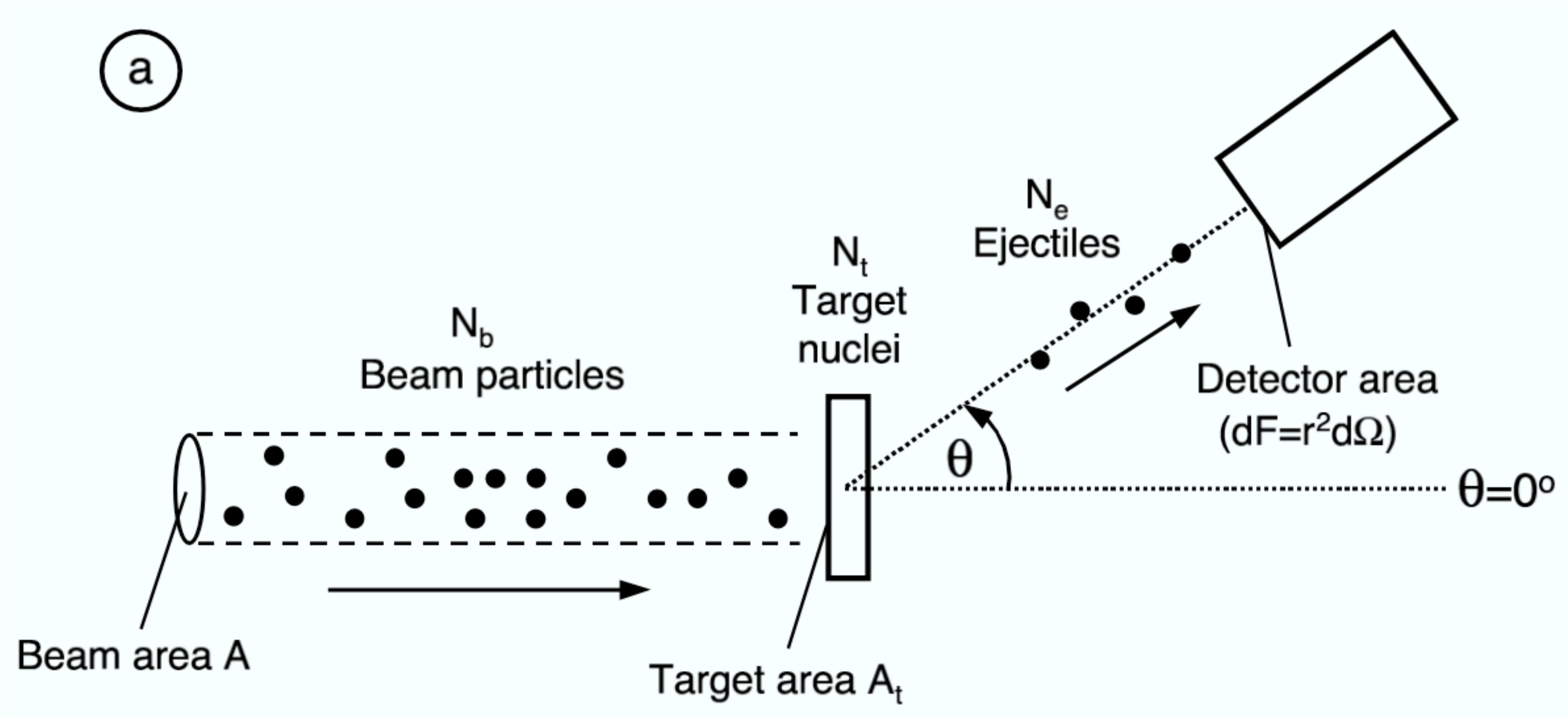
R-Matrix Theory for Nuclear Astrophysics

J. Skowronski

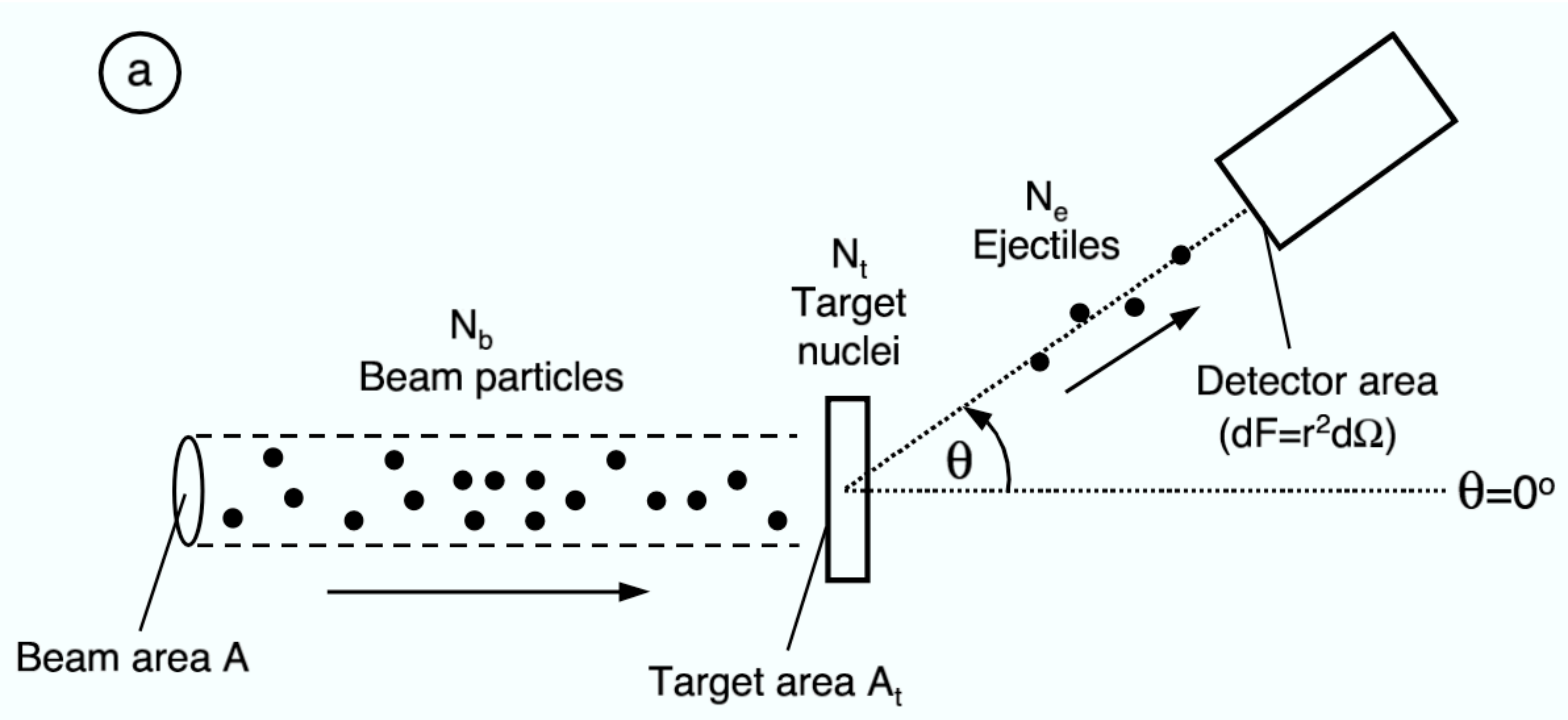
Introduction

Cross Section

$$\sigma = \frac{N_r}{N_p\ N_t}$$



Cross Section



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N_p = number of incoming particles

N_t = number of target particles

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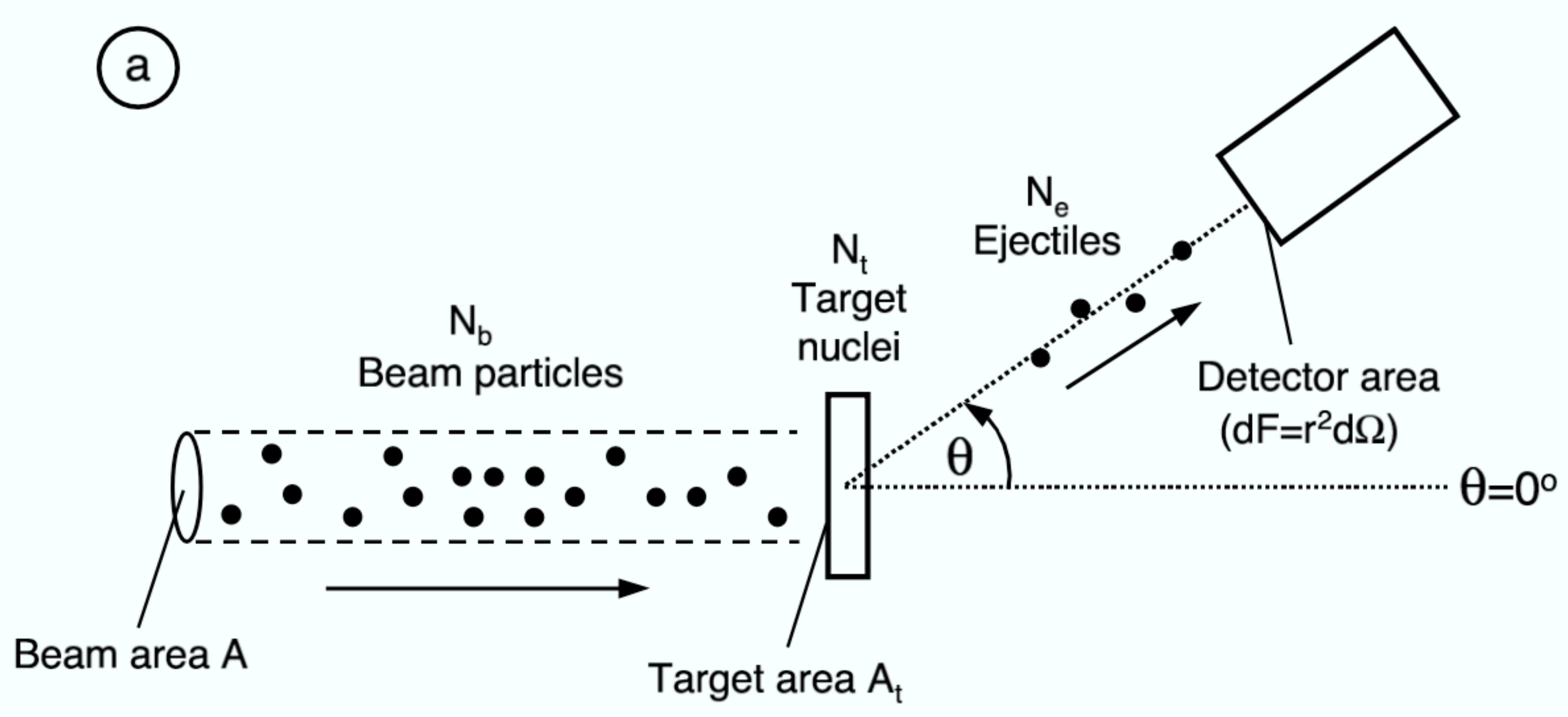

N_r = number of reactions

N_p = number of incoming particles

N_t = number of target particles

How to link this to theoretical values?

