Faddeev-AGS Calculation of Neutron Induced Nuclear Reaction on Deuteron within Wave-Packet Continuum Discretization Approach

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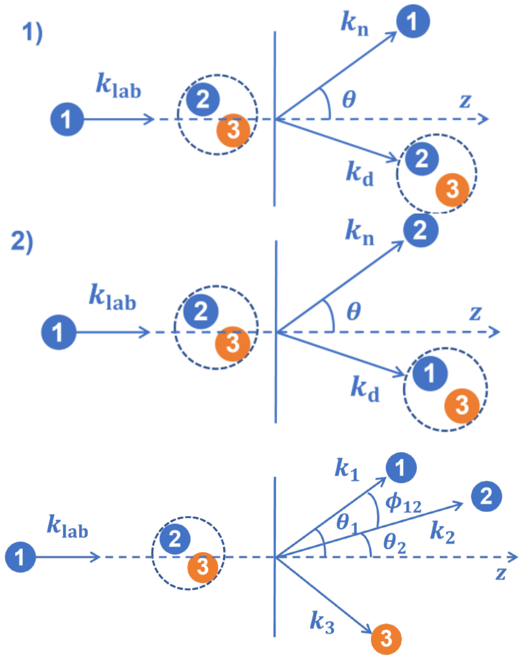
ISINN 2025-05-27

Outline

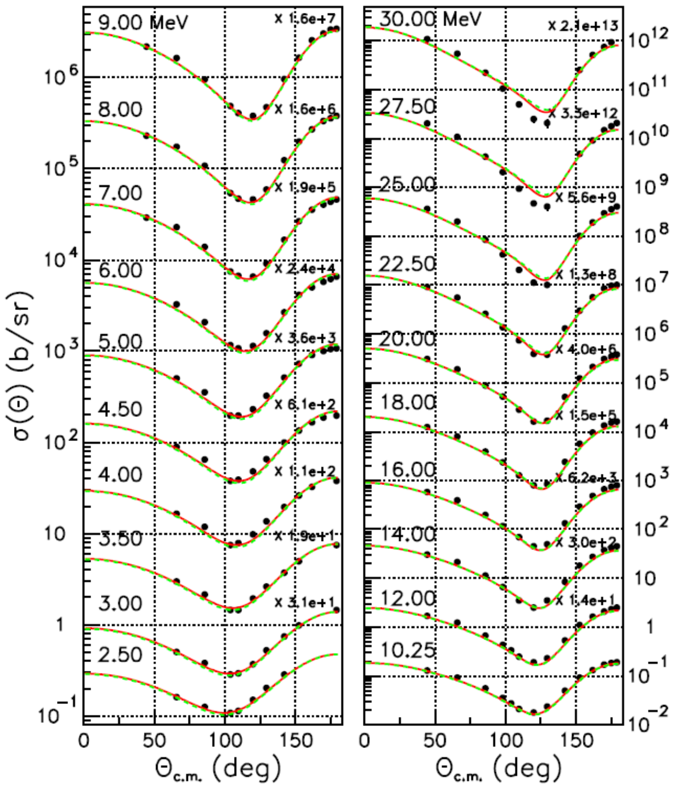
- Introduction
- Faddeev-AGS equation and WPCD approach
- Results and discussion
- Summary and outlook

Introduction

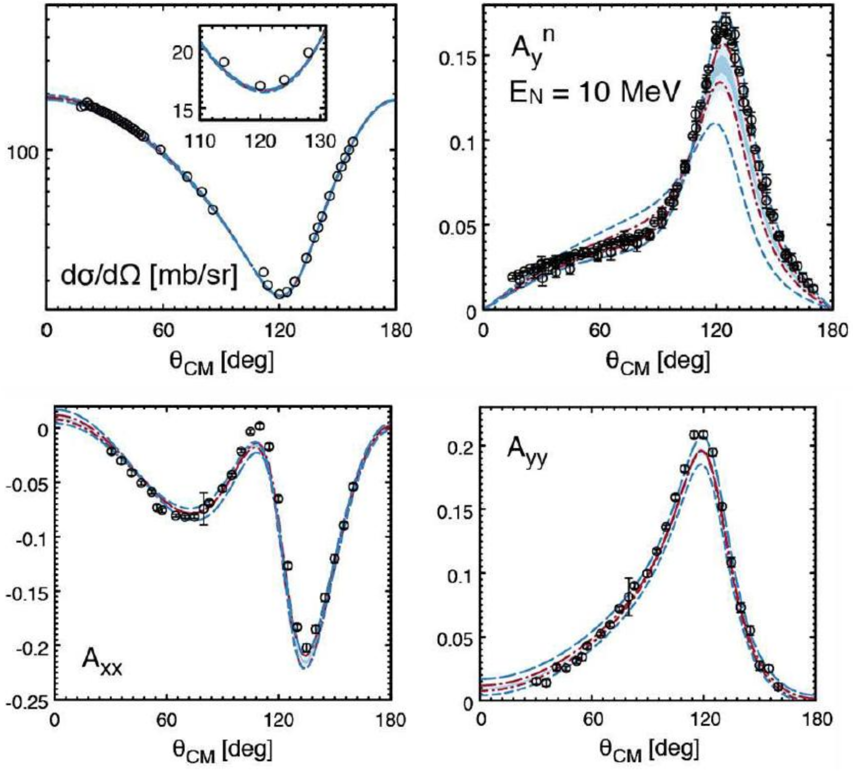
- n+d: Fundamental three-body nuclear reaction
  - Three nucleon system, well studied by Faddeev method
  - benchmark for nuclear interaction, no Coulomb force



n+d reaction



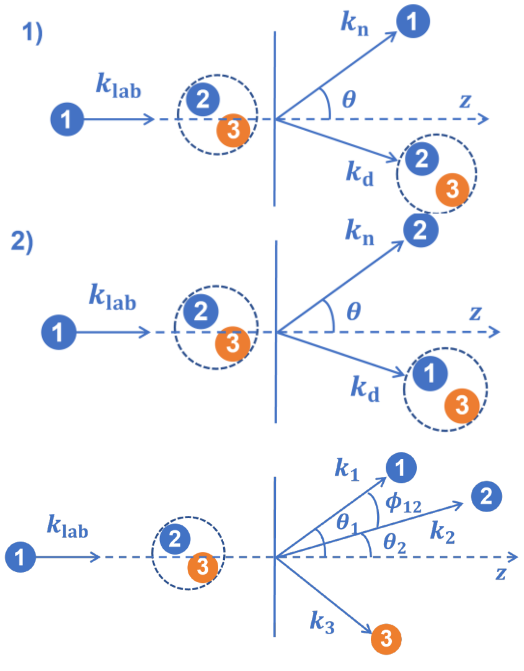
n+d elastic scattering
by Faddeev-AGS in JEFF-3.3



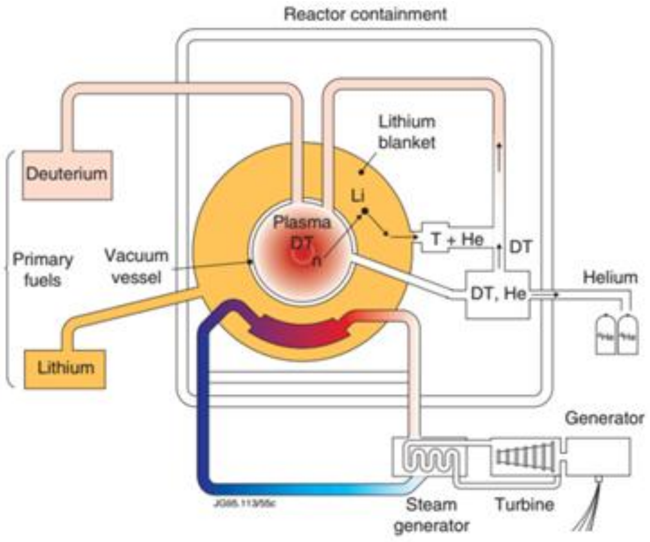
recent development for Ay puzzle
Epelbaum E, et al., Front. Phys. 8:98 (2020)

Introduction

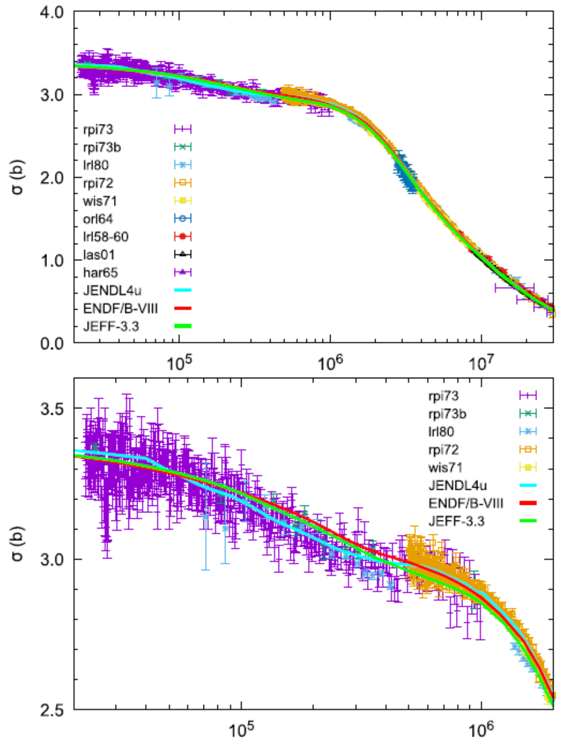
- **n+d: Fundamental three-body nuclear reaction**
  - Three nucleon system, well studied by Faddeev method
  - benchmark for nuclear interaction, no Coulomb force
  - requirement from nuclear data evaluation

