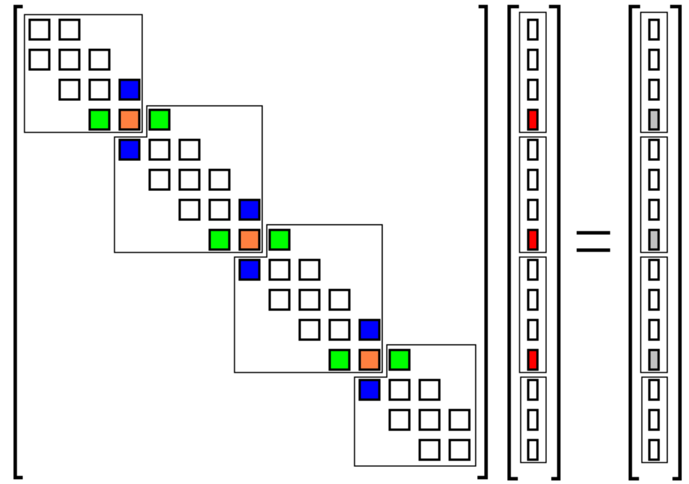
$$\begin{cases} \alpha_1 = -B_1^{-1} C_1, \qquad \beta_1 = B_1^{-1} F_1; \\ \alpha_i = -(B_i + A_i \alpha_{i-1})^{-1} C_i, \qquad \beta_i = (B_i + A_i \alpha_{i-1})^{-1} (F_i - A_i \beta_{i-1}), i = \overline{2, N-1}; \\ \beta_N = (B_N + A_N \alpha_{N-1})^{-1} (F_N - A_N \beta_{N-1}). \end{cases}$$

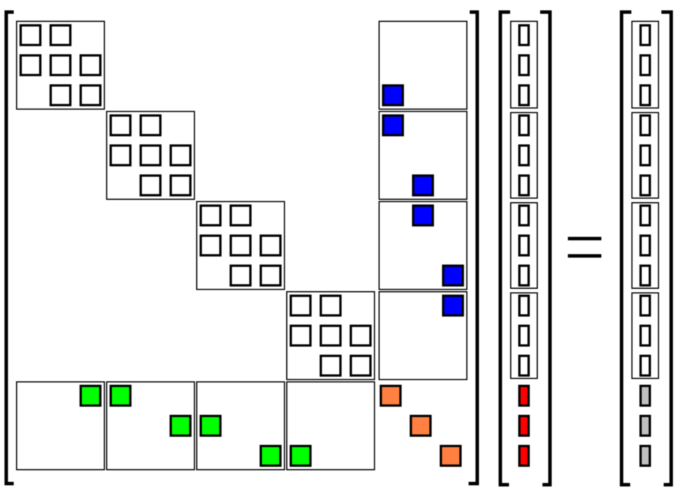
$$\begin{cases} X_N = \beta_N; \\ X_i = \alpha_i X_{i+1} + \beta_i, \qquad i = \overline{N-1, 1}; \end{cases}$$

# Parallelization

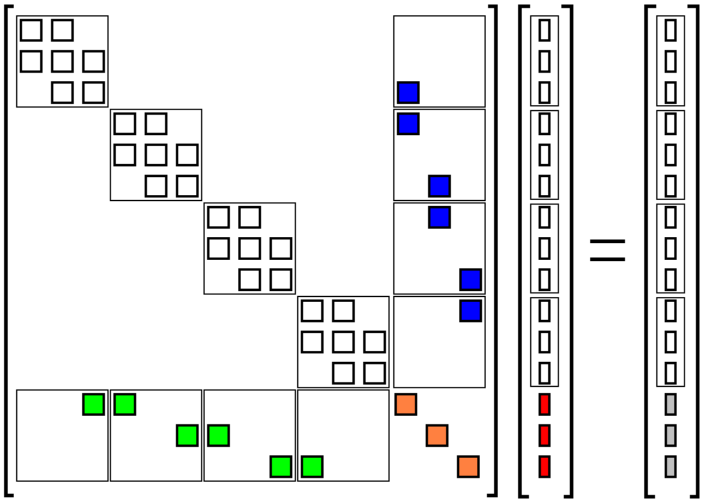
The sweeping algorithm is recursive and cannot be parallelized.
We have developed the domain decomposition algorithm
for block three-diagonal matrices







$$\begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_v \end{bmatrix} \begin{bmatrix} u \\ v \end{bmatrix} = \begin{bmatrix} b_{11} \\ b_v \end{bmatrix}$$



$$\begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_v \end{bmatrix} \begin{bmatrix} u \\ v \end{bmatrix} = \begin{bmatrix} b_{11} \\ b_v \end{bmatrix}$$

The initial linear equation can be rearranged into the form of some independent matrixes (white squares) and coupling matrix (orange squares) on the diagonal and additional blocks (green and blue).

---

$$\begin{cases} A_{11}u + A_{12}v = b_{11} \\ A_{21}u + A_v v = b_v \end{cases}$$

$$\begin{cases} u = A_{11}^{-1}b_{11} - A_{11}^{-1}A_{12}v \\ (A_v - A_{21}A_{11}^{-1}A_{12})v = b_v - A_{21}A_{11}^{-1}b_{11} \end{cases}$$

$$\begin{cases} u = -A_{11}^{-1}A_{12}v + A_{11}^{-1}b_{11} \\ A_{21}u + A_v v = b_v \end{cases}$$

The inversion of $A_{11}$ is reduced to the independent inversions of block diagonal matrixes (white squares).