Schrödinger Equation (1)

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(r)\right]\psi(r) = E\psi(r)$$

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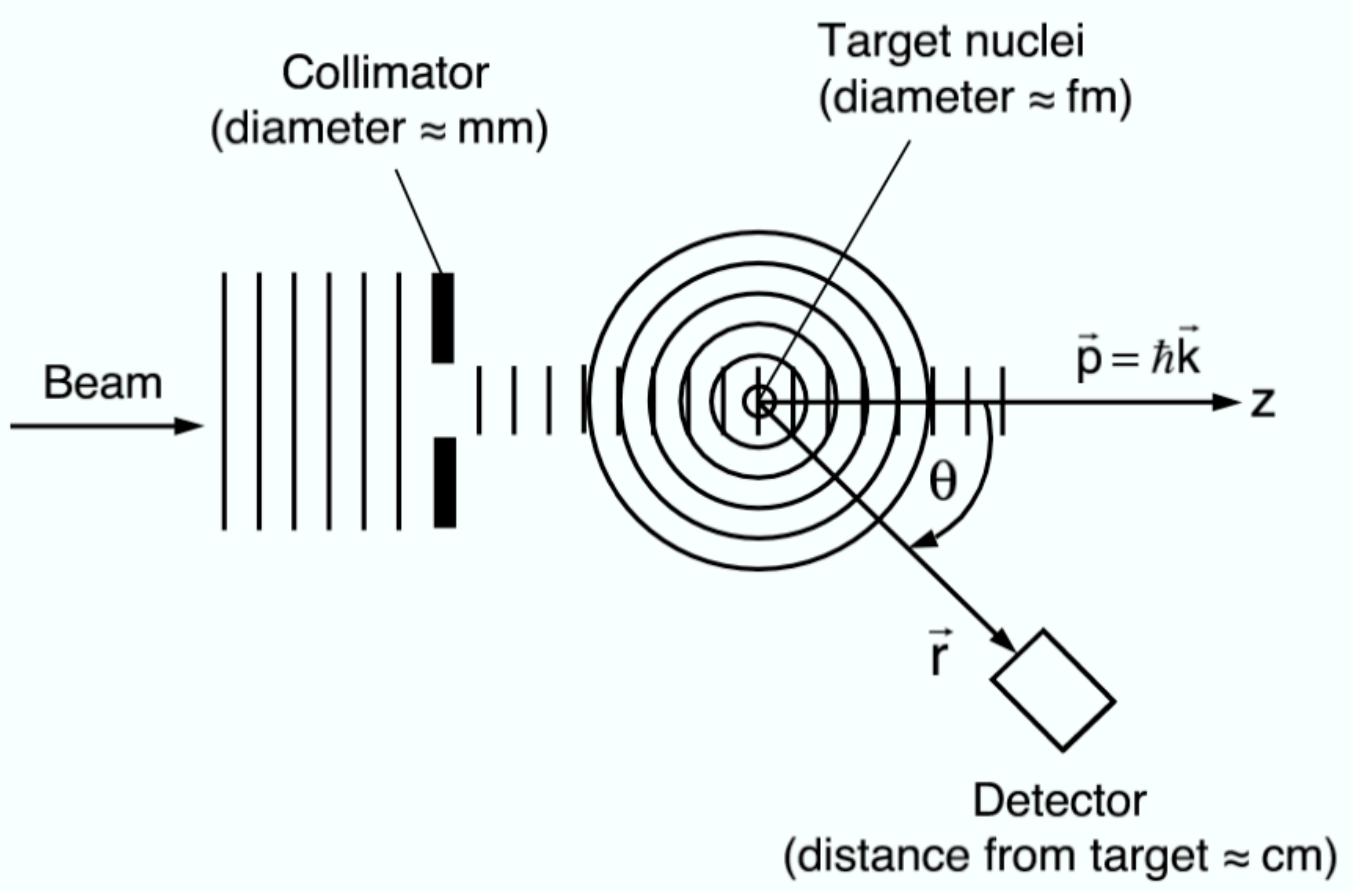
For $r \to \infty$ we can obtain a solution for **generic** $V(r)$:

$$\psi(r) = N\left[e^{ikr} + f(\theta)\frac{e^{ikr}}{r} \right]$$



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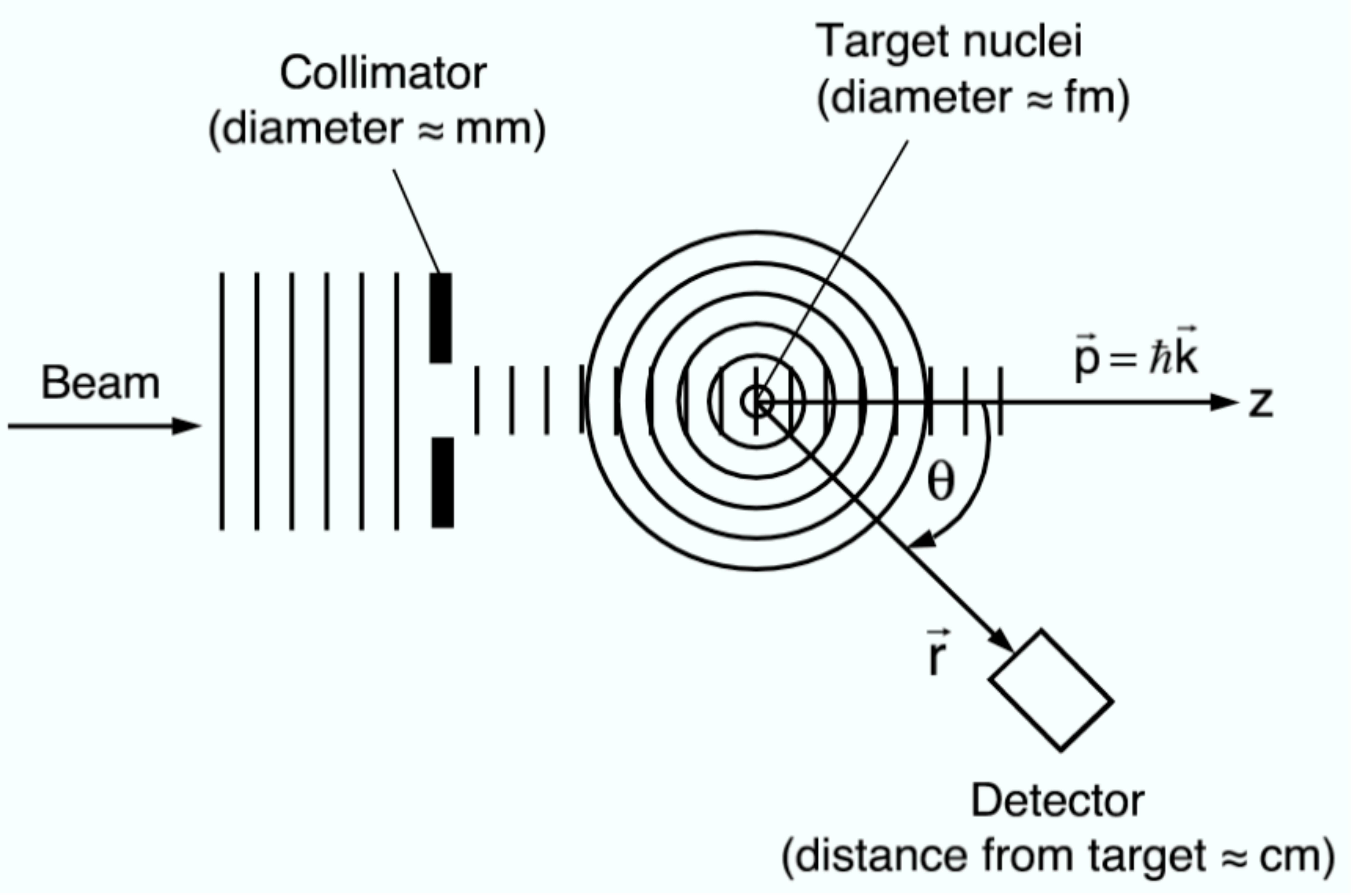
$$\psi(r) = N\Big[\underbrace{e^{ikr}}_{\psi_i(r)} + f(\theta)\underbrace{\frac{e^{ikr}}{r}}_{\psi_o(r)}\Big]$$

Incoming Plane Wave

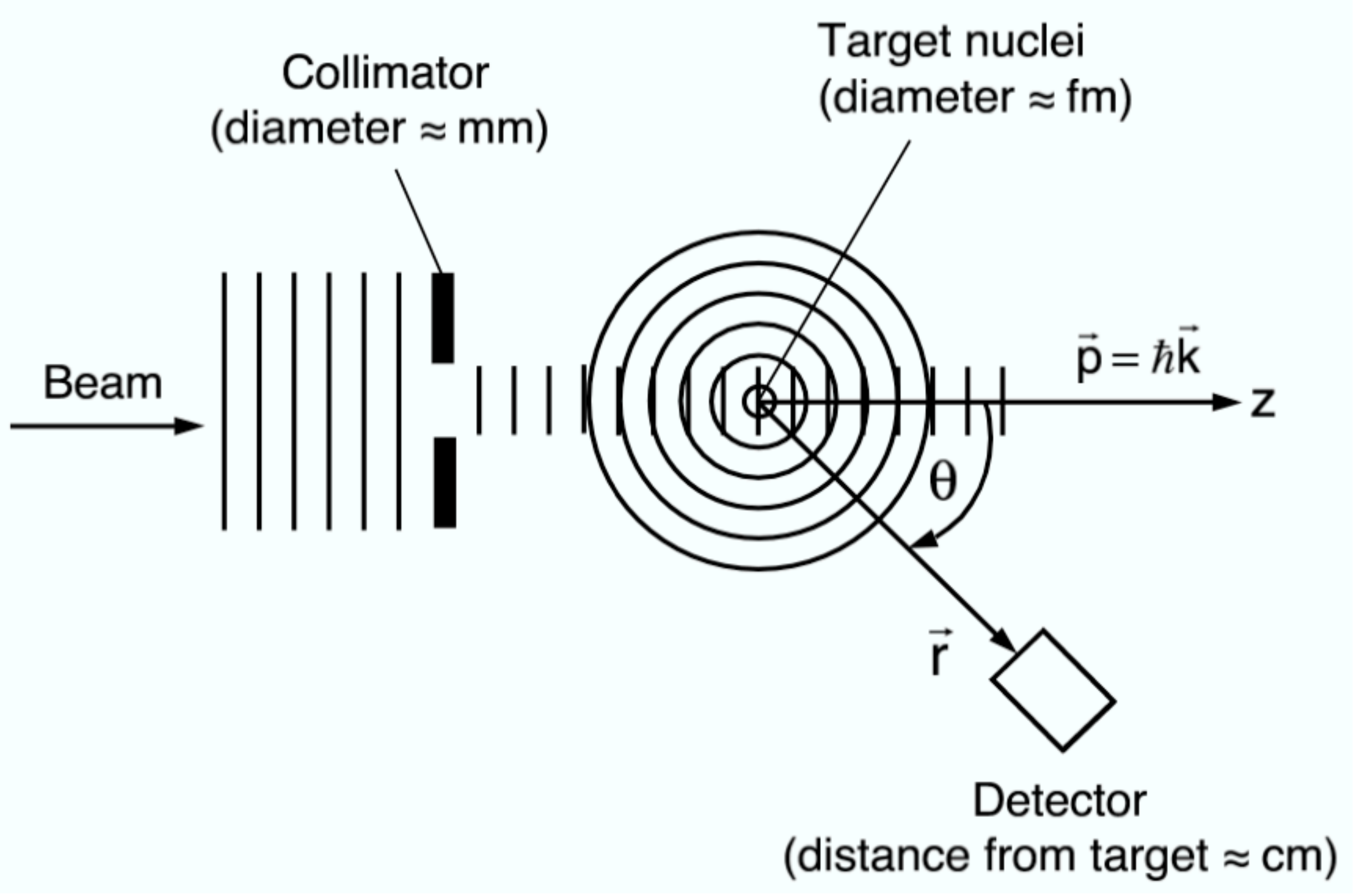
Outgoing Spherical Wave



Scattering Amplitude

Incoming current density: $j_i = v_i |\psi_i(r)|^2 \longrightarrow j_i = v_i N^2$

Outgoing current density: $j_o = v_o |\psi_o(r)|^2 \longrightarrow j_o = v_o N^2 |f(\theta)|^2 \frac{1}{r^2}$



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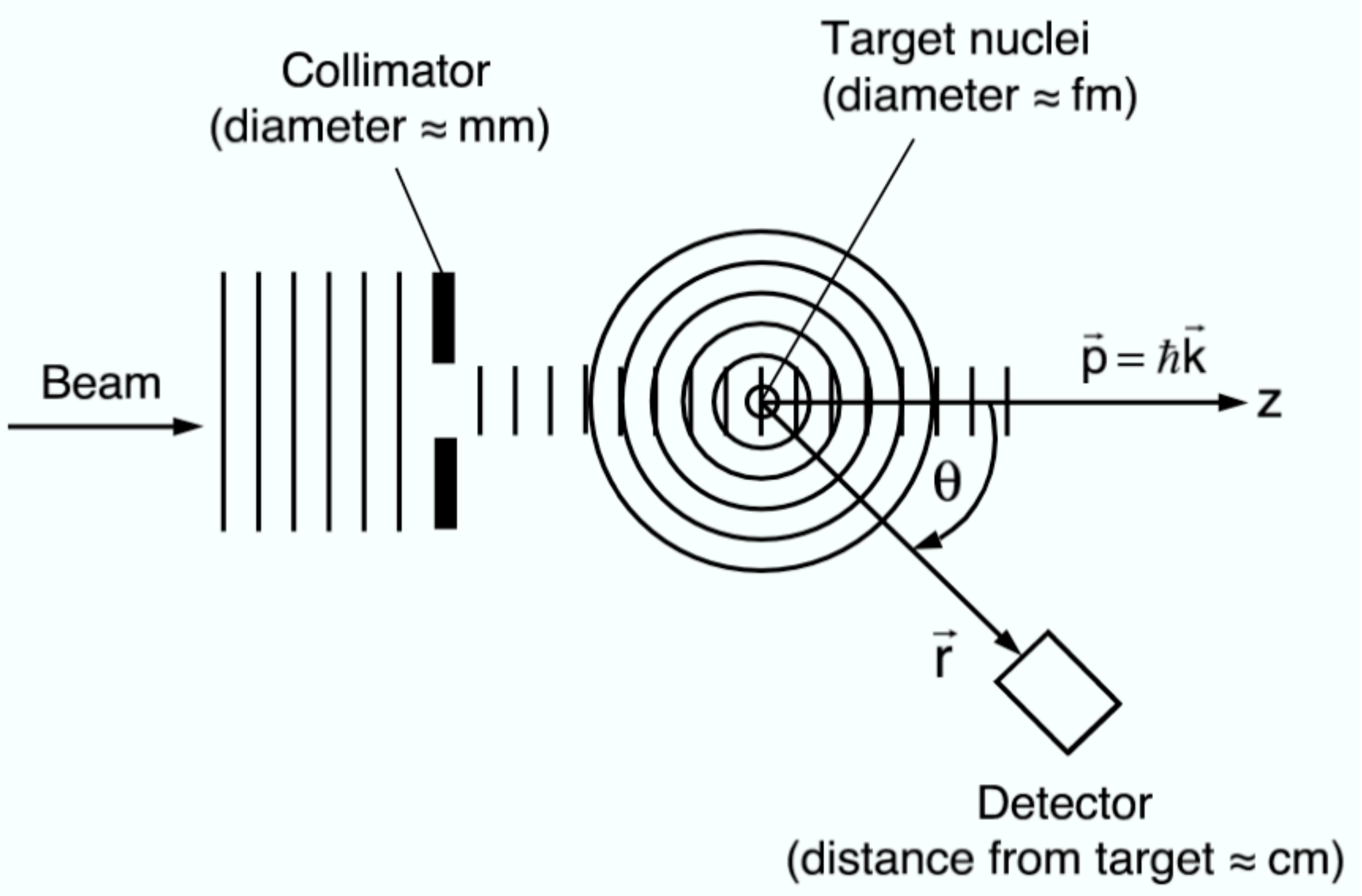
$v_i = v_o$ for **elastic scattering**