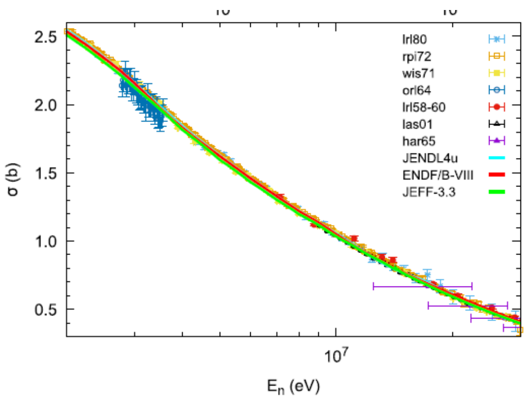


n+d reaction



d(n,2n)p: an important source of neutron breeding in fusion reactor



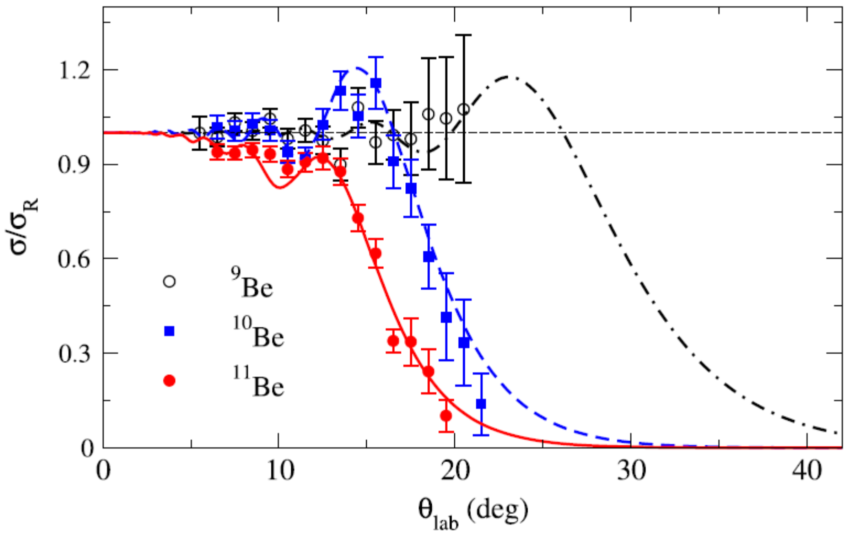


n+d reaction data in ENDF/B, JEFF and JENDL

Introduction

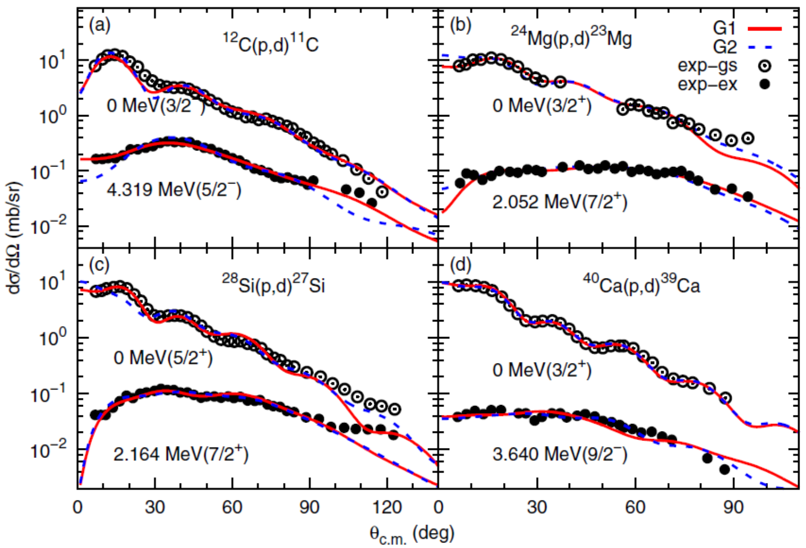
- Three-body model in nuclear reactions
  - extensively used, various theoretical approaches
  - nuclear structure, reaction, astrophysics

elastic scattering



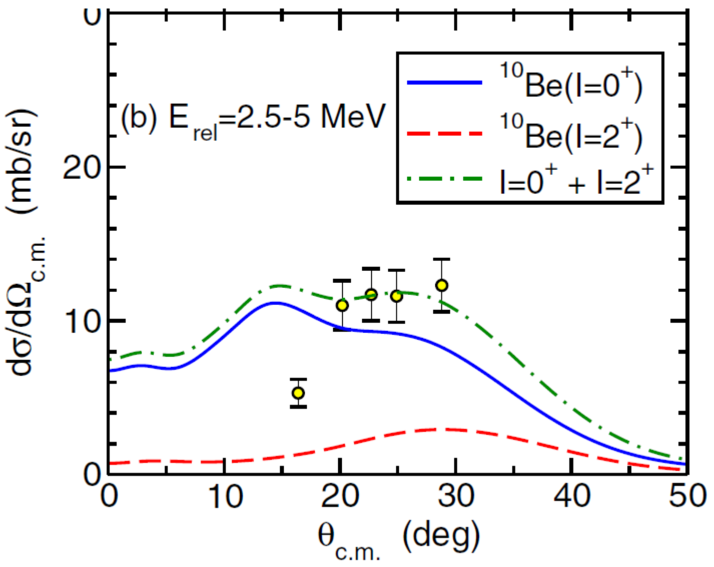
extract optical potentials, rms radii, density distributions…
F.F.Duan, et al., PLB 811(2020)135942

rearrangement



extract spin, parity, spectroscopic factors…
Y. P. Xu, et al., PRC 98, 044622 (2018)

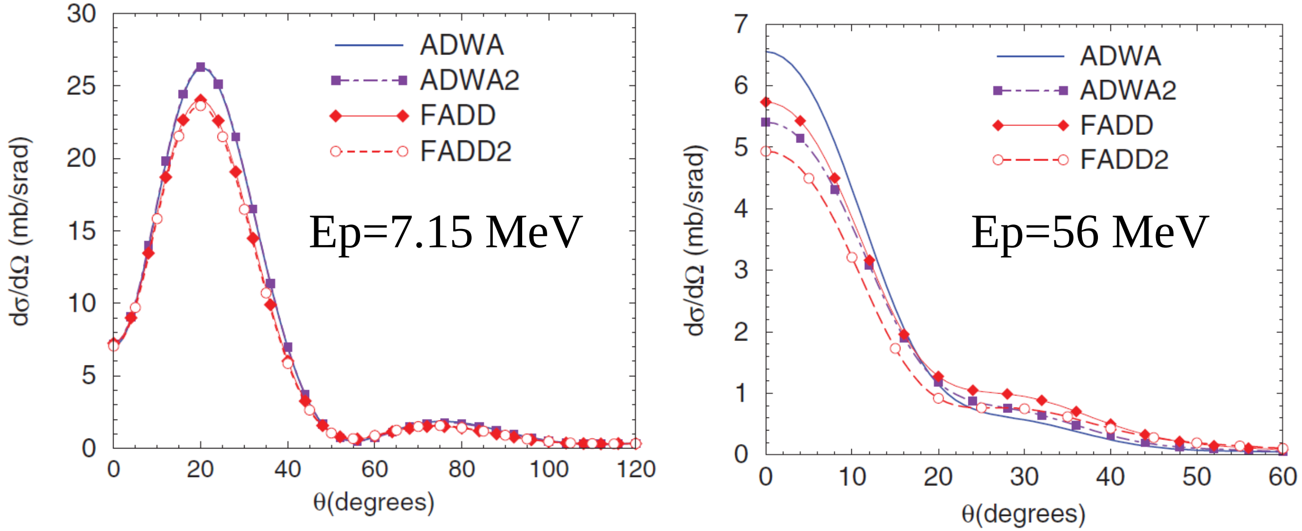
breakup



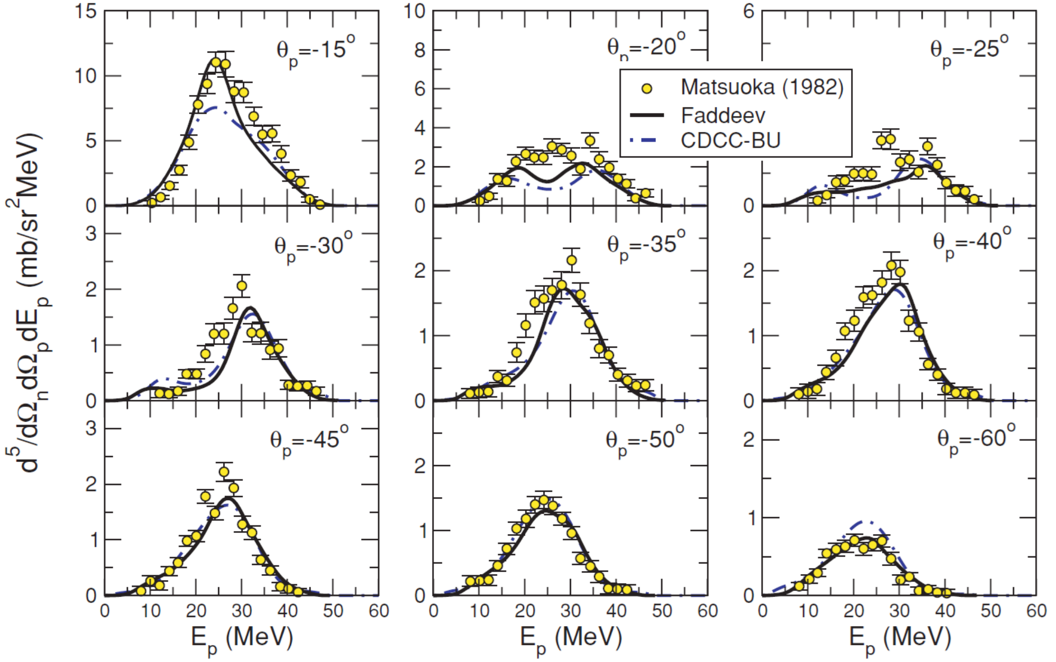
cluster structure, outgoing particles…
R. de Diego, et al., PRC 95, 044611 (2017)