**For matrix operations the LAPACK library has been used (http://www.netlib.org/lapack/)**

The following three situations have been studied:

1) Solving the system and calculation of the amplitudes using **sweeping algorithm without parallelization**

2) Solving the system and calculation of the amplitudes using **the sweeping algorithm with parallel LAPACK subroutines in Intel MKL 10.0 library (OpenMP parallelization)**

3) Solving the system and calculation of the amplitudes using **the domain decomposition method with the MPI parallelization on the supercomputer cluster**

# Comparison of the times using the different types of parallelization

| Algorithm & Parallelization | Full time (minutes) |
|---|---|
| sweeping alg.<br>no parallelization | 632 |
| sweeping alg. +<br>Intel MKL<br>Open MP, 4 CPU | 287 |
| domain decomposition +<br>MPI, 64 CPU | 56 |
| domain decomposition +<br>MPI, 48 CPU | 80 |
| domain decomposition +<br>MPI, 32 CPU | 98 |

**Parameters of the system:**

Each block is 1000x1000

3000 blocks along the diagonal

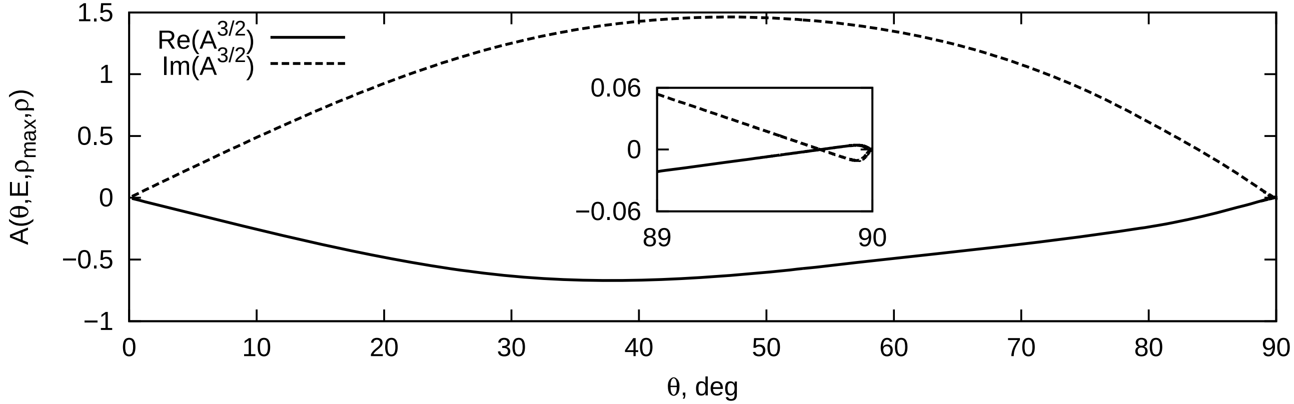
**The full time includes:**

- construction of blocks
- solving the system
- calculation of the amplitudes

The calculation of the amplitudes is parallelized in case of using the MPI parallelization.

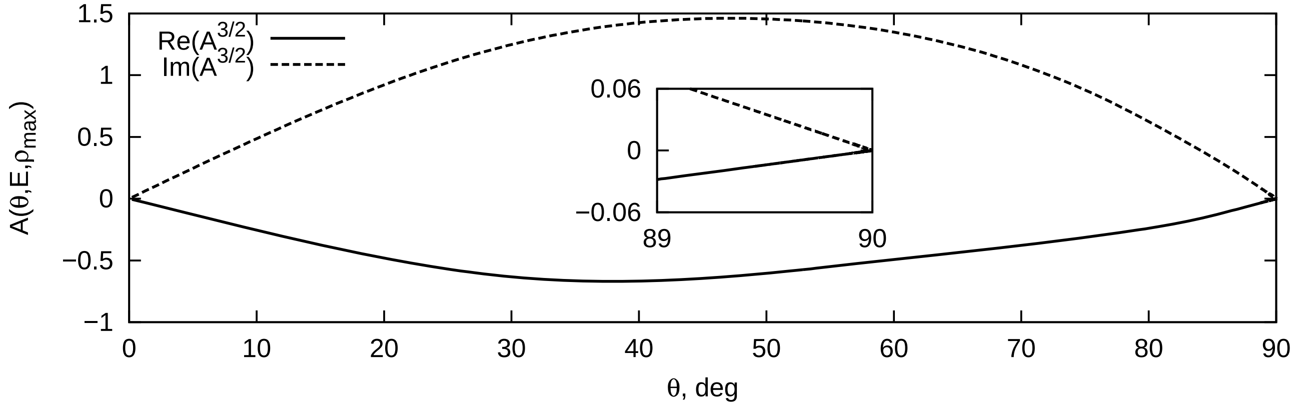
# Results for amplitudes

- The breakup amplitude: J=3/2 (quartet)