$$\boxed{\frac{d\sigma}{d\Omega} = \frac{j_o r^2}{j_i} = |f(\theta)|^2}$$

Differential Cross Section
=
Scattering Amplitude



Schrödinger Equation (2)

$$\frac{d^2u}{dr^2} + \frac{2m}{\hbar^2}\left[E - V(r) - \frac{l(l+1)\hbar^2}{2mr^2}\right]u = 0$$

What is the effect of the potential on the waveform?

Schrödinger Equation (2)

$$\frac{d^2u}{dr^2} + \frac{2m}{\hbar^2}\left[E - V(r) - \frac{l(l+1)\hbar^2}{2mr^2}\right]u = 0$$

$V(r) = 0,\, r \to \infty\colon\ u_l^{f.p.} = \sin(kr - l\frac{\pi}{2})$ ***spherical Bessel function***

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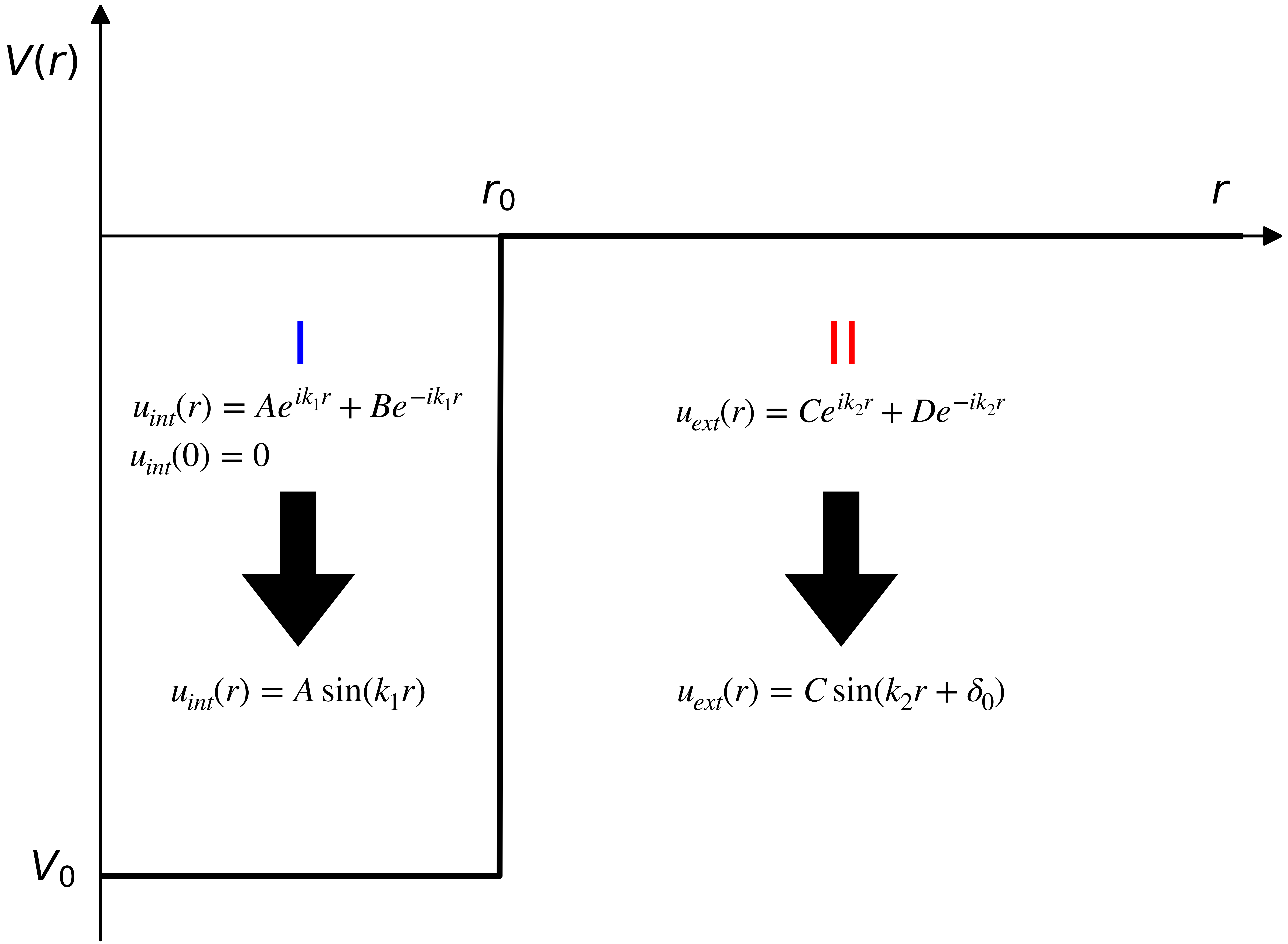
$V(r) \neq 0,\ r \to \infty$: $u_l = \sin(kr - l\frac{\pi}{2} + \delta_l)$ ⟶ differs by a **phase shift** δ_l

$$\boxed{\left(\frac{d\sigma}{d\Omega}\right)_{el} = \frac{1}{k^2}\sin^2\delta}$$

Square-Well Potential (1)



Continuity Condition

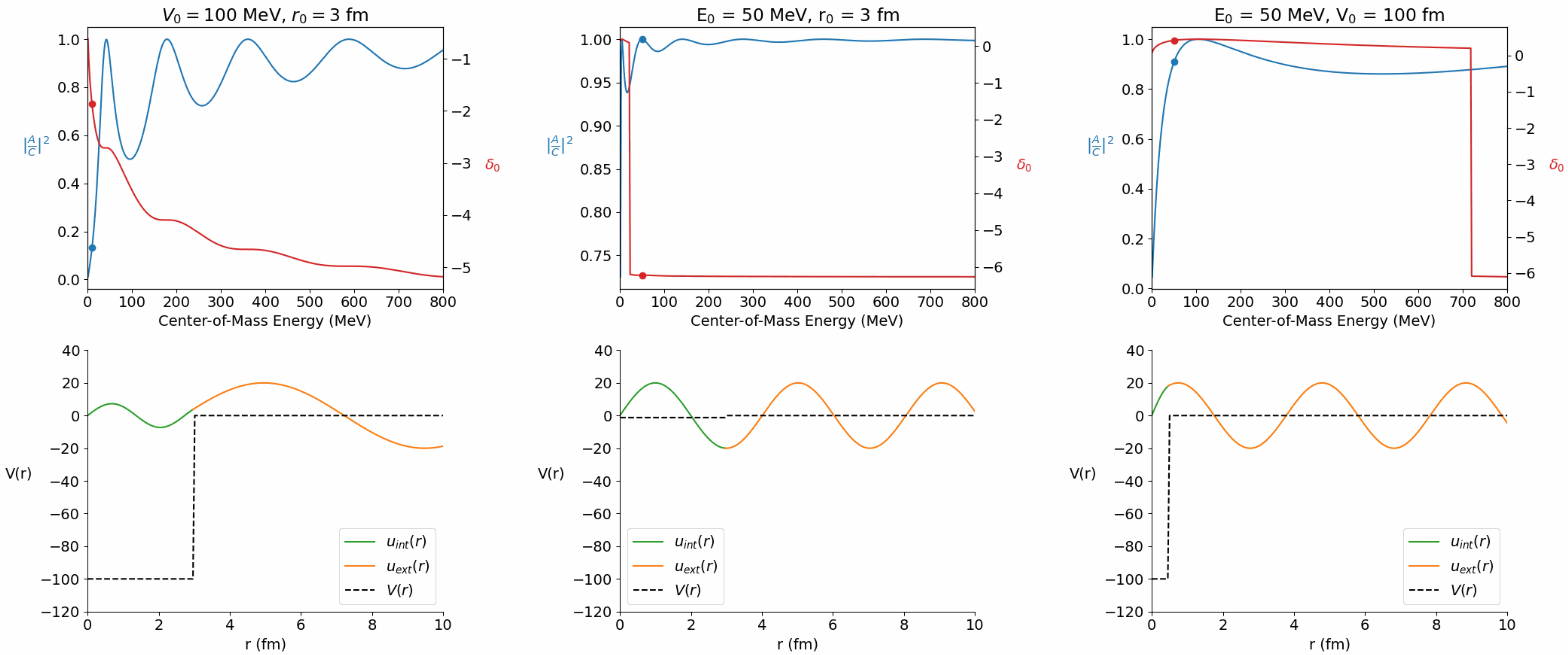
$$
\begin{cases}
u_{int}(r_0) = u_{ext}(r_0) \\[1ex]
\dfrac{du_{int}}{dr}(r_0) = \dfrac{du_{ext}}{dr}(r_0)
\end{cases}
$$

$$\downarrow$$

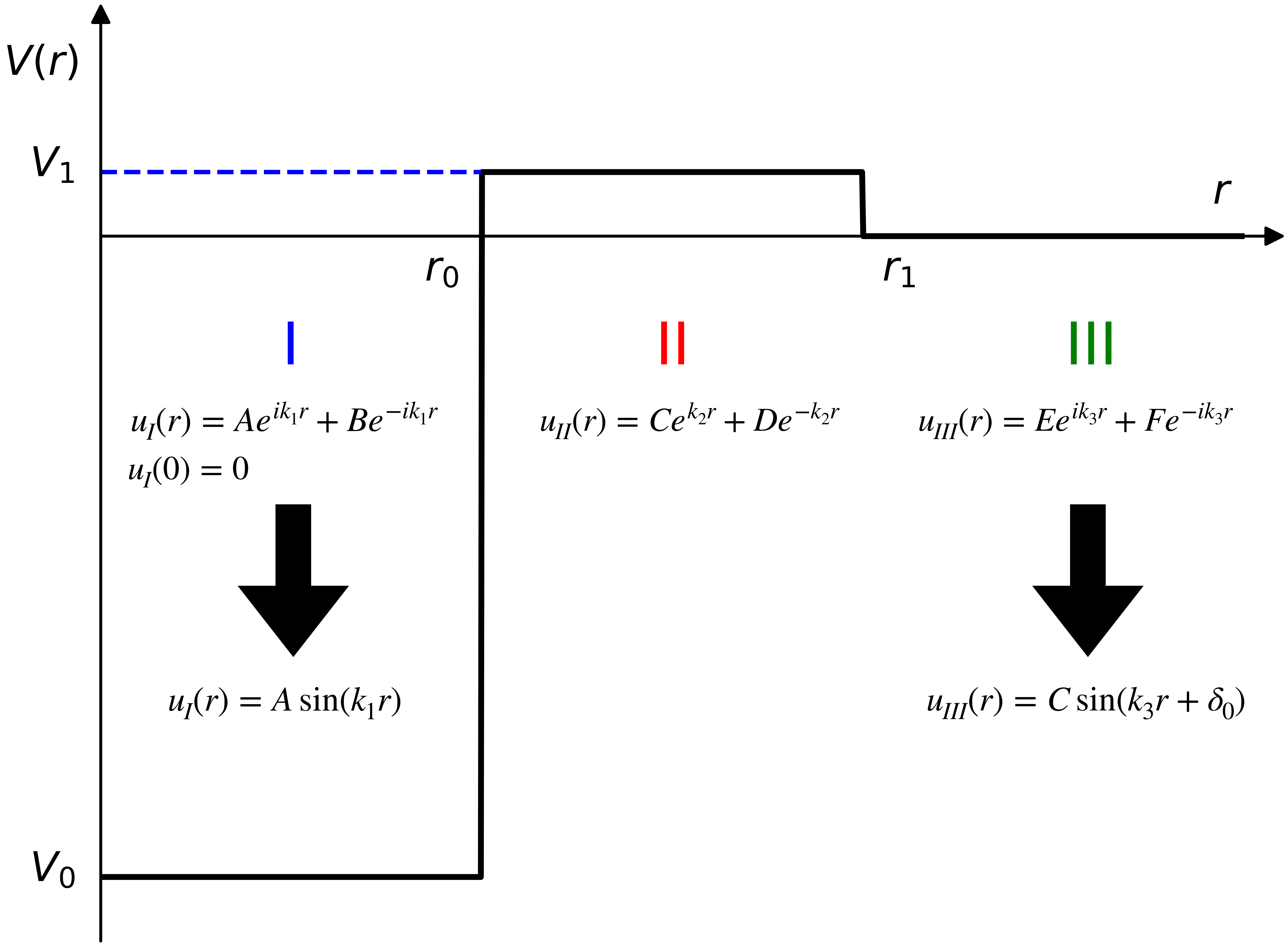
It is possible to solve it for $\left|\dfrac{A}{C}\right|$ and δ_0