Introduction

- **Three-body model in nuclear reactions**
  - breakup and rearrangement channels are handled independently in many cases
  - **what if rearrangement and breakup channels couple non-negligibly? — light nuclei reactions**
  - **Faddeev method:** fully includes elastic scattering, breakup and rearrangement channels



12C(p,d)11C, ADWA vs Faddeev
F. M. Nunes, et al., PRC 84, 034607 (2011)



12C(d,pn), CDCC vs Faddeev
A. Deltuva, et al., PRC 76, 064602 (2007)

Introduction

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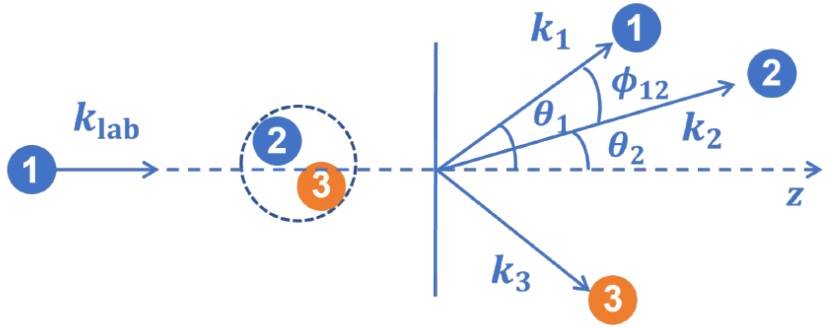
Reduce many-body to few(3)-body problem

- Isolate important degrees of freedom in a reaction
- Keep track of important channels
- Connect back to the many-body problem



start point n+d reaction

- solving Faddeev equation with Wave-Packet Continuum Discretization (WPCD) approach

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Faddeev-AGS equation

- **Three-body total Hamiltonian**

$$H = H_0 + \sum_{\alpha} v_\alpha$$

- **Faddeev equation**
  - L.D. Faddeev, Sov. Phys. JETP 12, 1014 (1961)

$$T = T_1 + T_2 + T_3$$

$$\begin{pmatrix} T_1 \\ T_2 \\ T_3 \end{pmatrix} = \begin{pmatrix} t_1 \\ t_2 \\ t_3 \end{pmatrix} + \begin{pmatrix} 0 & t_1 & t_1 \\ t_2 & 0 & t_2 \\ t_3 & t_3 & 0 \end{pmatrix} g_0 \begin{pmatrix} T_1 \\ T_2 \\ T_3 \end{pmatrix}$$

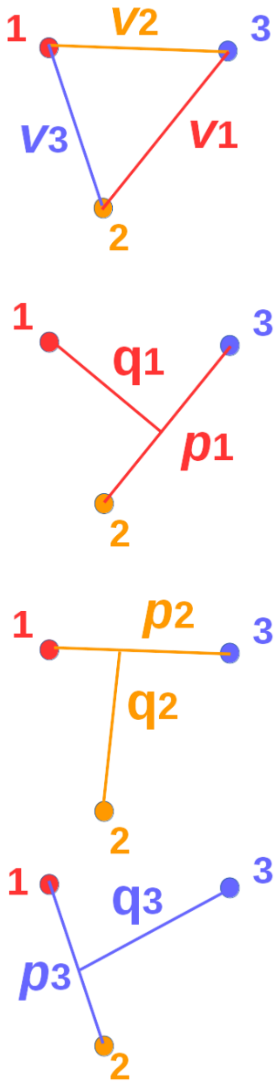
$$t_i = (1 - v_i g_0)^{-1} v_i$$

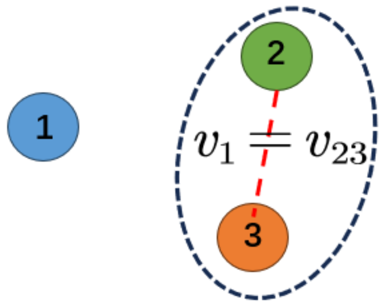
- **Faddeev-AGS equation**
  - E. O. Alt, et al., NPB 2, 167 (1967).

$$\langle \phi_\beta | U_{\beta\alpha} | \phi_\alpha \rangle \equiv \left\langle \phi_\beta \middle| v_\beta \middle| \Psi_\alpha^{(+)} \right\rangle$$

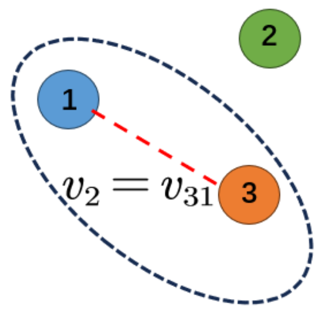
$$U_{\beta\alpha} = \bar{\delta}_{\alpha,\beta} G_0^{-1} + \sum_{\gamma} \bar{\delta}_{\gamma,\beta} t_\gamma G_0 U_{\gamma,\alpha}$$

$$U_{0\alpha} = G_0^{-1} + \sum_{\gamma} t_\gamma G_0 U_{\gamma,\alpha}$$

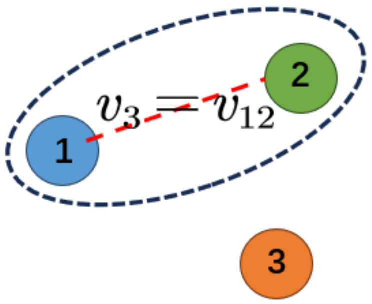




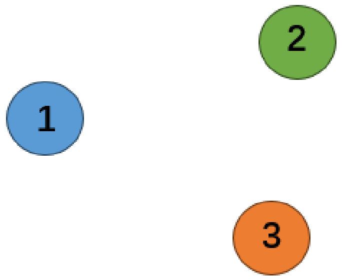
Asymptotic State
$\boldsymbol{\alpha}$
elastic scattering



Asymptotic State
$\boldsymbol{\beta}$
rearrangement



Asymptotic State
$\boldsymbol{\gamma}$
rearrangement



Asymptotic State
0
breakup

Faddeev-AGS equation

- Faddeev-AGS equation for n+d system

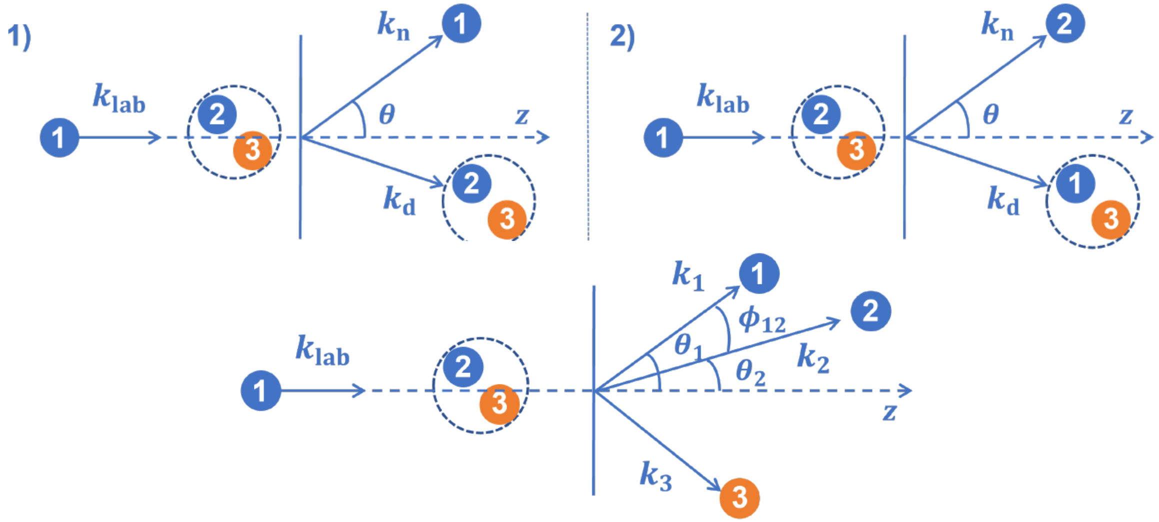
$$U = PG_0^{-1} + PtG_0U$$

$$P = P_{12}P_{23} + P_{13}\ P_{23}$$

$$G_0 = 1/(E + i0^+ - H_0)$$

$$U_0 = (1 + tG_0)U$$

- **Difficulties:**
  - t-matrix
    - varies with energy
    - pole at deuteron binding energy
  - G_0
    - logarithmic singularity at breakup threshold
  - P
    - variable integration limits