$$E_{lab} = 14.1\, MeV$$

$$\rho = \rho_{\max} = 1400\, fm$$

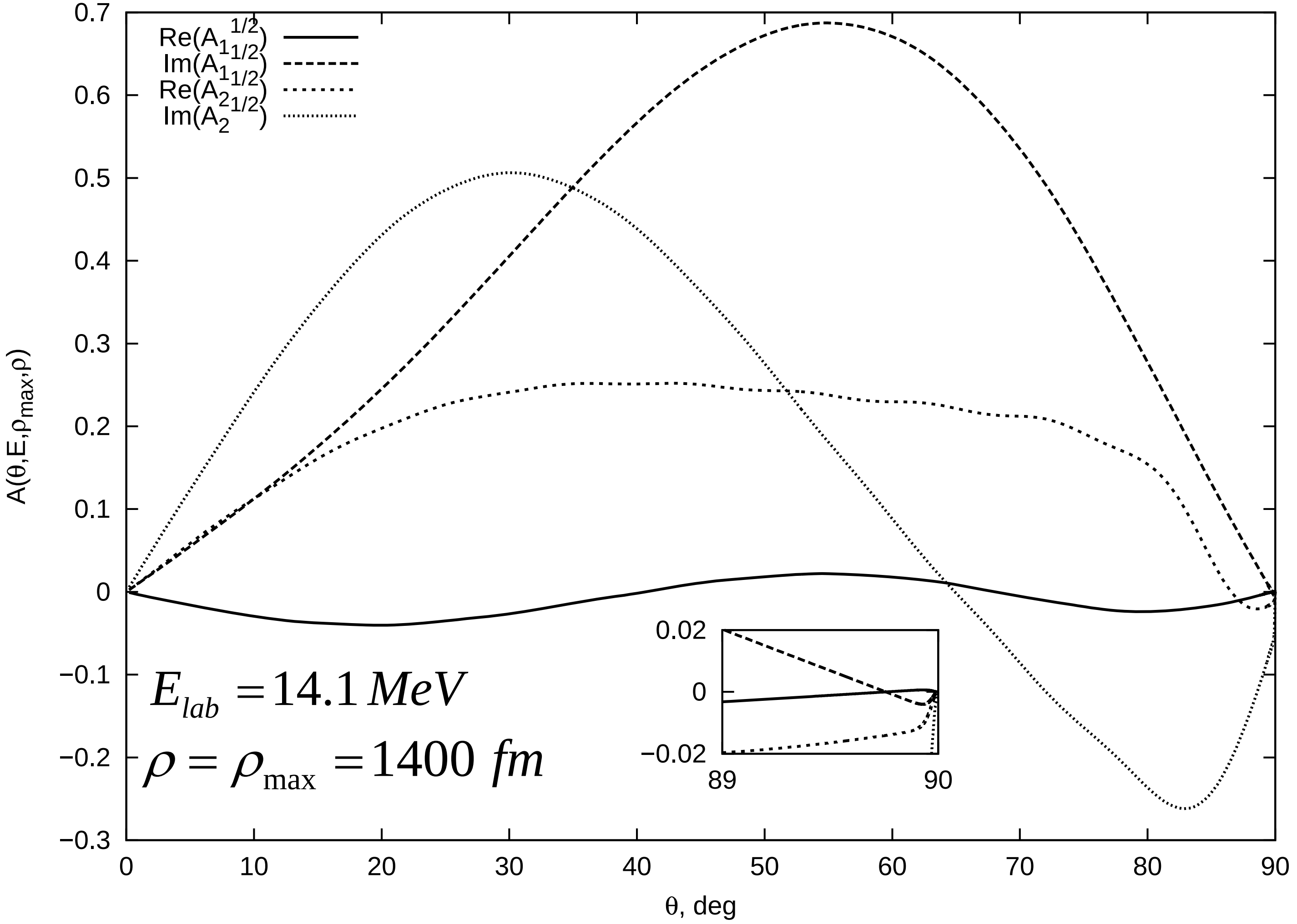



$$E_{lab} = 14.1\, MeV$$

$$\rho = \infty, \rho_{\max} = 1400\, fm$$

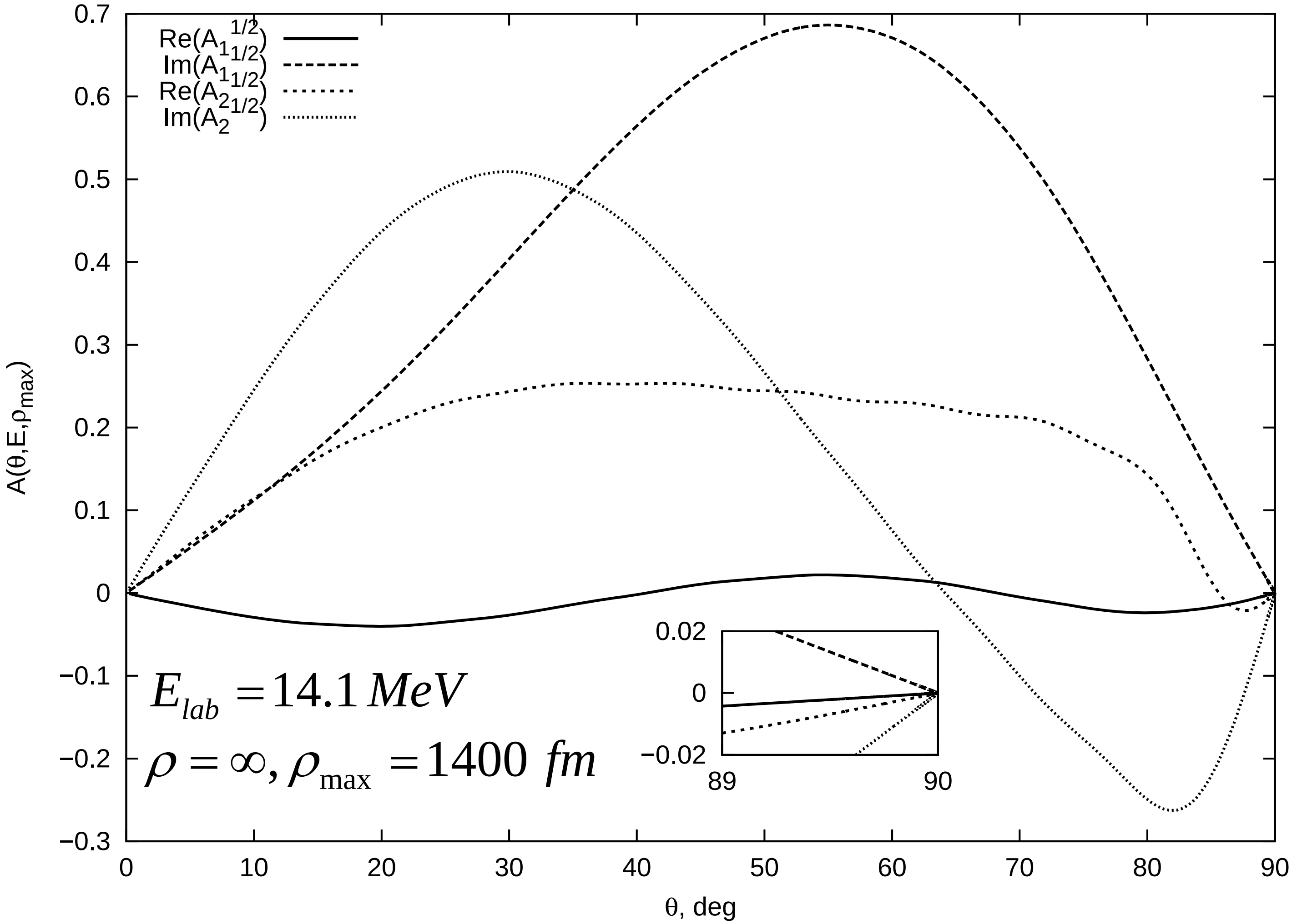
$$A_i^J\left(\theta, E, \rho_{\max}\right) = \lim_{\rho \to \infty} A_i^J\left(\theta, E, \rho_{\max}, \rho\right) = \sum_{k=1}^{N_\phi} a_{i,k}^J (E, \rho_{\max}) \frac{2}{\sqrt{\pi}} \sin 2k\theta$$

- The breakup amplitude: J=1/2 (doublet)