Square-Well Potential (2)

Varying CoM Energy | *Varying Potential Depth* | *Varying Potential Radius*



Square-Well Barrier (1)



Continuity Condition

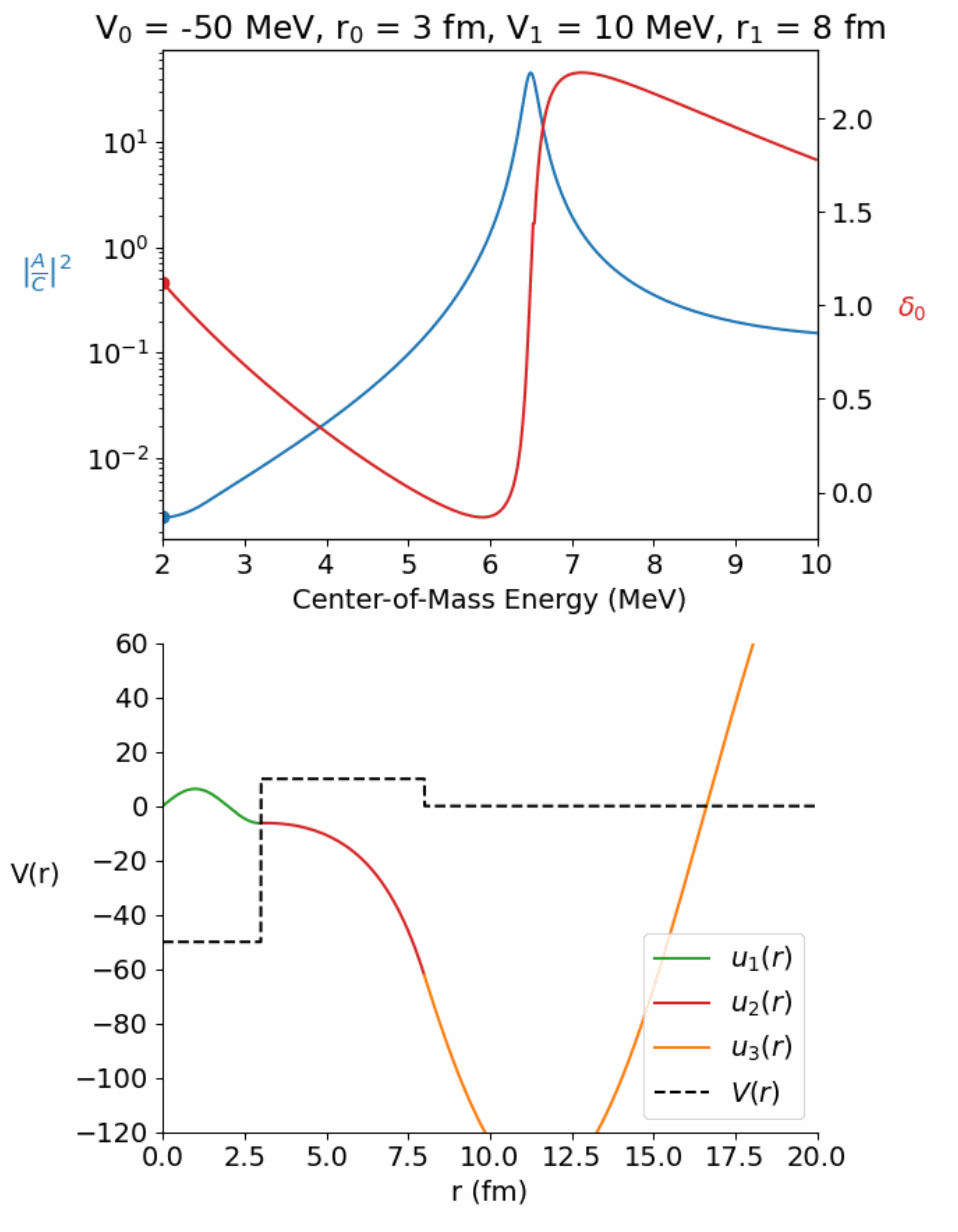
$$
\begin{cases}
u_I(r_0) = u_{II}(r_0) \\
\dfrac{du_I}{dr}(r_0) = \dfrac{du_{II}}{dr}(r_0) \\
u_{II}(r_1) = u_{III}(r_1) \\
\dfrac{du_{II}}{dr}(r_1) = \dfrac{du_{III}}{dr}(r_1)
\end{cases}
$$

$\downarrow$

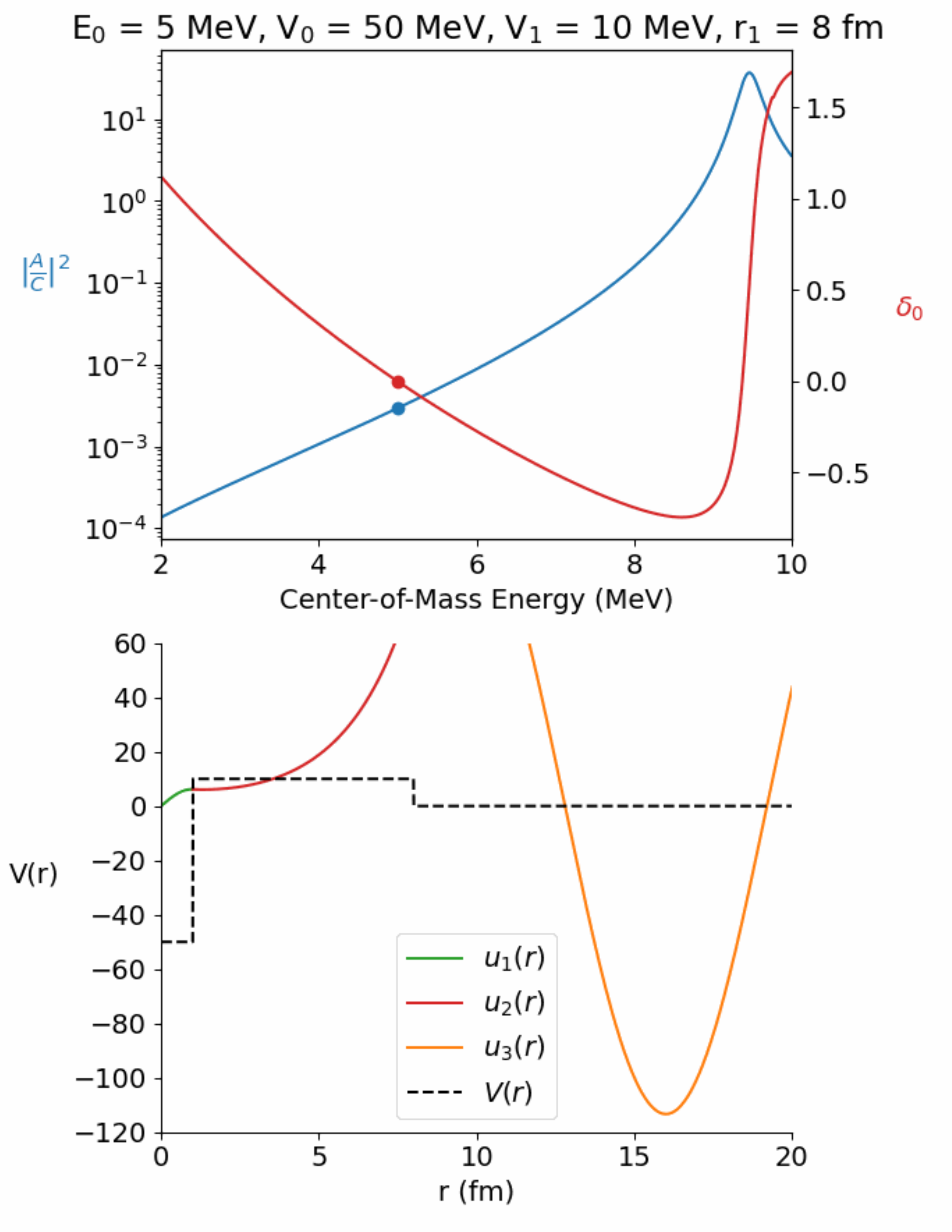
It is possible to solve it for $|\dfrac{A}{F}|$ and δ_0

Square-Well Barrier (2)