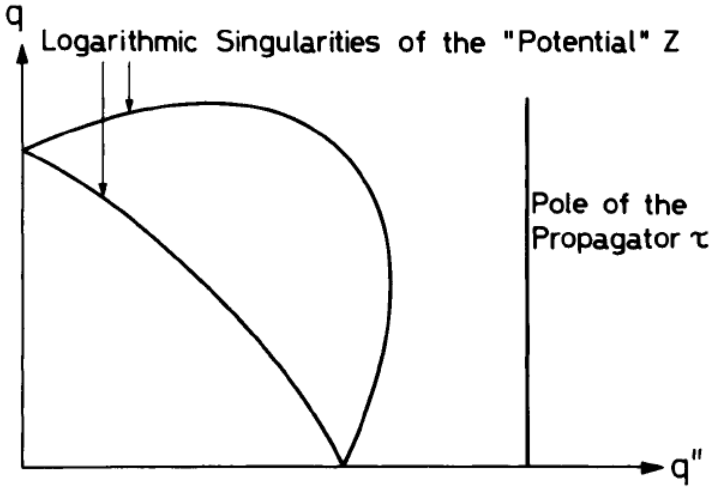


Fig. 16. Position of singularities in the kernel of Eq. (5.62)

Faddeev-AGS equation

- Faddeev-AGS equation for n+d system

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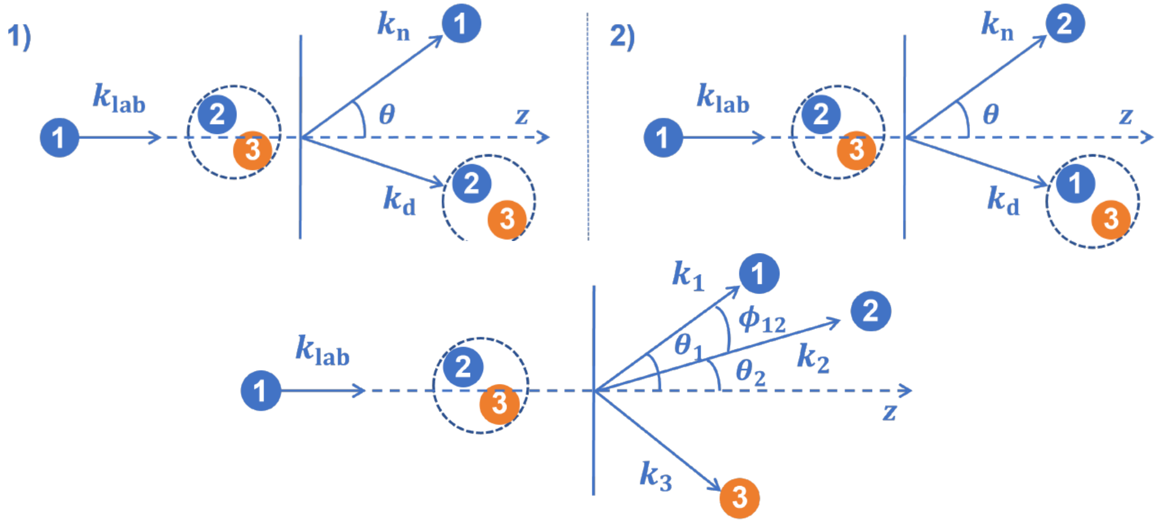


- **Difficulties:**
  - t-matrix
    - varies with energy
    - pole at deuteron binding energy
  - G_0
    - logarithmic singularity at breakup threshold
  - P
    - variable integration limits

$$\langle p'q'\alpha'|P|pq\alpha\rangle = \int_{-1}^{+1} dx\ \frac{\delta(p'-\pi_1)}{p'^{l'+2}}\frac{\delta(p-\pi_2)}{p^{l+2}}G_{\alpha'\alpha}(q'qx)$$

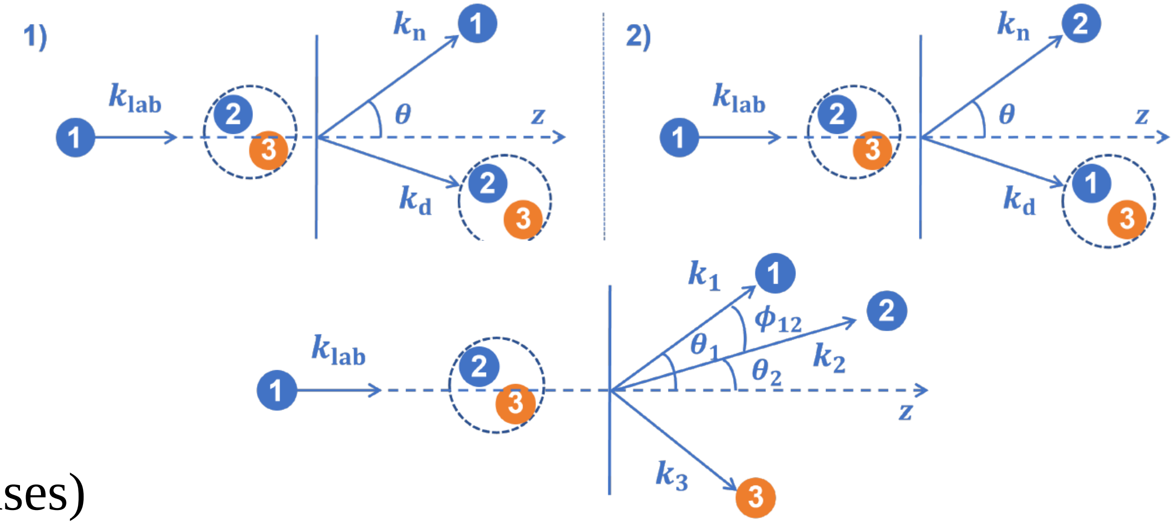
$$\langle pq\alpha|\hat{T}|\phi\rangle = \langle pq\alpha|\hat{t}P|\phi\rangle + \sum_{\alpha'}\sum_{\alpha''}\int_0^\infty dq'\ q'^2 \int_{-1}^{+1} dx\ \frac{\hat{t}_{\bar{\alpha}\bar{\alpha}'}(p,\pi_1,E-(3/4m)q^2)}{\pi_1^{l'}}$$
$$\times G_{\alpha'\alpha''}(qq'x)\frac{1}{E+i\epsilon-q^2/m-q'^2/m-qq'x/m}$$
$$\times\left(\delta_{\alpha''\alpha_d}\frac{\langle\pi_2q'\alpha''|\hat{T}|\phi\rangle}{\pi_2^{l''}}\frac{1}{E+i\epsilon-(3/4m)q^2-\epsilon_d}+\bar{\delta}_{\alpha''\alpha_d}\frac{\langle\pi_2q'\alpha''|\hat{T}|\phi\rangle}{\pi_2^{l''}}\right)$$

Faddeev-AGS equation

- Equivalent form
  - O.A. Rubtsova, et al., Ann. Phys. 360 (2015) 613–654

$$U = Pv + PvG_1U$$

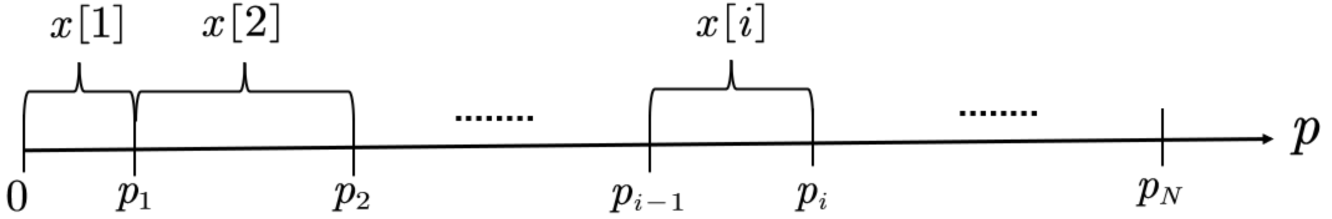
$$G_1 = 1/(E + i0^+ - H_0 - v)$$



- **Properties:**
  - v: no pole and no energy-dependence (in many cases)
  - G_1: diagonally matrix within the eigen-states of $H_0 + v$