$$A_i^J(\theta, E, \rho_{\max}, \rho) = \sum_{k=1}^{N_\phi} a_{i,k}^J(E, \rho_{\max})\phi_k(\rho \mid \theta)$$

- <u>The breakup amplitude</u>: J=1/2 (doublet)




$$A_i^J(\theta, E, \rho_{\max}) = \lim_{\rho\to\infty} A_i^J(\theta, E, \rho_{\max}, \rho) = \sum_{k=1}^{N_\phi} a_{i,k}^J(E, \rho_{\max}) \frac{2}{\sqrt{\pi}} \sin 2k\theta$$

# Results: the breakup amplitude

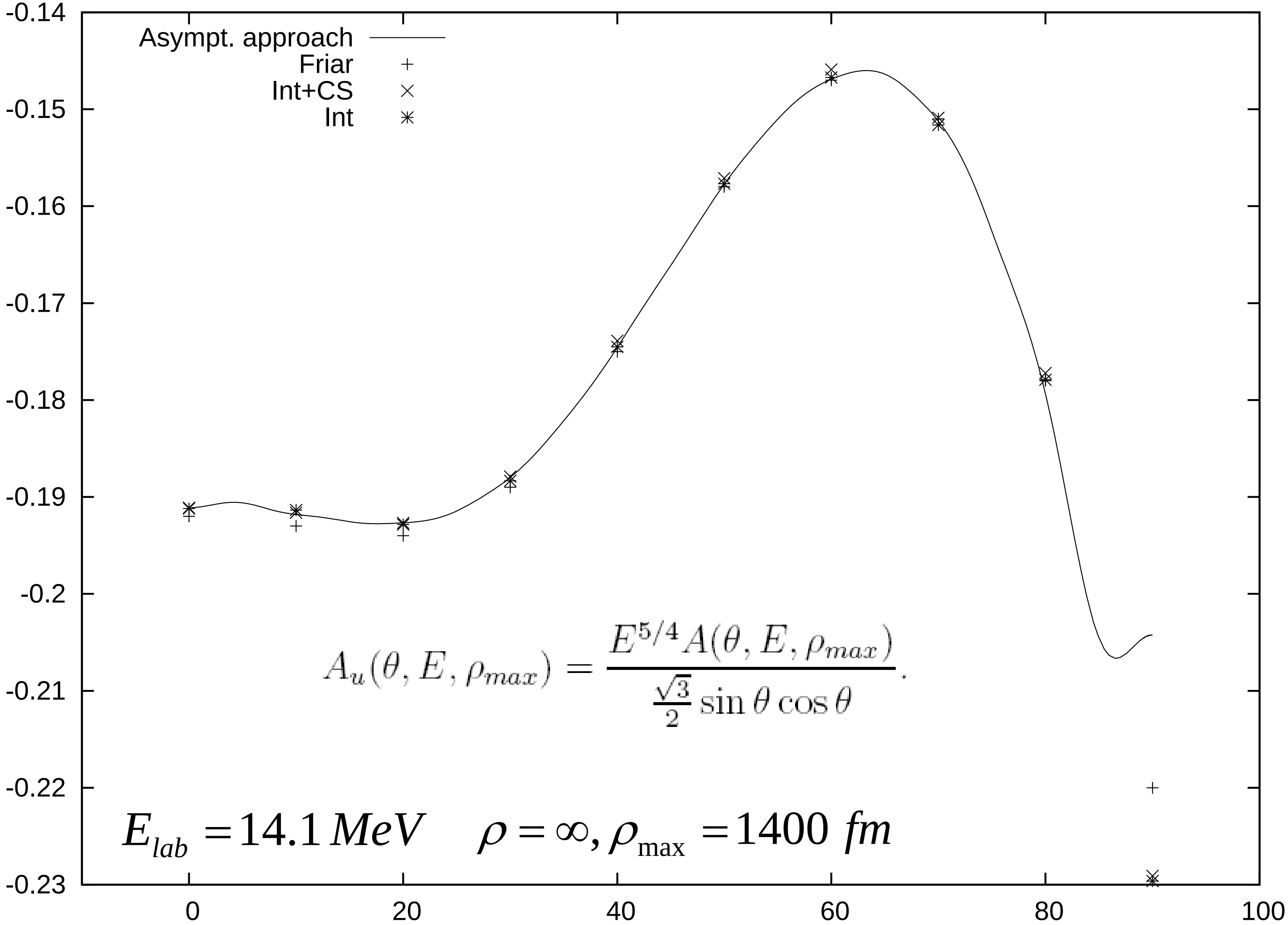
Compare the obtained values of the breakup amplitude