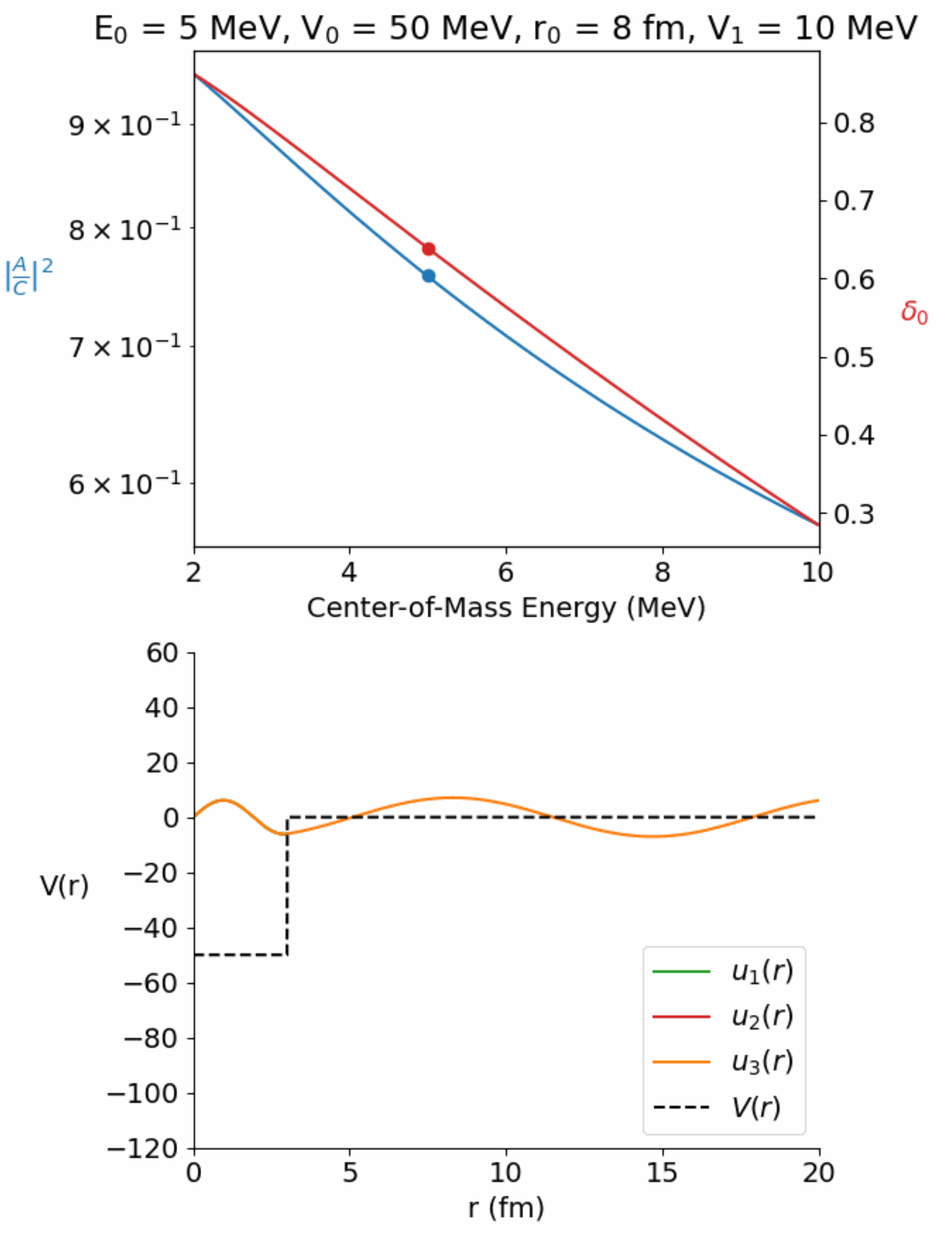
Varying CoM Energy



Varying Potential Radius

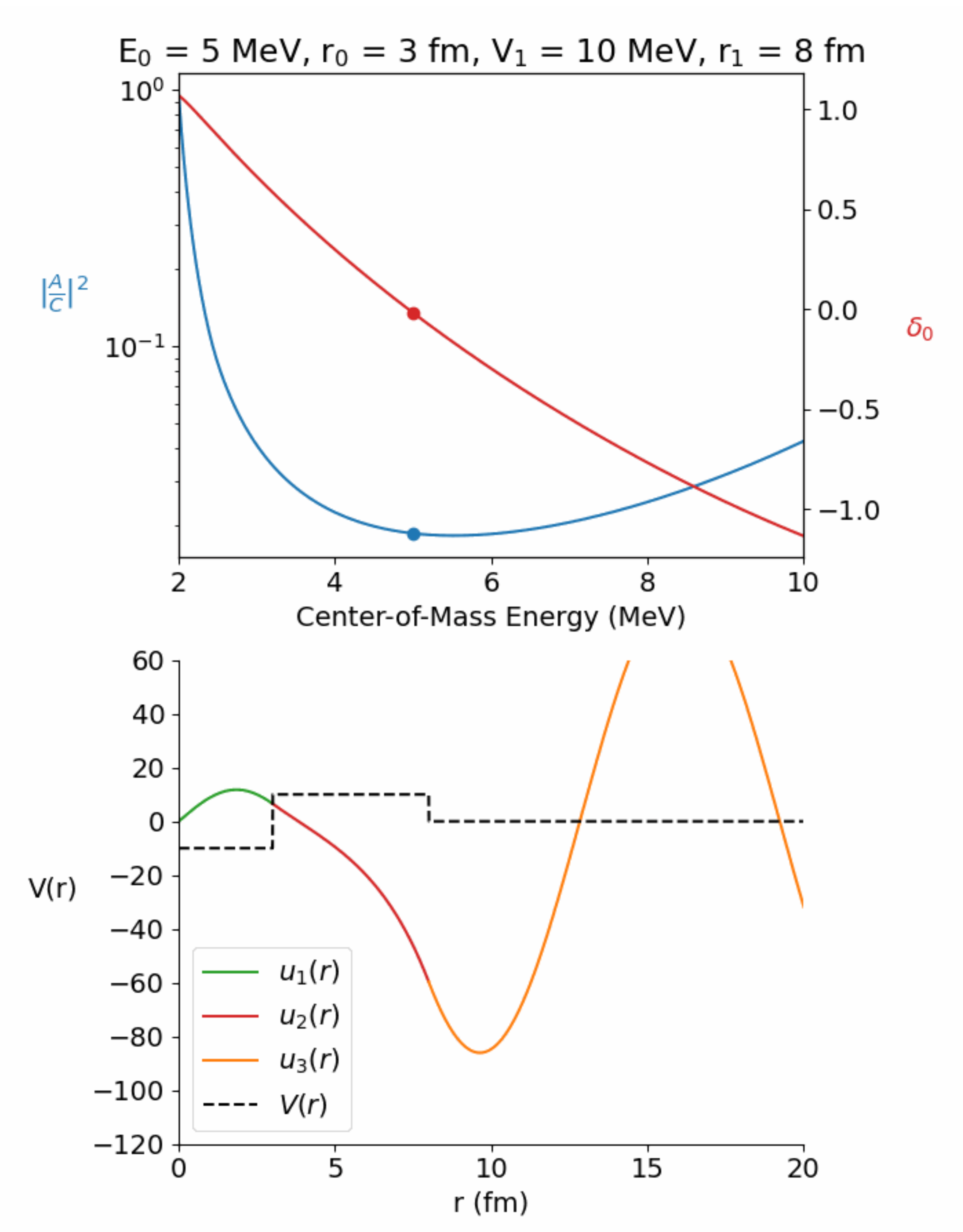


Varying Barrier Radius

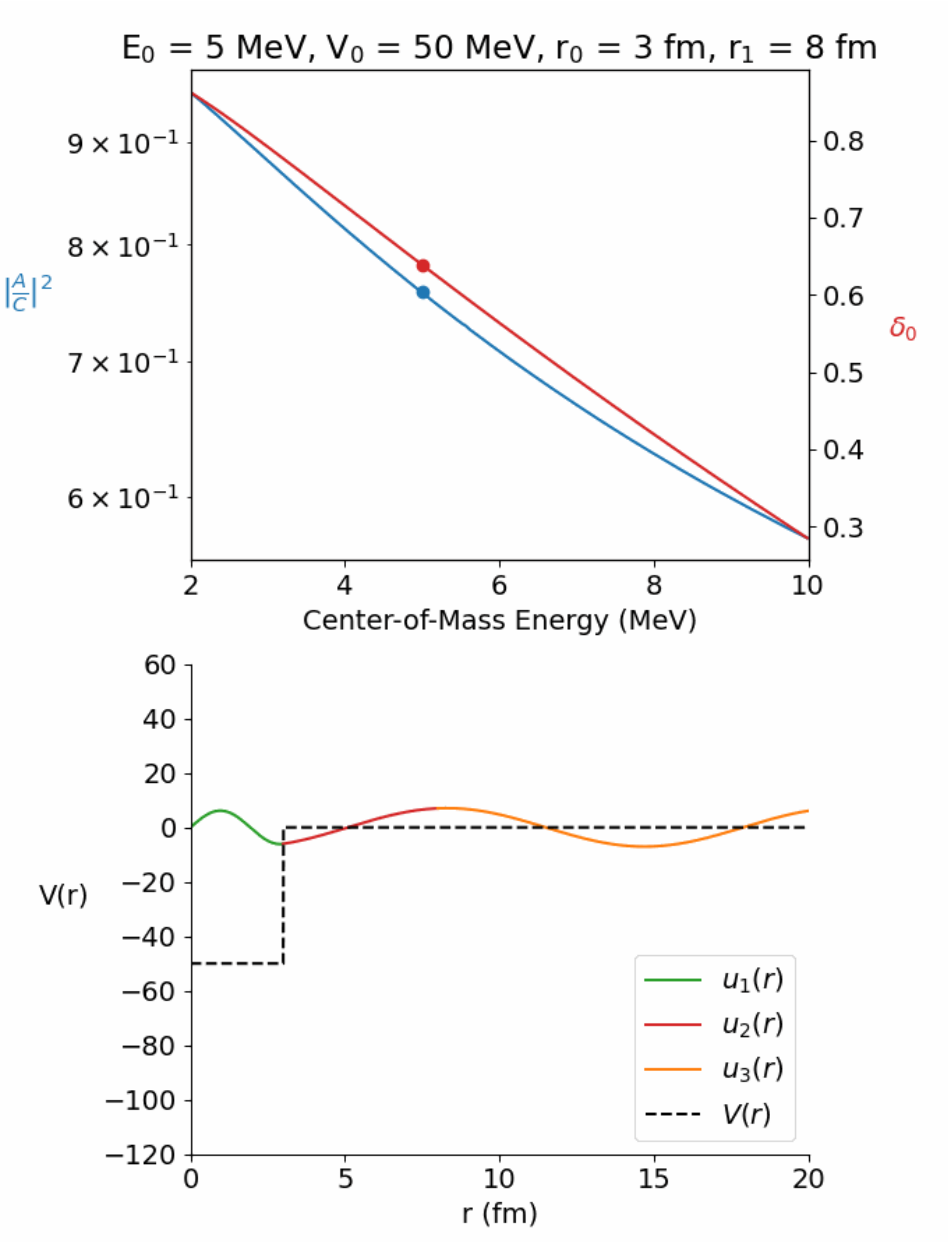


Square-Well Barrier (3)