WPCD approach – 2-body system

- continuum momentum space → discrete momentum interval



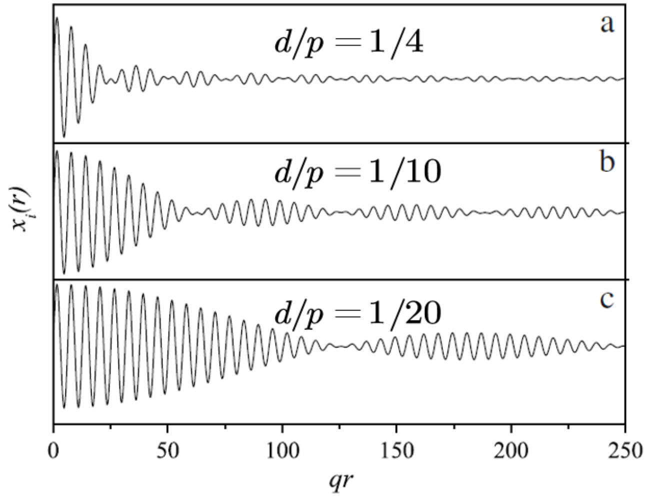
- Orthogonal basis based on wave packets (WP)

$$|x[i]\rangle = \frac{1}{\sqrt{B}} \int_{p_{i-1}}^{p_i} p\,dp\, w(p)\, |p\rangle,\ B = \int_{p_{i-1}}^{p_i} dp\ |w(p)|^2$$

momentum WP: $w(p) = 1,\ B = p_i - p_{i-1}$

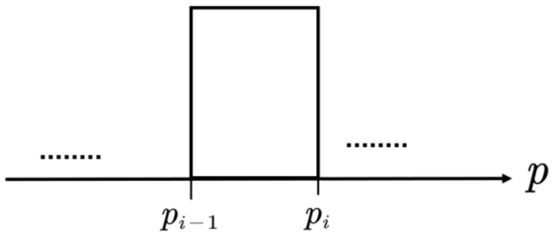
energy WP: $w(p) = \sqrt{\frac{p}{m}},\ B = \frac{p_i^2}{2m} - \frac{p_{i-1}^2}{2m} = E_i - E_{i-1}$

$\langle x[i] \,|\, x[j] \rangle = \delta_{ij}$



coordinate space
S-wave with ω =1

$$px_i(p) = \frac{f_i(p)[\theta(p - p_{i-1}) - \theta(p - p_i)]}{\sqrt{B_i}}$$



momentum space
step-like function if ω=1

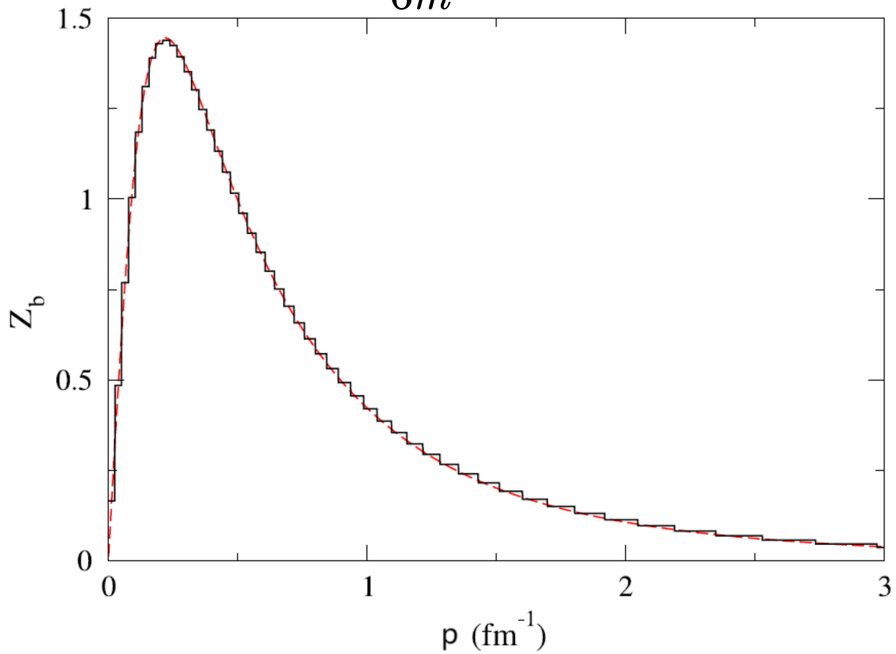
WPCD approach – 2-body system

- Compare: Bound state and scattering phase shift

$$\langle \boldsymbol{x}|\varepsilon - h|\boldsymbol{x}\rangle = 0$$

$$\langle x[i]|h|x[j]\rangle = \langle x[i]|h_0|x[j]\rangle + \langle x[i]|v|x[j]\rangle$$

$$\langle x[i]|h_0|x[j]\rangle = \frac{\delta_{ij}}{6m}\left(p_i^2 + p_{i-1}^2 + p_i p_{i-1}\right)$$

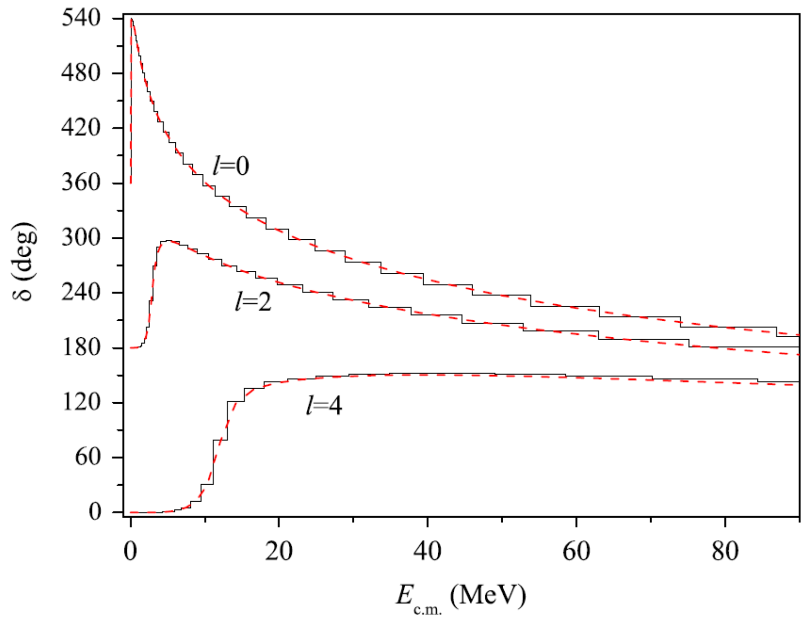


deuteron bound state wave function in momentum space

$$\boldsymbol{t} = \boldsymbol{v} + \boldsymbol{v}\boldsymbol{g_o}\boldsymbol{t}$$

$$\langle x[i]|g_0|x[j]\rangle = \langle x[i]|\frac{1}{p^2/2m + i0^+ - h_0}|x[j]\rangle$$

$$= \frac{\delta_{ij} m}{p(p_i - p_{i-1})}\left[\ln\left(\frac{p - p_{i-1}}{p - p_i}\right) + \ln\left(\frac{p + p_i}{p + p_{i-1}}\right) - i\pi\,\Theta\left(p \in [p_{i-1}, p_i]\right)\right]$$



$\alpha - \alpha$ scattering phase shift

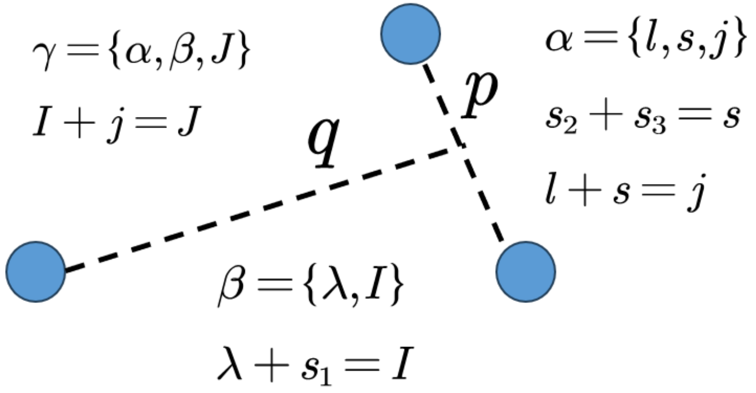
WPs are constructed by Coulomb wave function

O.A. Rubtsova, et al., Ann. Phys. 360 (2015) 613–654

WPCD approach – 3-body system

- Three-body total Hamiltonian

$$H = H_0 + \sum_\alpha v_\alpha$$



- Channel Hamiltonian

$$H_1 = H_0 + v = h_0^q \otimes h_1^p$$

$$h_1^p = h_0^p + v$$

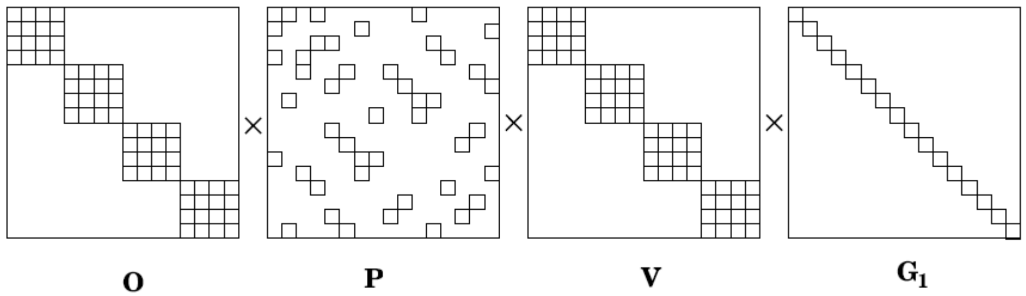
- 3-body wave packet
  - direct product of q WP y_i and p pseudo states(including bound states) φ_n
  - pseudo states are generated from h_1^p diagonalization with p WPs
  - approximate the eigen-states of H_1

$$\left|Z_{ni}^{\gamma}\right\rangle = |\varphi_n y_i \gamma\rangle$$

WPCD approach – 3-body system

- Equivalent form of Faddeev-AGS equation

$$U = Pv + PvG_1 U$$



- integral equation → linear equation

$$\mathbb{U} = \mathbb{P}\mathbb{v}_1 + \mathbb{P}\mathbb{v}_1\mathbb{G}_1\mathbb{U}$$

$$\mathbb{G}_1 = \sum_{n,i,\gamma} |Z_{ni}^{\gamma}\rangle G_{ni}^{\gamma} \langle Z_{ni}^{\gamma}|$$

$$[\mathbb{P}]_{n,i,m,j}^{\gamma,\gamma'} \equiv \left\langle Z_{ni}^{\gamma} \middle| P \middle| Z_{mj}^{\gamma'} \right\rangle = \left\langle Z_{ni}^{\gamma}(1) \middle| Z_{mj}^{\gamma'}(2) \right\rangle + \left\langle Z_{ni}^{\gamma}(1) \middle| Z_{mj}^{\gamma'}(3) \right\rangle$$