$$A_u(\theta, E, \rho_{max}) = \frac{E^{5/4} A(\theta, E, \rho_{max})}{\frac{\sqrt{3}}{2}\sin\theta\cos\theta}.$$

for some values of hyper-angle as $\rho_{\max} \to \infty$ with the results of other authors

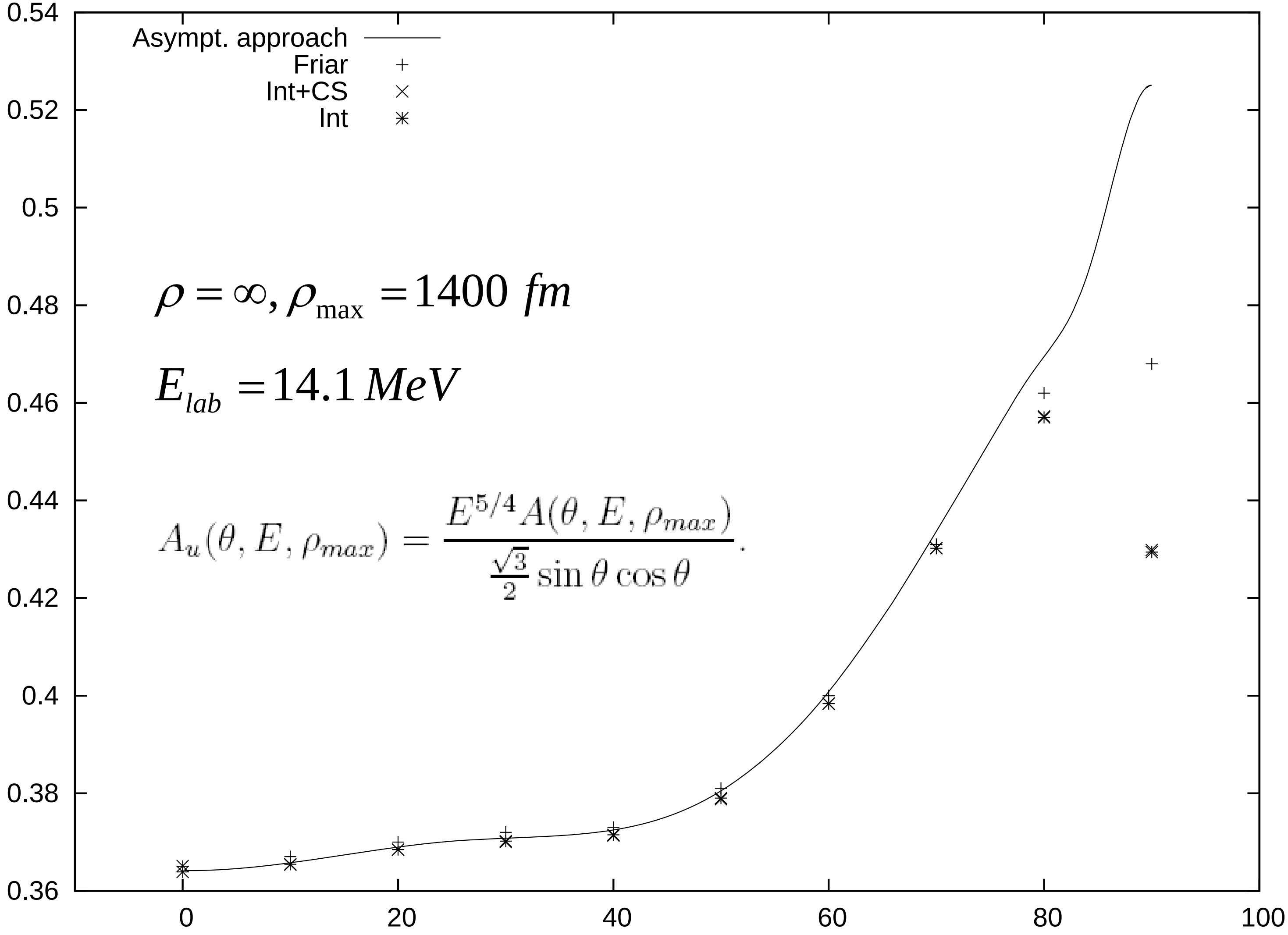
| $\theta$, deg | 0 | 10 | 20 | 30 | 40 | 50 | 60 | 70 | 80 | 90 |
|---|---|---|---|---|---|---|---|---|---|---|
| 14.1 MeV, quartet | | | | | | | | | | |
| J.L. Friar, Phys Rev C **51** 2356 (1995) | | | | | | | | | | |
| $\mathrm{Re}(A_u^{3/2})$ | -1.92[-1] | -1.93[-1] | -1.94[-1] | -1.89[-1] | -1.75[-1] | -1.58[-1] | -1.47[-1] | -1.51[-1] | -1.78[-1] | -2.20[-1] |
| $\mathrm{Im}(A_u^{3/2})$ | 3.65[-1] | 3.67[-1] | 3.70[-1] | 3.72[-1] | 3.73[-1] | 3.81[-1] | 4.00[-1] | 4.31[-1] | 4.62[-1] | 4.68[-1] |
| P. Belov, S. Yakovlev, Asymptotic approach (2012) | | | | | | | | | | |
| $\mathrm{Re}(A_u^{3/2})$ | -1.91[-1] | -1.92[-1] | -1.93[-1] | -1.88[-1] | -1.74[-1] | -1.58[-1] | -1.47[-1] | -1.51[-1] | -1.79[-1] | -2.04[-1] |
| $\mathrm{Im}(A_u^{3/2})$ | 3.64[-1] | 3.66[-1] | 3.69[-1] | 3.71[-1] | 3.73[-1] | 3.80[-1] | 4.01[-1] | 4.34[-1] | 4.69[-1] | 5.25[-1] |
| P. Belov, S. Yakovlev, Integral representation (2012) | | | | | | | | | | |
| $\mathrm{Re}(A_u^{3/2})$ | -1.91[-1] | -1.91[-1] | -1.93[-1] | -1.88[-1] | -1.75[-1] | -1.58[-1] | -1.47[-1] | -1.52[-1] | -1.78[-1] | -2.29[-1] |
| $\mathrm{Im}(A_u^{3/2})$ | 3.64[-1] | 3.65[-1] | 3.68[-1] | 3.70[-1] | 3.71[-1] | 3.79[-1] | 3.98[-1] | 4.30[-1] | 4.57[-1] | 4.29[-1] |
| P. Belov, S. Yakovlev, Integral representation with complex scaling (2012) | | | | | | | | | | |
| $\mathrm{Re}(A_u^{3/2})$ | -1.91[-1] | -1.92[-1] | -1.93[-1] | -1.88[-1] | -1.74[-1] | -1.57[-1] | -1.46[-1] | -1.51[-1] | -1.77[-1] | -2.29[-1] |
| $\mathrm{Im}(A_u^{3/2})$ | 3.65[-1] | 3.65[-1] | 3.68[-1] | 3.70[-1] | 3.71[-1] | 3.79[-1] | 3.98[-1] | 4.30[-1] | 4.57[-1] | 4.30[-1] |