Varying Potential Depth



Varying Barrier Height



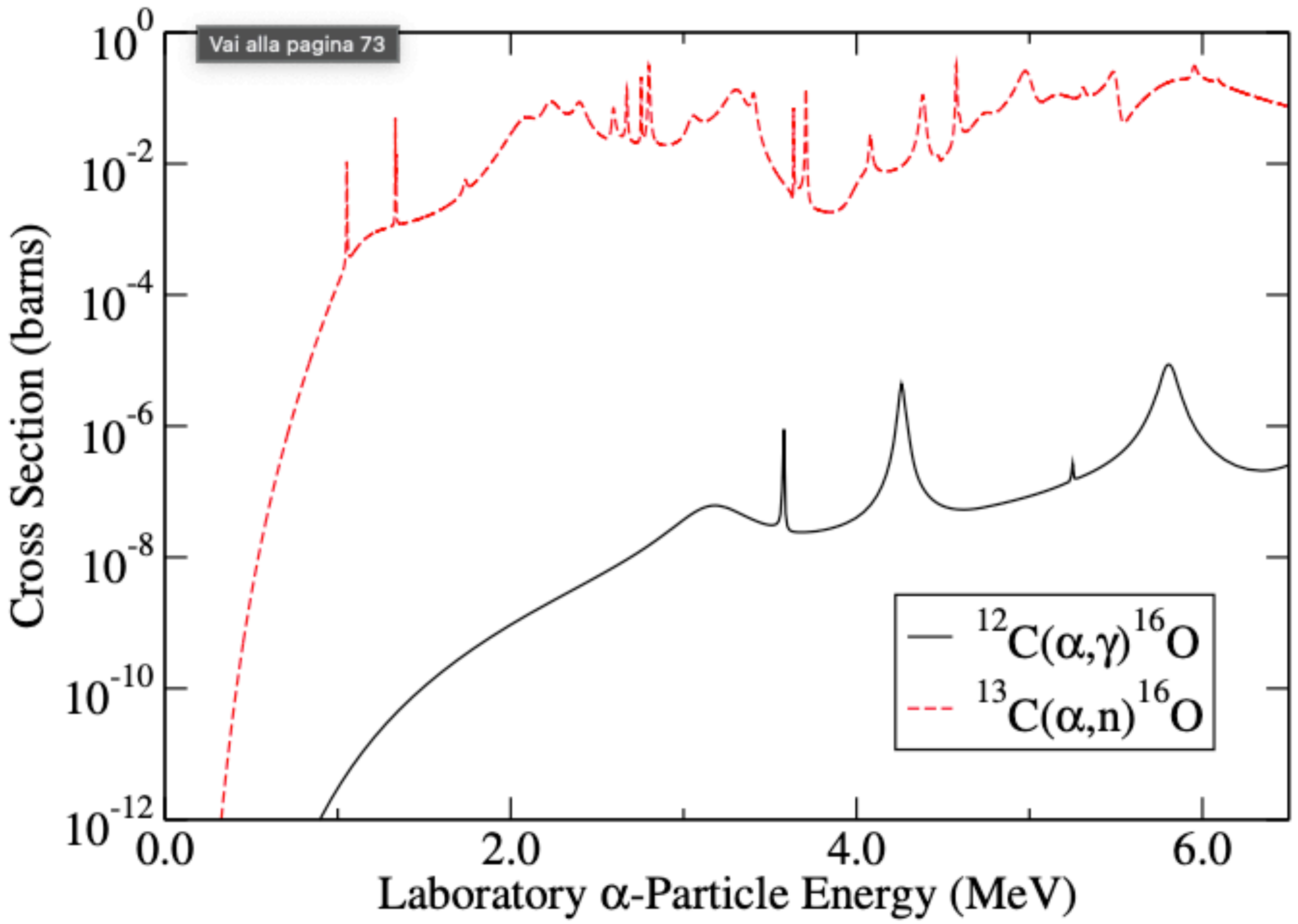
Calculating Cross Section

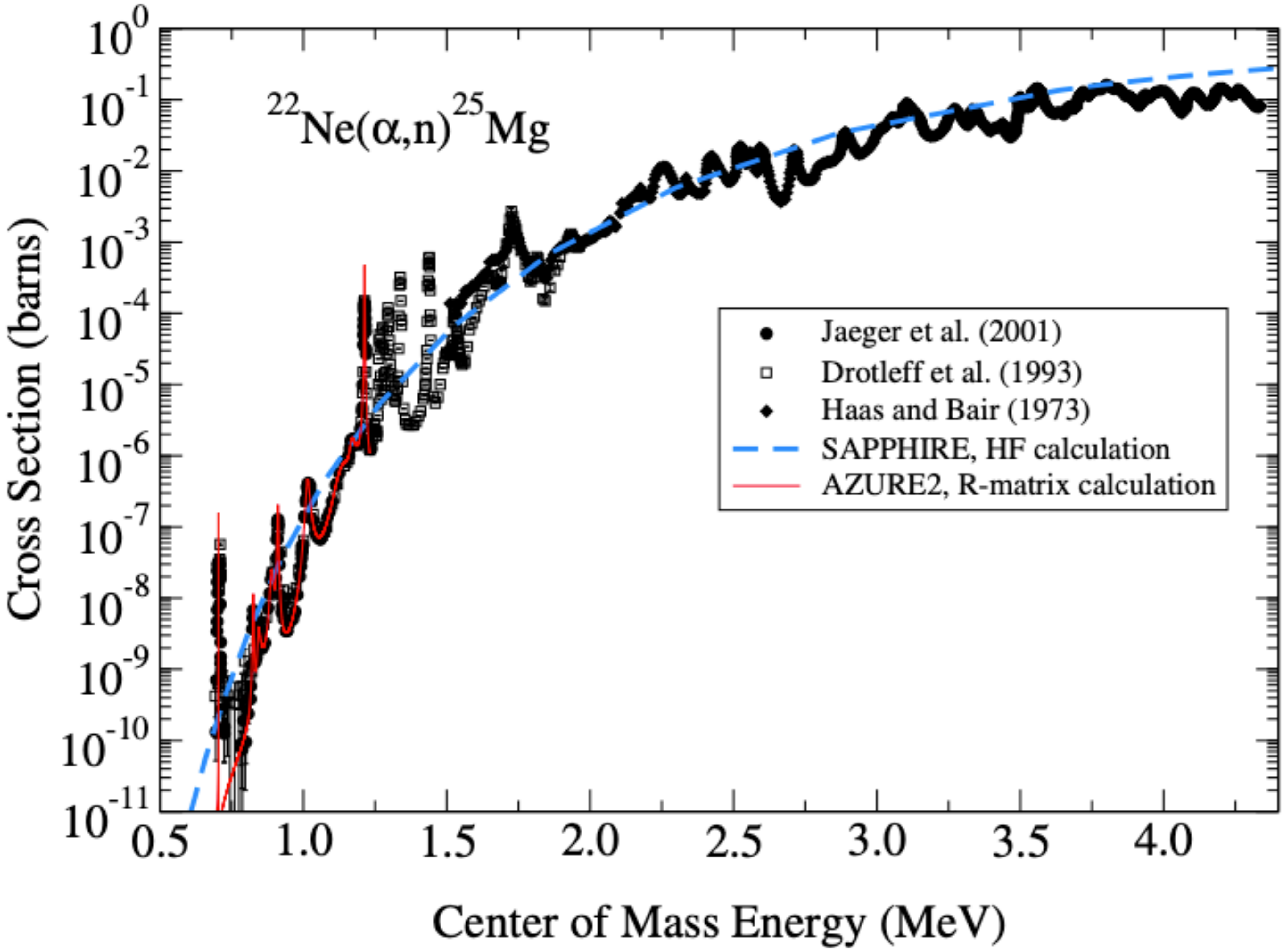
$$\boxed{\frac{d\sigma}{d\Omega} = \frac{j_o r^2}{j_i} = |f(\theta)|^2}$$

→ We can try to calculate the cross section…

See Jupyter Notebooks

Measuring Cross Section





Many more resonances than previous calculations

Single-Particle Limit

Conclusion: single-particle models are not able to describe the real cross sections

Problem: it is computationally unfeasible to introduce individual nucleons

Solution

R-Matrix Theory

R-Matrix Theory

References

Main References

- Lane and Thomas (1958), doi.org/10.1103/RevModPhys.30.257
- Descouvemont and Baye (2010), arxiv.org/abs/1001.0678v1
- Brune (2004), arxiv.org/abs/nucl-th/0502087v1

AZURE2

- Azuma et al. (2010), doi.org/10.1103/PhysRevC.81.045805
- Odell et al. (2022), doi.org/10.3389/fphy.2022.888476

Introduction

- **No reference to specific potential** (no absolute cross section)
- Two regions: **interior** ($r < R_0$) and **exterior** ($r > R_0$)
- Exterior ***observables***: penetration and phase shift
- Interior ***parameters***: reduced widths

Assumptions

1. Well-defined **spherical** surface at $r = R_0$
2. **No nuclear interaction** outside the radius

Logarithmic Derivative (1)

Continuity: $u_l^{in}(R_0) = u_l^{out}(R_0)$ + $\left(\dfrac{du_l^{in}(r)}{dr}\right)_{r=R_0} = \left(\dfrac{du_l^{out}(r)}{dr}\right)_{r=R_0}$

Definition: $f_l = R_0\left(\dfrac{1}{u_l(r)}\dfrac{du_l(r)}{dr}\right)_{r=R_0} = R_0\left(\dfrac{d\ln u_l(r)}{dr}\right)_{r=R_0}$

$$\downarrow$$

$$f_l(u_l^{in}) = f_l(u_l^{out})$$

Logarithmic Derivative (2)

Let's take the wave function in the exterior region r > R_0:

$$\psi_{out} = Ae^{ikr} + Be^{-ikr} = \ldots = \frac{1}{kr} e^{i\delta_0} \sin(kr + \delta_0) = \frac{u_{out}(r)}{r}$$

Now we can calculate f_0 and solve it for $e^{i2\delta_0}$:

$$e^{i2\delta_0} = \frac{f_0 + ikR_0}{f_0 - ikR_0} e^{-2ikR_0}$$

→ It is possible to calculate the cross section!

$$\sigma_0 = \frac{\pi}{k^2} \frac{-4kR_0 \mathrm{Im}\, f_0}{(\mathrm{Re}\, f_0)^2 + (\mathrm{Im}\, f_0 + -kR)^2}$$

Logarithmic Derivative (3)

Missing Ingredient: logarithmic derivative at the boundary f_0

1. Approximate interior wave function in the **closest vicinity of the boundary**

$$u_I(r) = Ae^{iKr} + Be^{-iKr}$$

2. Introduce **phase shift** ζ and **absorption coefficient** $q \geq 0$

$$A = Be^{2i\zeta}e^{-2q}$$

3. Calculate the logarithmic derivative

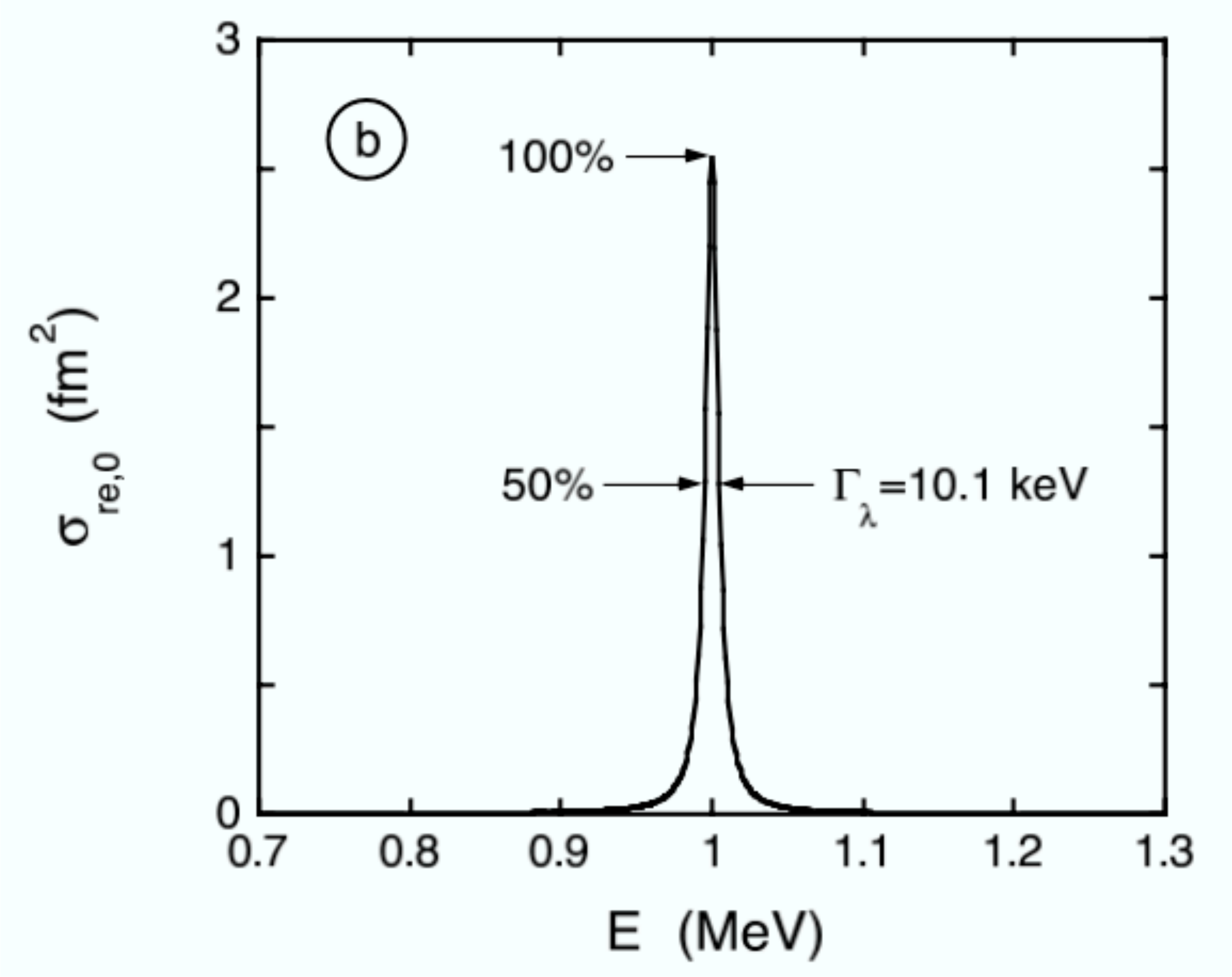
4. Expand the derivative around the resonance, E_λ, assuming $q \sim 0$

Logarithmic Derivative (4)

$$\sigma_0 = \frac{\pi}{k^2} \frac{\dfrac{(2kR)(2qKR)}{(\partial f_0/\partial E)_{E_\lambda,\ q=0}}}{(E - E_\lambda)^2 + \dfrac{(qKR + kR)^2}{(\partial f_0/\partial E)_{E_\lambda,\ q=0}}}$$

Breit-Wigner Formula

$$\sigma_0 = \frac{\pi}{k^2} \frac{\Gamma_{\lambda e}\Gamma_{\lambda r}}{(E - E_\lambda)^2 + \Gamma_\lambda^2/4}$$



$$\Gamma_{\lambda e} = -\frac{2kR}{(\partial f_0/\partial E)_{E_\lambda,\ q=0}}$$ **Particle Width**

$$\Gamma_{\lambda r} = -\frac{2qKR}{(\partial f_0/\partial E)_{E_\lambda,\ q=0}}$$ **Reaction Width**

$$\Gamma_\lambda = \Gamma_{\lambda e} + \Gamma_{\lambda r}$$ **Total Width**

$$\gamma_{\lambda e}^2 = -\left(\frac{\partial f_0}{\partial E}\right)^{-1}_{E_\lambda,\ q=0}$$ **Reduced Width**

R-matrix

If we assume only an **elastic process** ($q = 0$): $f_0 = (E - E_\lambda)\left(\frac{\partial f_0}{\partial E}\right)_{E_\lambda, q=0}$

Then we define the **R-function** as: $\frac{1}{f_0} = \frac{(\partial f_0/\partial E)^{-1}_{E_\lambda, q=0}}{E - E_\lambda} = \frac{\gamma^2_{\lambda e}}{E - E_\lambda} = \mathscr{R}$

⟶ the value at each E is obtained by **summing over all resonances** λ

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$\longrightarrow$ the value at each E is obtained by **summing over all resonances** λ

Usually **other reaction channels** are present as well, so we define the **R-matrix**:

$$\mathscr{R}_{cc'} = \sum_\lambda \frac{\gamma_{\lambda c}\gamma_{\lambda c'}}{E - E_\lambda}$$

R-matrix Problems

- Channel radius, R_0, is arbitrary and have **no precise physical meaning**

$\longrightarrow$ different radii means **different widths** (but **consistent cross sections**)

$\longrightarrow$ good practice is to put it **slightly bigger** than possible nuclear interaction

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- The widths, γ_λ, depends on boundary conditions

  ⟶ their values can be **unphysical** (i.e. formal) and **imaginary**

  ⟶ only the **Brune boundary condition** gives physical meaning

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  ⟶ their values can be **unphysical** (i.e. formal) and **imaginary**

  ⟶ only the **Brune boundary condition** gives physical meaning

- Not all the resonances can be included due to computational limits

  ⟶ **background levels** (i.e. poles) at high energies are usually inserted

Why and How

Why do we need phenomenology?