- elastic scattering amplitude

$$A_{el}^{\gamma}(q_0) \approx \frac{2m}{3q_0} \frac{\left\langle Z_{1j_0}^{\gamma} \middle| U \middle| Z_{1j_0}^{\gamma} \right\rangle}{d_{j_0}}$$

- breakup amplitude

$$T = tG_0U = vG_1U$$

$$\mathbb{T}_{n,i,1j_0}^{\gamma} \equiv \frac{\left\langle Z_{ni}^{\gamma} \middle| U \middle| Z_{1j_0}^{\gamma} \right\rangle}{\sqrt{d_{j_0} d_k d_j}}$$

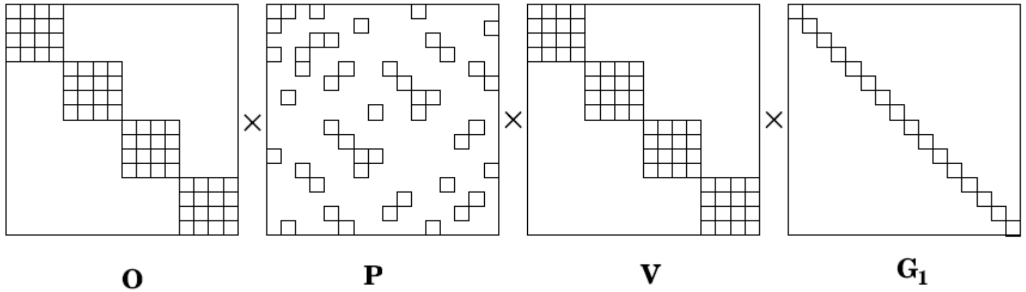
$$T^{\gamma}(p,q) \approx e^{i\delta(p_n)} \frac{\mathbb{T}_{n,i,1j_0}^{\gamma}}{p_n q_i q_0}$$

$$A_{bu}^{\gamma}(\theta) = \frac{4\pi m}{3\sqrt{3}} q_0 K^4 e^{\frac{i\pi}{4}} T^{\gamma}(p,q)$$

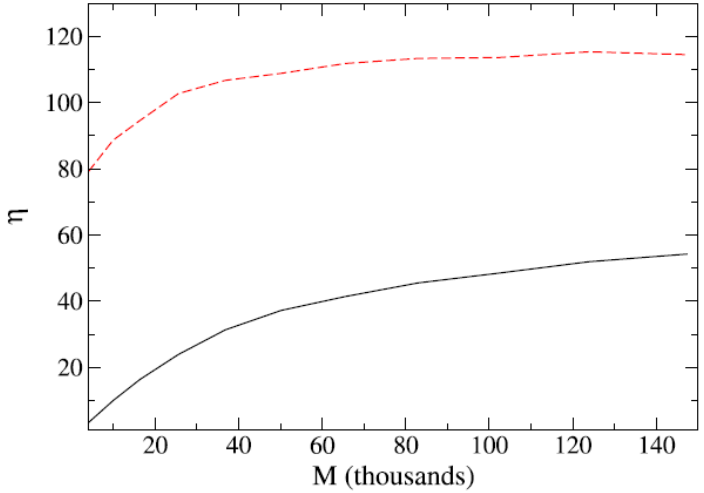
WPCD approach – 3-body system

- Equivalent form of Faddeev-AGS equation

  $U = Pv + PvG_1U$



- **Advantages within WPCD approach**
  - all singularities are smoothed and represented by complex number
  - eigen-states of H_1 are represented by 3-body WP basis
  - channel green function G_1 has analytical form
  - P matrix element depends on WP basis only, independent from other operators
  - GPU-enabled calculations



GPU speed-up ratio

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- **Results and discussion**
- Summary and outlook

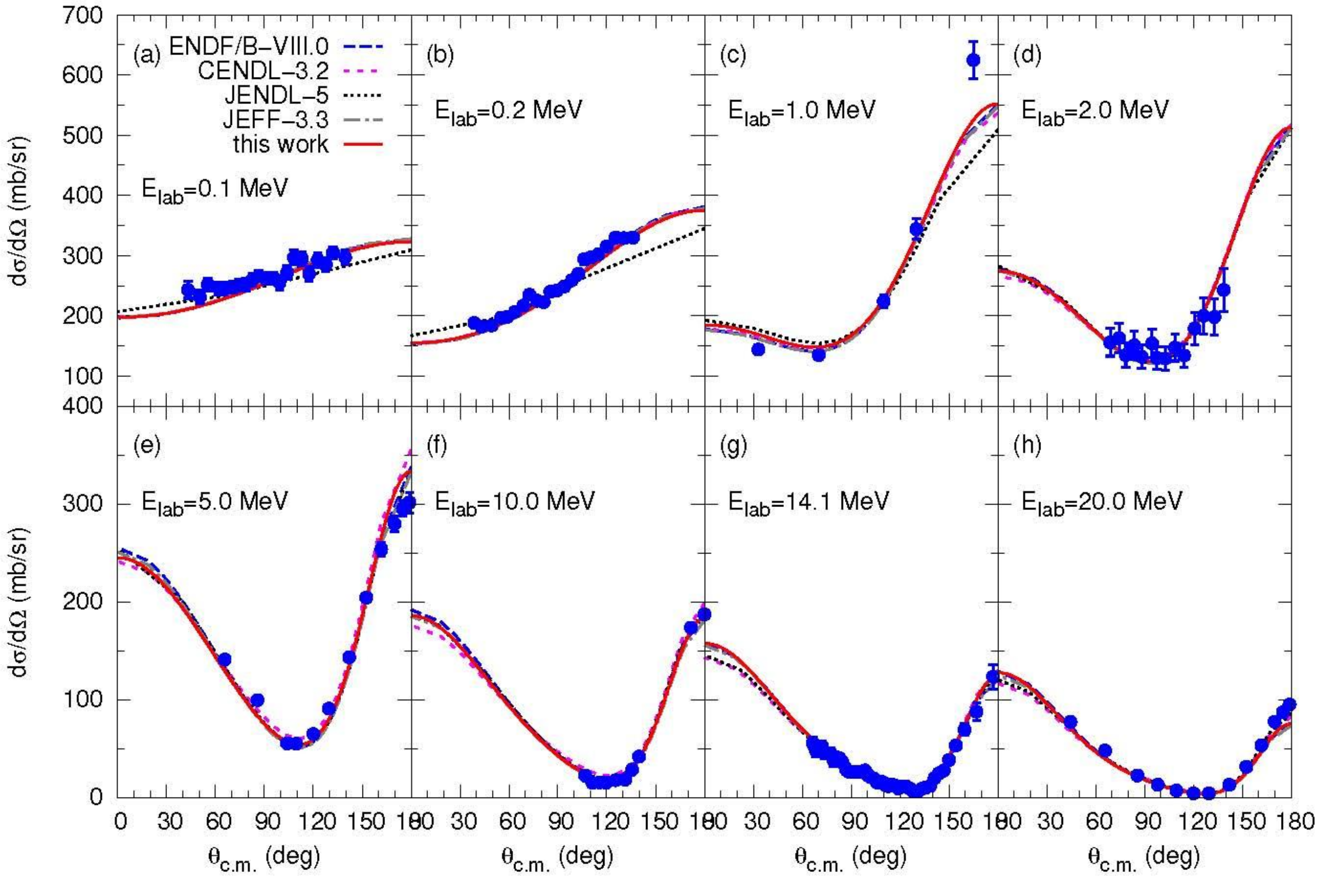
Results and discussion

n+d elastic scattering (Nijmegen potential)

- Elastic scattering S-matrix can be obtained from solutions directly

$$S = \langle \varphi_b q_0 | U | \varphi_b q_0 \rangle \approx \frac{\left\langle Z^{\gamma}_{1 j_0} \middle| U \middle| Z^{\gamma}_{1 j_0} \right\rangle}{d_{j_0}}$$

$$A^{\gamma}_{el}(q_0) \approx \frac{2m}{3q_0} \frac{\left\langle Z^{\gamma}_{1 j_0} \middle| U \middle| Z^{\gamma}_{1 j_0} \right\rangle}{d_{j_0}}$$



Yan Li, et al., AEST， 56, 860 (2022)