## The real part of the breakup amplitude $A_u$




The results obtained by different groups and methods are presented. Solid line is our result using the asymptotic approach, dots are results of J.L. Friar (PRC 51 2356 (1995)) and our calculations carried out using the integral representation (Int) and integral representation with complex scaling (Int+CS).

# The imaginary part of the breakup amplitude Au



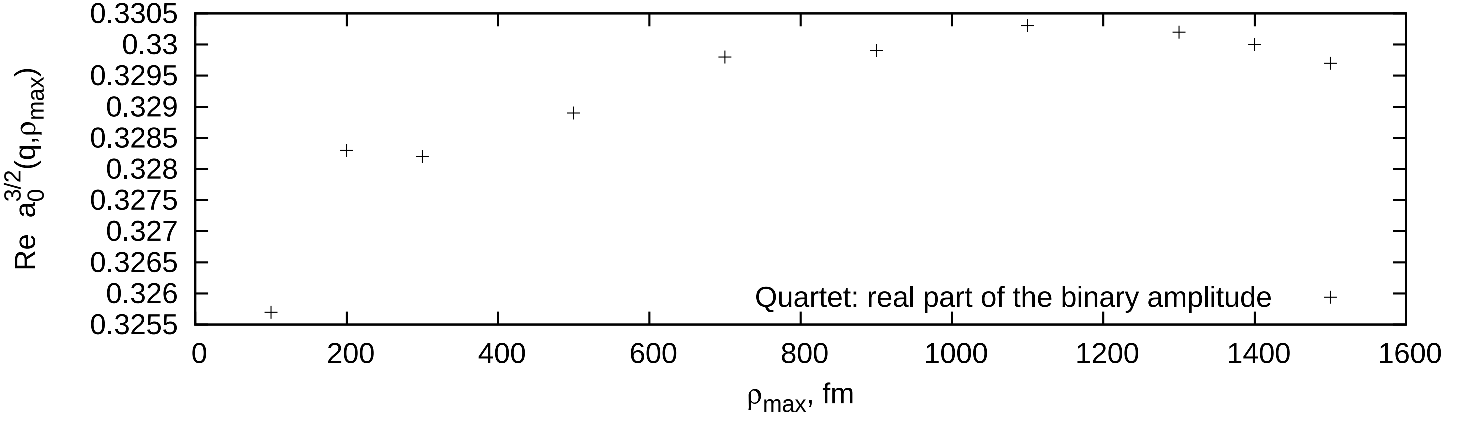

The results obtained by different groups and methods are presented. Solid line is our result using the asymptotic approach, dots are results of J.L. Friar (PRC 51 2356 (1995)) and our calculations carried out using the integral representation (Int) and integral representation with complex scaling (Int+CS).