1. Usually we can not measure the cross section at astrophysical energies, e.g. **1 - 100 keV range**

2. The only way of getting the cross section is by **extrapolating** the measured data

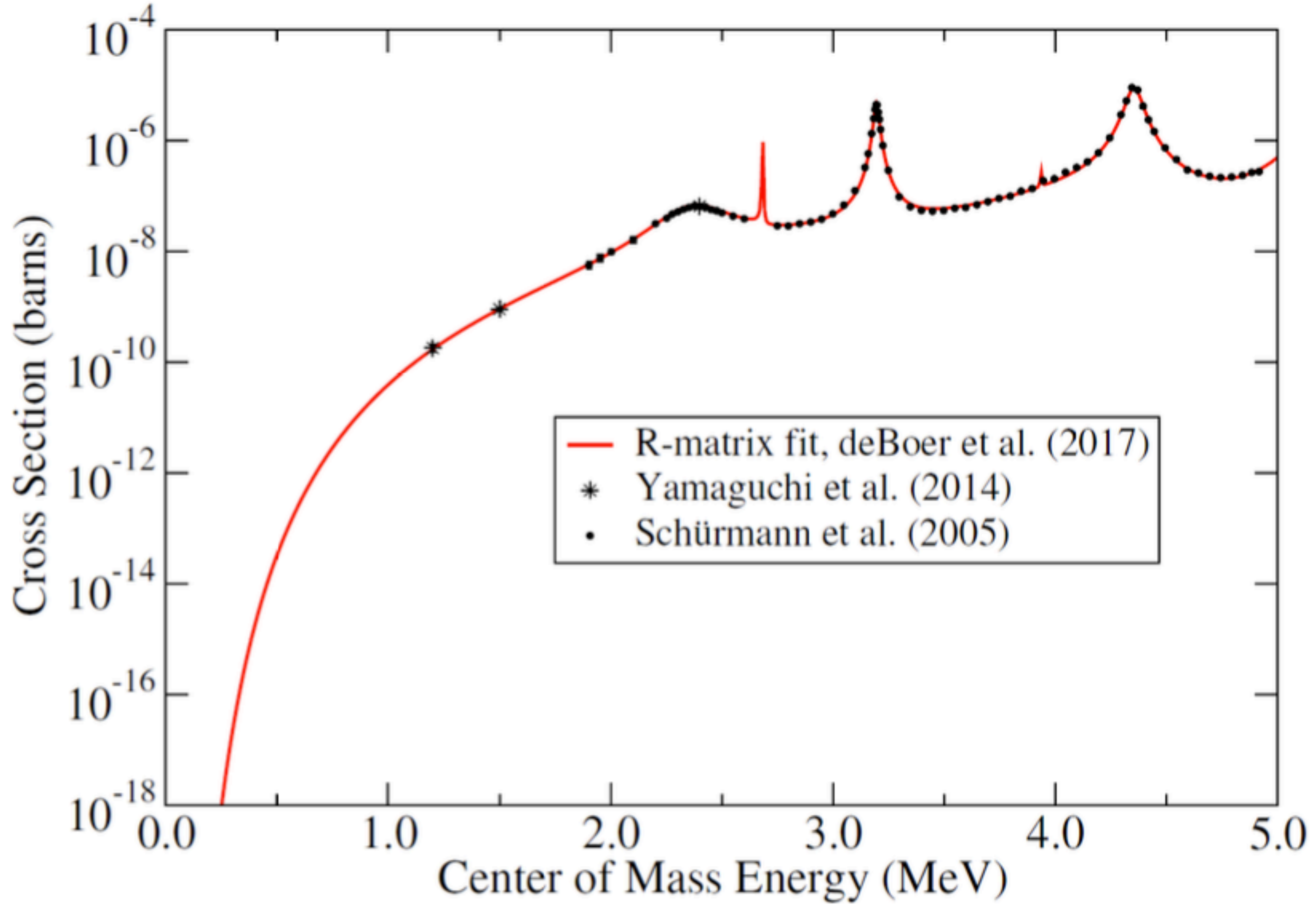
3. R-matrix permits us to use **meaningful physical information** to try to parametrise the cross section

4. It permits to not only use **direct data**, i.e. measured cross sections, but also **indirect data** as spectroscopic factors, decay lifetimes etc.

What do we use it for?

- **Astrophysics**: extrapolate a charged particle cross section from some higher energy region that is experimental accessible down in energy to a region that can't be measured but is important for stellar environments

$^{12}C(\alpha,\gamma)^{16}O$



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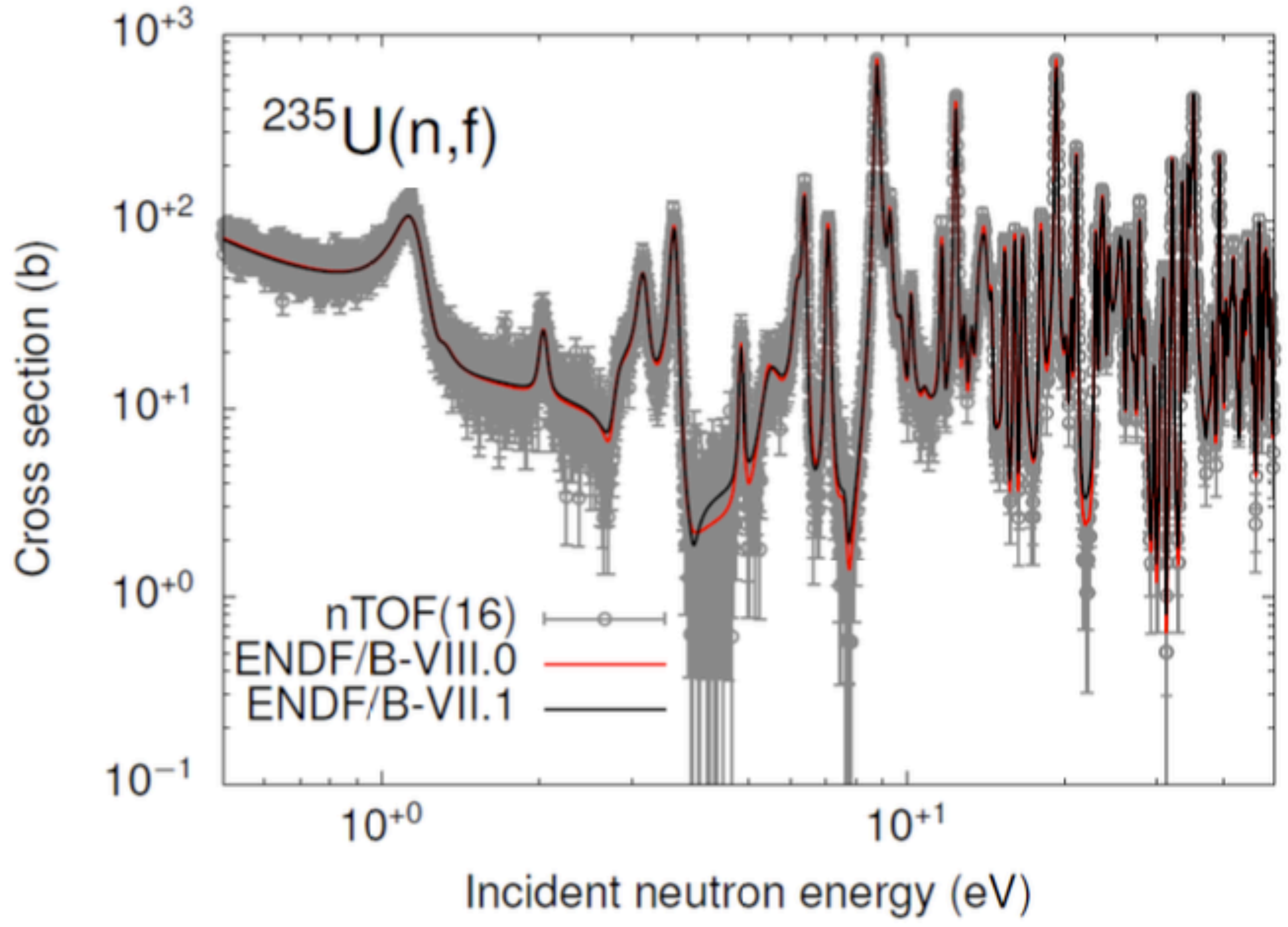
- **Nuclear Engineering:** simultaneously evaluate a broad set of data from different measurements and maybe even through different reaction channels, very important for nuclear safeguards



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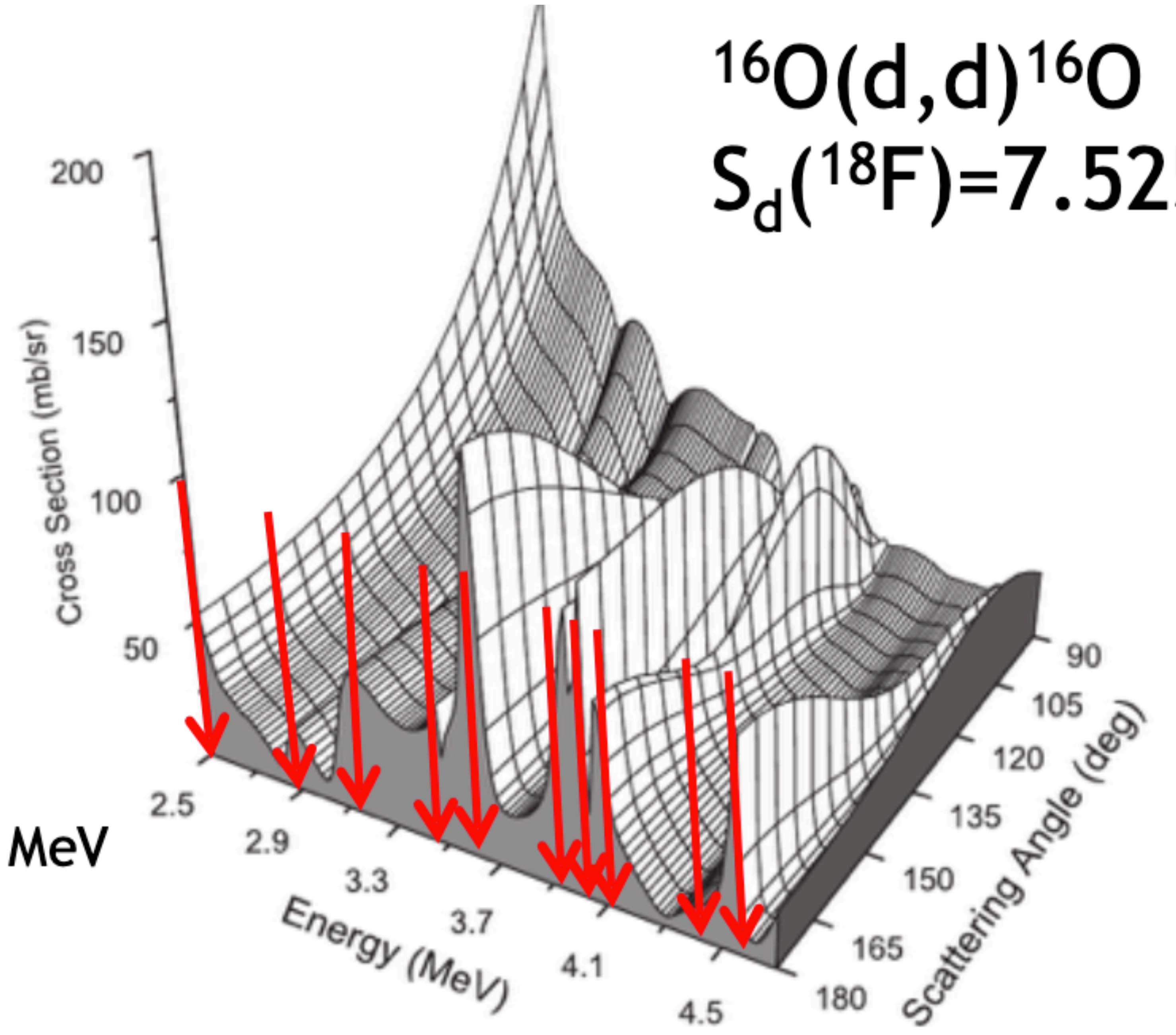
- **Material Studies:** precise evaluation of elastic cross section data at different angles can be used for the study of materials in samples

$^{16}O(d,d)^{16}O$
$S_d(^{18}F)=7.525$ MeV



$E_x=9.747$ MeV

$E_x=11.525$ MeV

What determines the cross section?