Results and discussion

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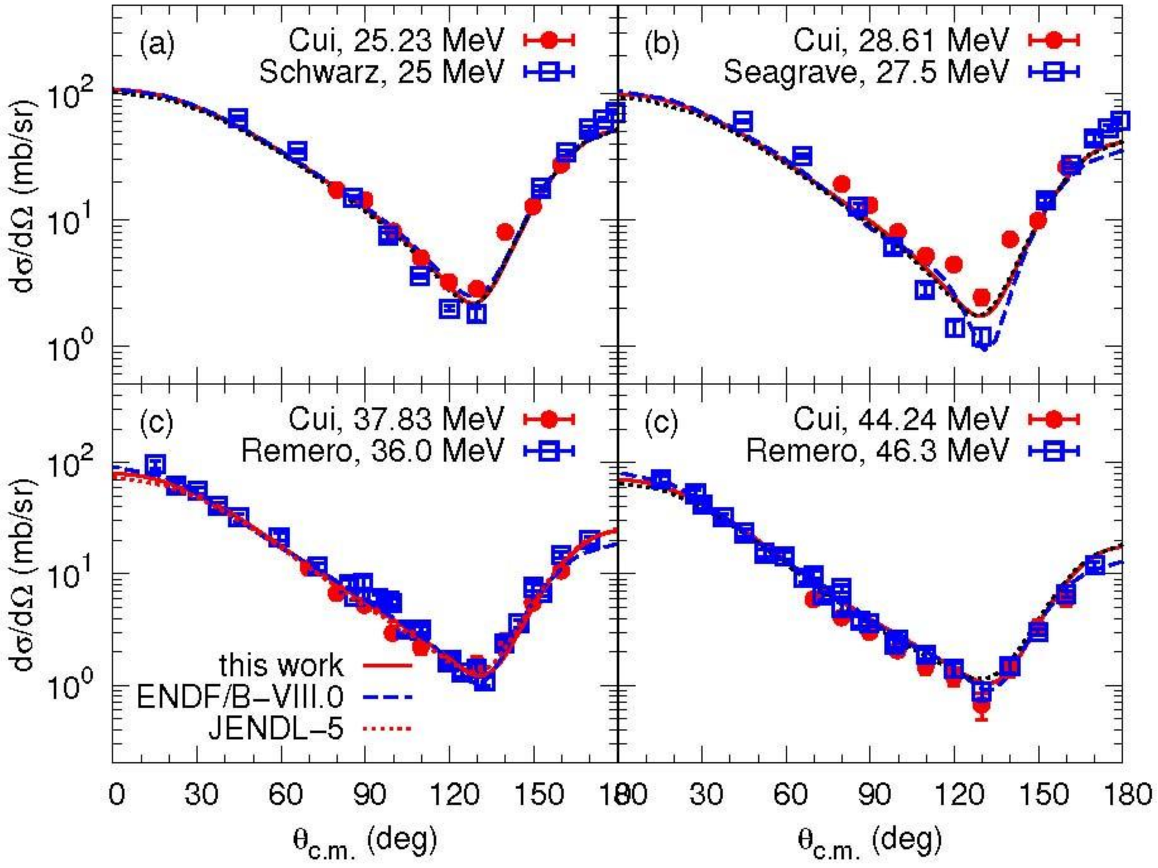


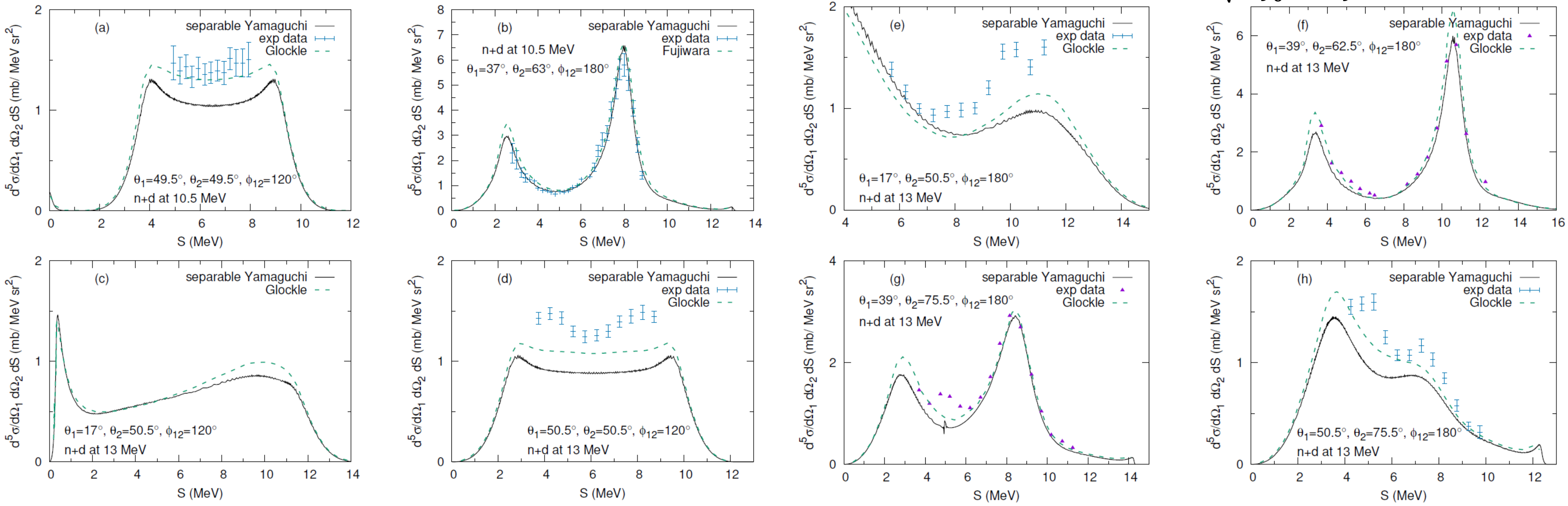
Yan Li, et al., AEST，56, 860 (2022)

Results and discussion

n+d breakup (Yamaguchi potential)

- breakup T-matrices can be obtained simply by multiplying a phase shift factor on solutions if the potential is in the single channel case

$$T = tG_0U = vG_1U \approx e^{i\delta(p_n)} \frac{\left\langle Z^{\gamma}_{ni} \middle| U \middle| Z^{\gamma}_{1j_0} \right\rangle}{\sqrt{d_{j_0} d_k d_j}}$$

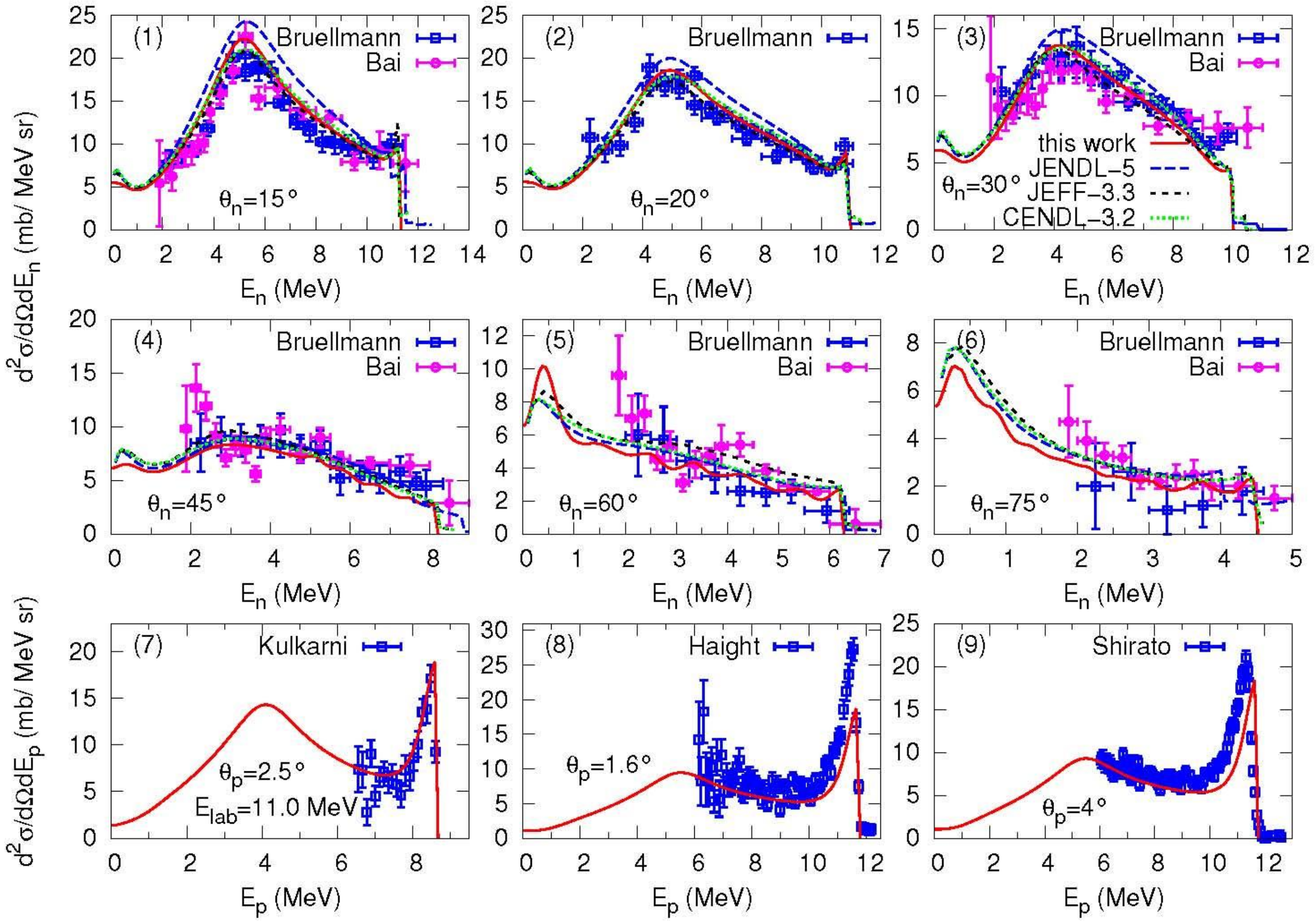


Results and discussion

- n+d breakup (Yamaguchi potential)