# Results: the binary amplitude

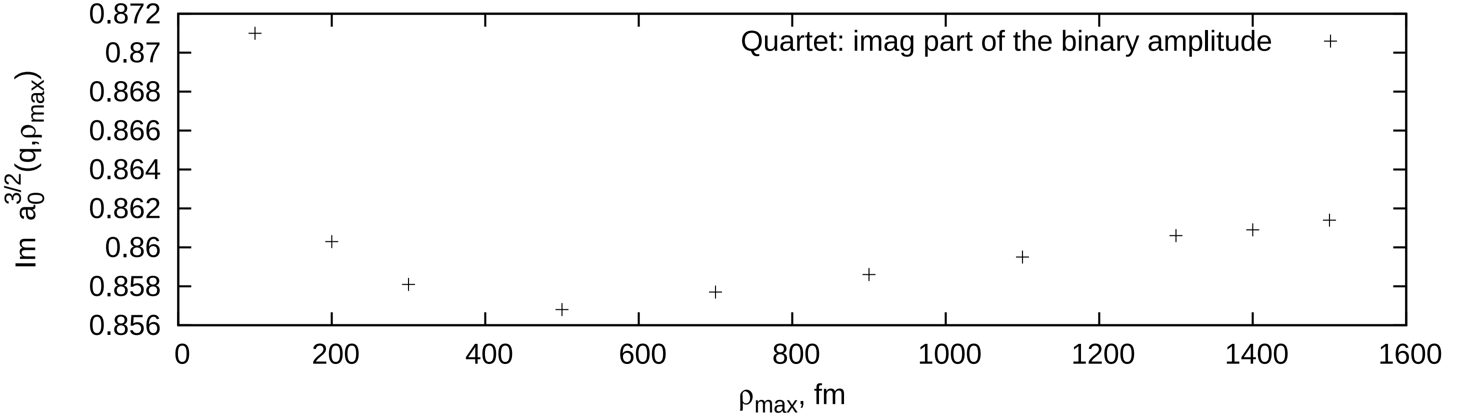
The $\rho_{\max}$ -dependence of the binary amplitude $a_0^{3/2}$, inelasticity $\eta^{3/2}$, phase shift $\delta^{3/2}$ and a parameter $\Lambda^{3/2}$, defining the accuracy of the calculation

| $\rho_{max}$ | $\mathrm{Re}(a_0^{3/2})$ | $\mathrm{Im}(a_0^{3/2})$ | $\eta^{3/2}$ | $\delta^{3/2}$ | $\Lambda^{3/2}$ |
|---|---|---|---|---|---|
| 100 | 0.3257 | 0.8710 | 0.9873 | 69.36 | 1.0307 |
| 200 | 0.3283 | 0.8603 | 0.9749 | 68.83 | 0.9956 |
| 300 | 0.3282 | 0.8581 | 0.9716 | 68.75 | 0.9879 |
| 500 | 0.3289 | 0.8568 | 0.9706 | 68.67 | 0.9854 |
| 700 | 0.3298 | 0.8577 | 0.9732 | 68.66 | 0.9906 |
| 900 | 0.3299 | 0.8586 | 0.9746 | 68.69 | 0.9930 |
| 1100 | 0.3303 | 0.8595 | 0.9763 | 68.71 | 0.9965 |
| 1300 | 0.3302 | 0.8606 | 0.9778 | 68.76 | 0.9994 |
| 1400 | 0.3300 | 0.8609 | 0.9781 | 68.78 | 0.9998 |
| 1500 | 0.3297 | 0.8614 | 0.9784 | 68.81 | 1.0014 |

# The plots of the real and imaginary parts of the binary amplitude




$$E_{lab} = 14.1\,MeV$$



The inelasticity $\eta^{3/2}$, phase shift $\delta^{3/2}$ and a parameter $\Lambda^{3/2}$ showing the accuracy of the calculations for different energies.

| $E_{lab}$, МэВ | 4.0 | 14.1 | 42.0 |
|---|---|---|---|
| $J = 3/2$, квартет | | | |
| $\eta^{3/2}$ | 0.9998 | 0.9781 | 0.9031 |
| $\delta^{3/2}$ | 101.48 | 68.78 | 37.66 |
| $\Lambda^{3/2}$ | 0.9996 | 0.9998 | 0.9995 |
| $J = 1/2$, дублет | | | |
| $\eta^{1/2}$ | 0.9646 | 0.4648 | 0.5021 |
| $\delta^{1/2}$ | 143.59 | 105.40 | 41.21 |
| $\Lambda^{1/2}$ | 1.0002 | 0.9997 | 1.0002 |