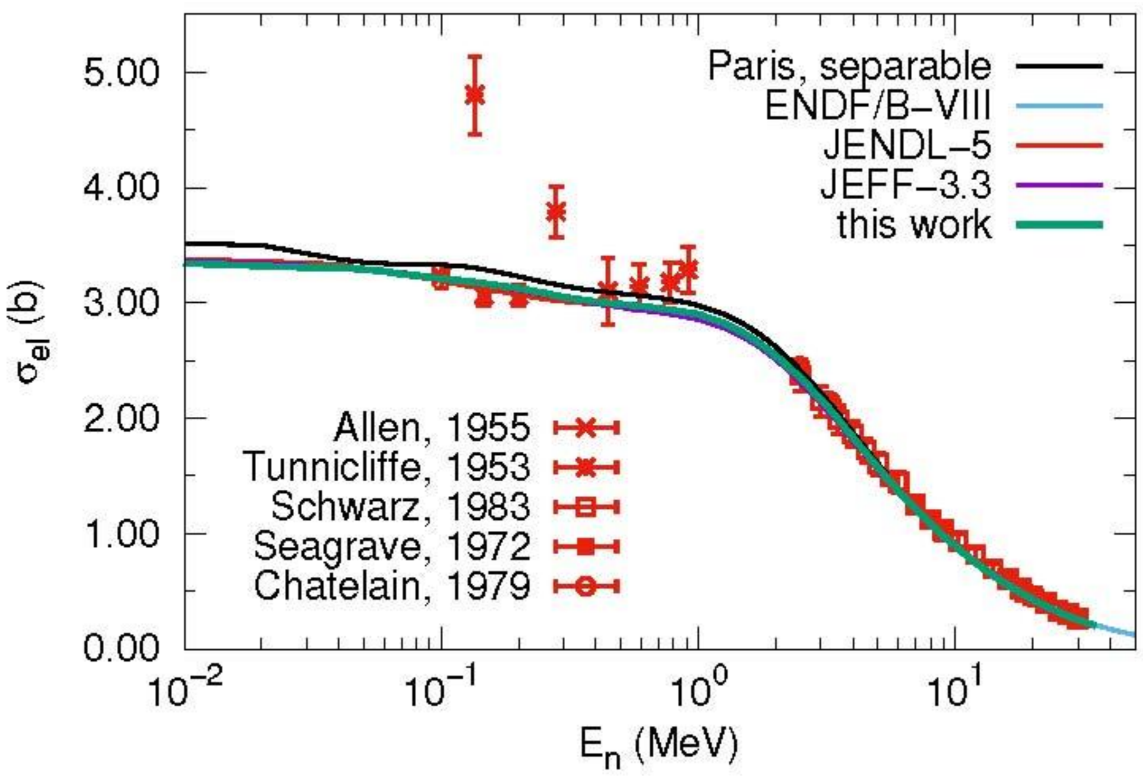
Outgoing neutron

Outgoing proton

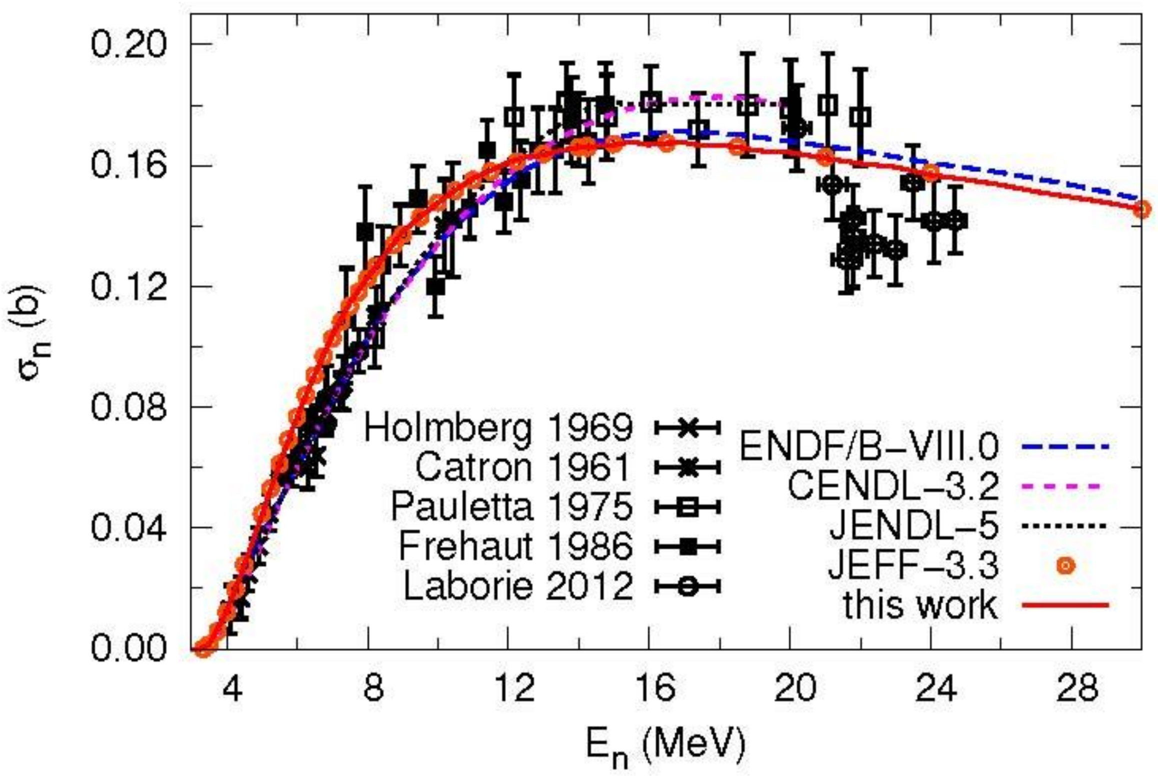


Results and discussion

◻ n+d reaction cross section



elastic reaction cross section



breakup reaction cross section

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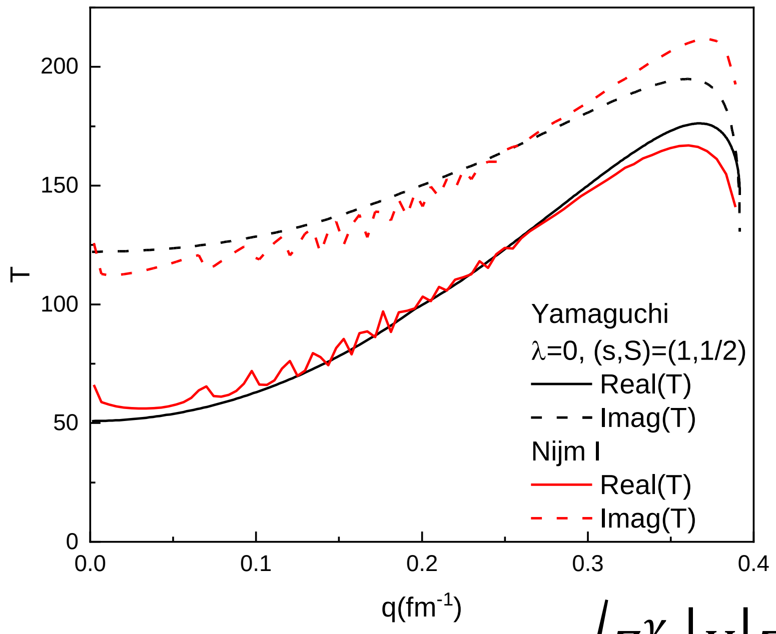
Summary and outlook

- We have solved Faddeev-AGS equation for n+d reaction within WPCD approach
  - ☑ elastic scattering (S-wave interaction, realistic nuclear force)
  - ☑ breakup (S-wave interaction)

- We are working on n+d breakup reaction calculations with realistic nuclear force



$$T \approx \begin{bmatrix} cos\theta & -sin\theta \\ sin\theta & cos\theta \end{bmatrix} e^{i\delta(p_n)} \frac{\langle Z^{\gamma}_{ni} | U | Z^{\gamma}_{1j_0} \rangle}{\sqrt{d_{j_0} d_k d_j}}$$

- We plan to extend the application of Faddeev-AGS equation and WPCD approach into
  - n-induced reactions on light nuclei
  - d-induced reactions
  - etc

- To build an effective tool for spectroscopic factor analysis and outgoing particle cross section calculations.

Thanks for your attention!