- <u>Comparison with the results of other authors</u>

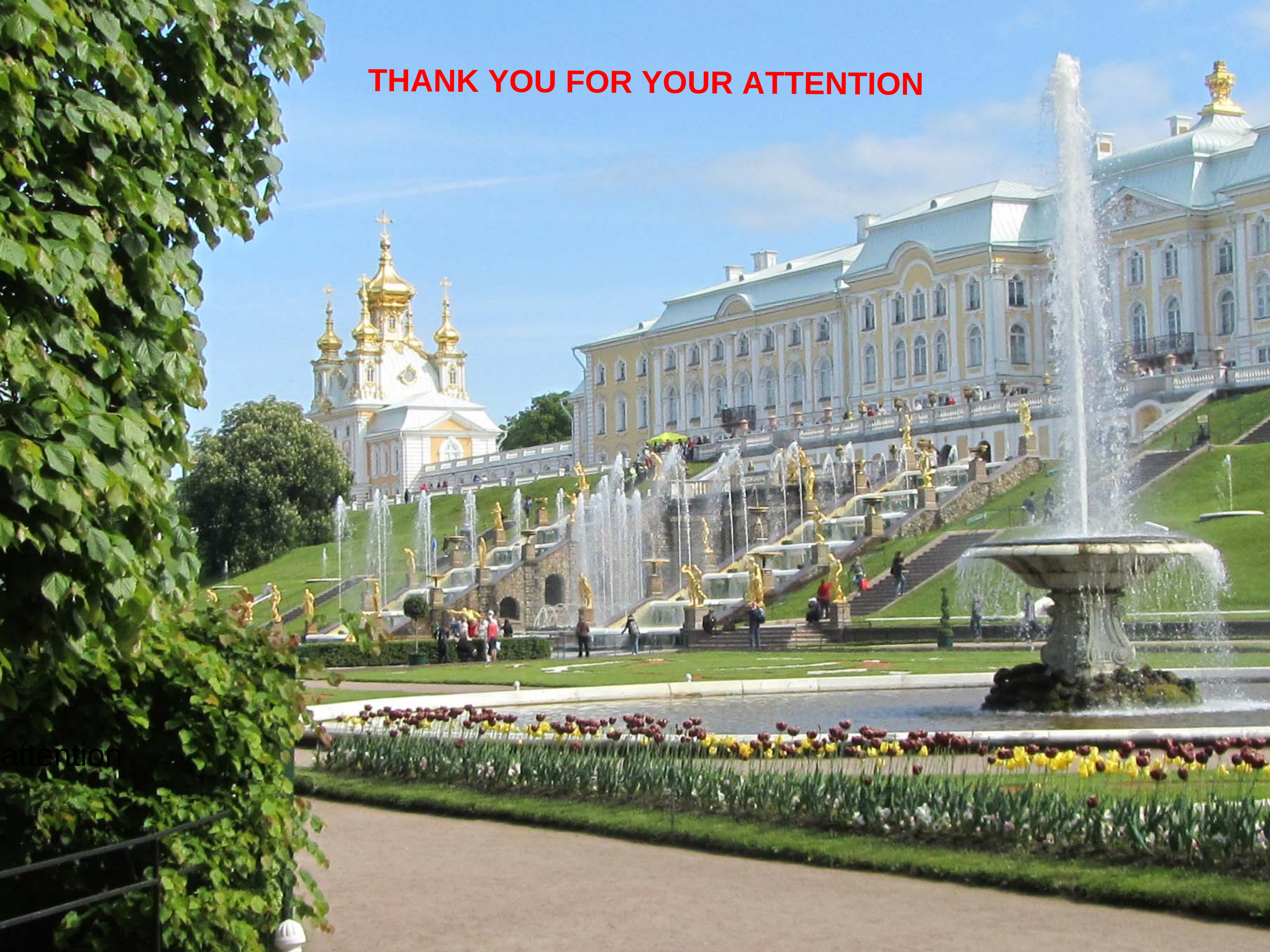
| Quartet | | | |
|---|---|---|---|
| Energy | Parameter | This work | [1] |
| 14 MeV | $\eta$ | 0.9781 | 0.9782 |
| | $\delta$ | 68.78 | 68.95 |
| 42 MeV | $\eta$ | 0.9031 | 0.9035 |
| | $\delta$ | 37.66 | 37.71 |
| Doublet | | | |
| 14 MeV | $\eta$ | 0.4648 | 0.4648 |
| | $\delta$ | 105.40 | 105.48 |
| 42 MeV | $\eta$ | 0.5021 | 0.5024 |
| | $\delta$ | 41.21 | 41.43 |

[1] *Payne G.L., Friar J.L., et al.* Phys. Rev. C **51** 2356 (1995)

# Conclusions

- Method 1: The orthonormal basis related to the two-body subsystem Hamiltonian is constructed. The asymptotic boundary condition is modified in terms of this basis. The breakup amplitude is represented by the linear combination of basis functions which allows the extrapolation of this amplitude to infinity exclusively by the properties of the basis functions. The coefficients of the linear combination together with the binary amplitude are numerically obtained from the comparison with the asymptotic.
- Method 2: The exterior complex scaling is used for reducing the asymptotic boundary conditions to zero. The binary and breakup amplitudes are obtained from their integral representation.
- The methods include solving the system of linear algebraic equations. The domain decomposition method which allows the parallelization of the solution process has been applied and reduced the overall time of calculation up to 10 times.

$$A_i^J\left(\theta, E, \rho_{\max}\right) = \lim_{\rho\to\infty} A_i^J\left(\theta, E, \rho_{\max}, \rho\right) = \sum_{k=1}^{N_\phi} a_{i,k}^J(E, \rho_{\max}) \frac{2}{\sqrt{\pi}} \sin 2k\theta$$


THANK YOU FOR YOUR ATTENTION
attention