Components	Type of measurement
• Tails of higher resonances	Direct, Indirect
• Sub-threshold resonances	Lifetime, Coulex, Indirect
• Non-resonant (direct) capture	Direct, Transfer

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Components	Type of measurement
• Tails of higher resonances	Direct, Indirect
• Sub-threshold resonances	Lifetime, Coulex, Indirect
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Direct: measure directly the cross section, angular distribution etc.

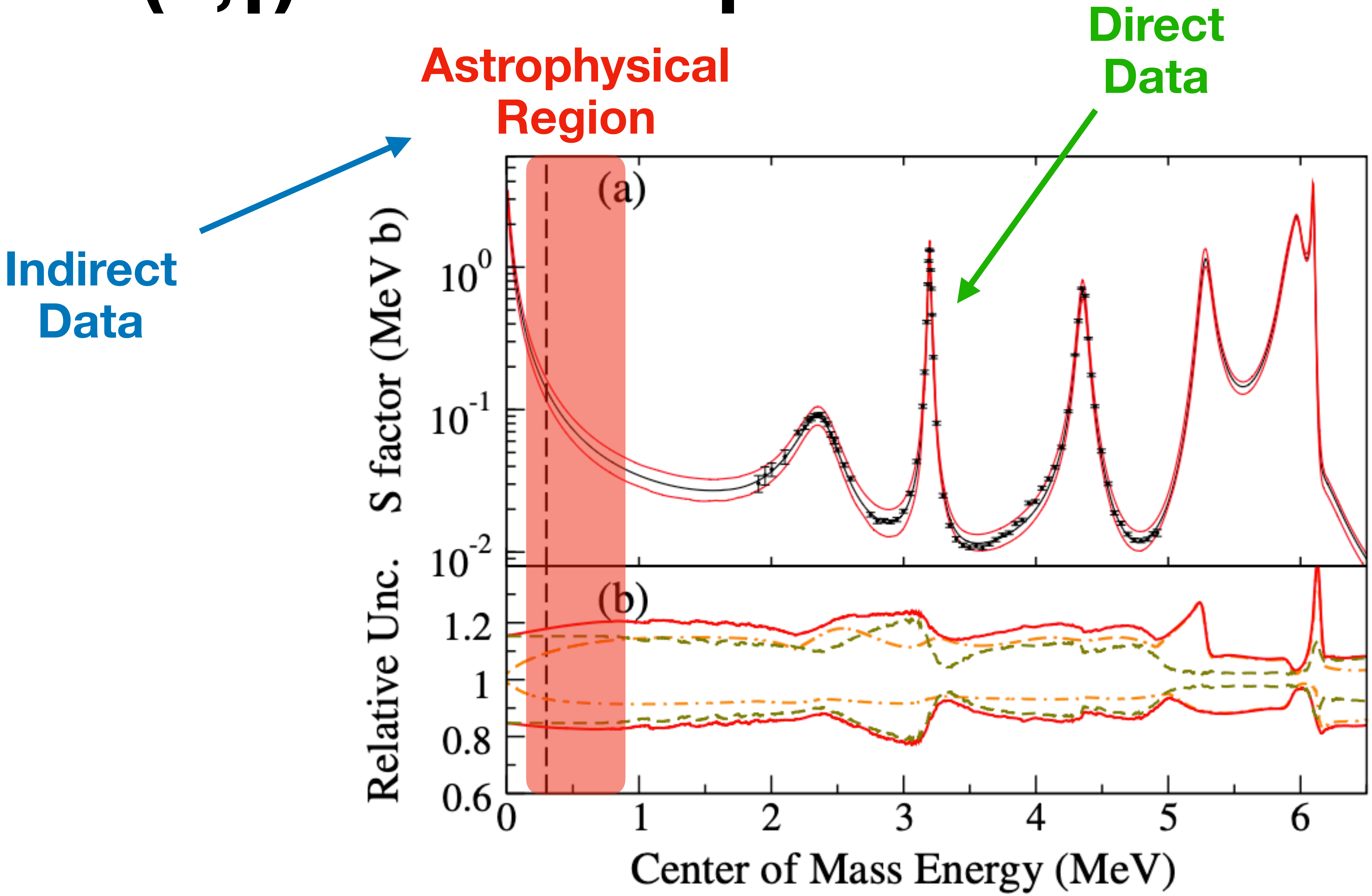
Indirect: measure the same excited state with different reaction channels

Lifetime: measure the lifetime of the state and convert to total width

Transfer: measure the spectroscopic factors for each state

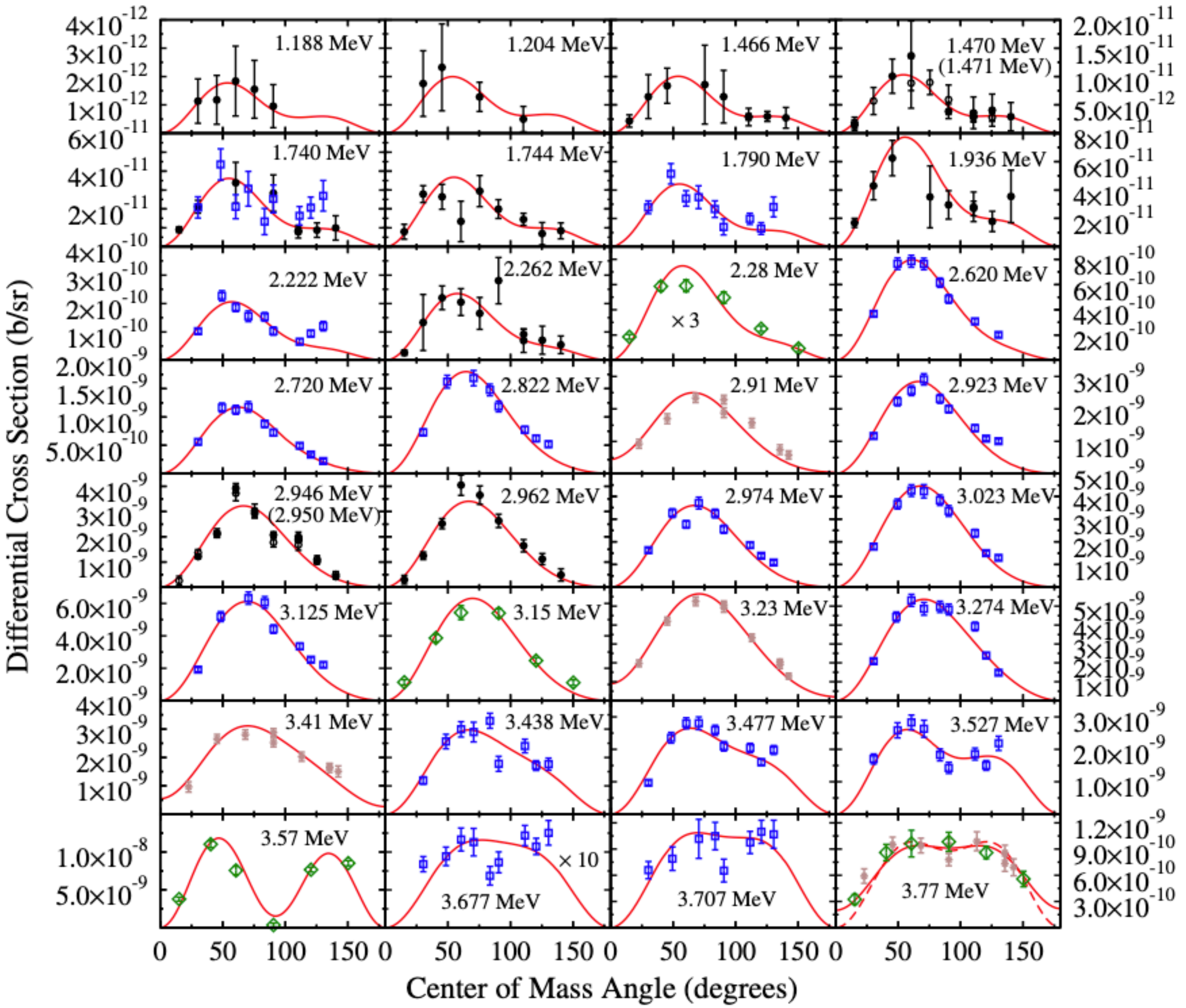
Coulex: measure the transition strength and convert to the total width

$^{12}C(\alpha,\gamma)^{16}O$ - Example



$^{12}C(\alpha,\gamma)^{16}O$ - Example

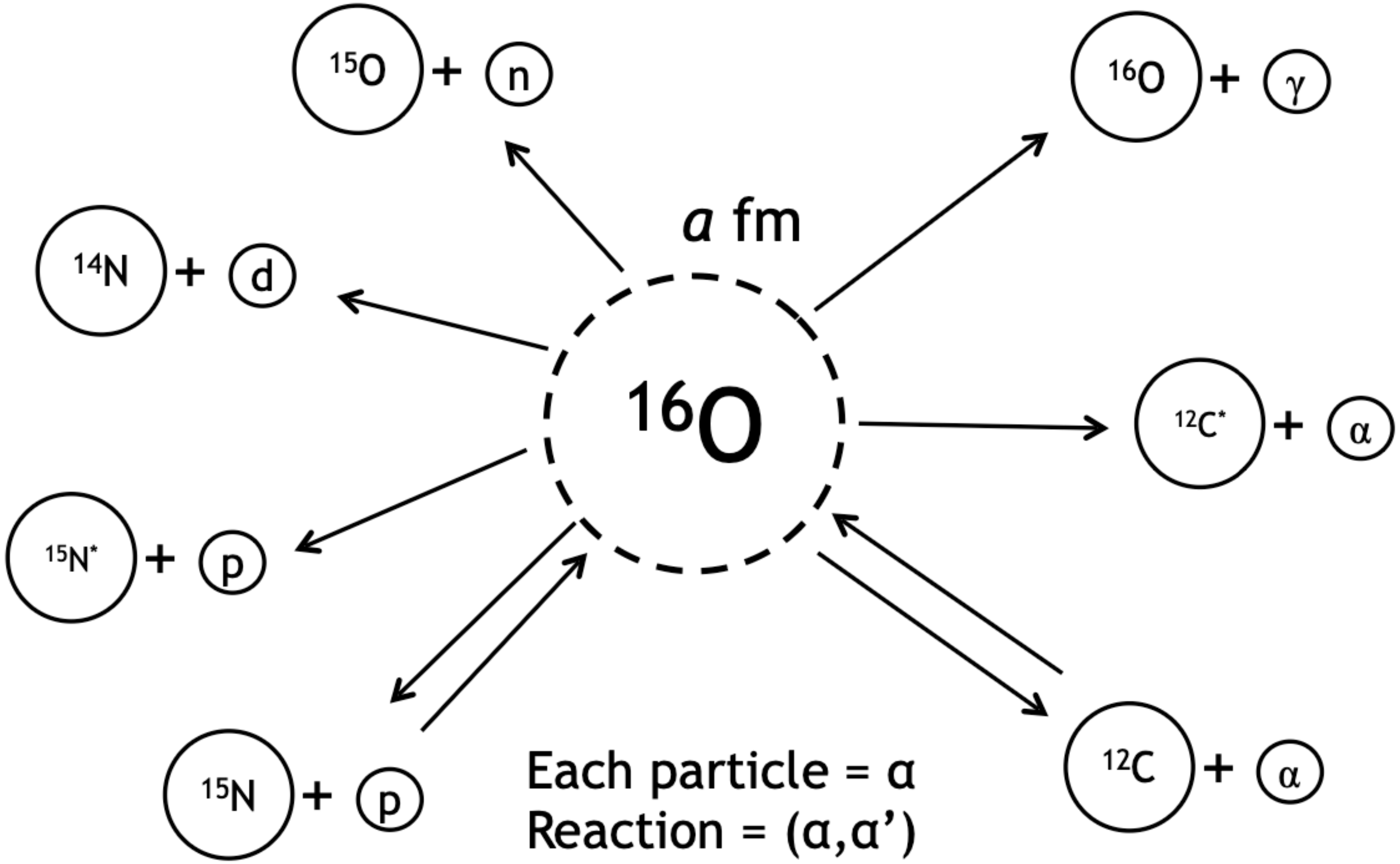
Angular distributions can be used as well



$^{12}C(\alpha,\gamma)^{16}O$ - Example

All of these populate the same compound nucleus

We can retrieve precious physical information from each reaction channel



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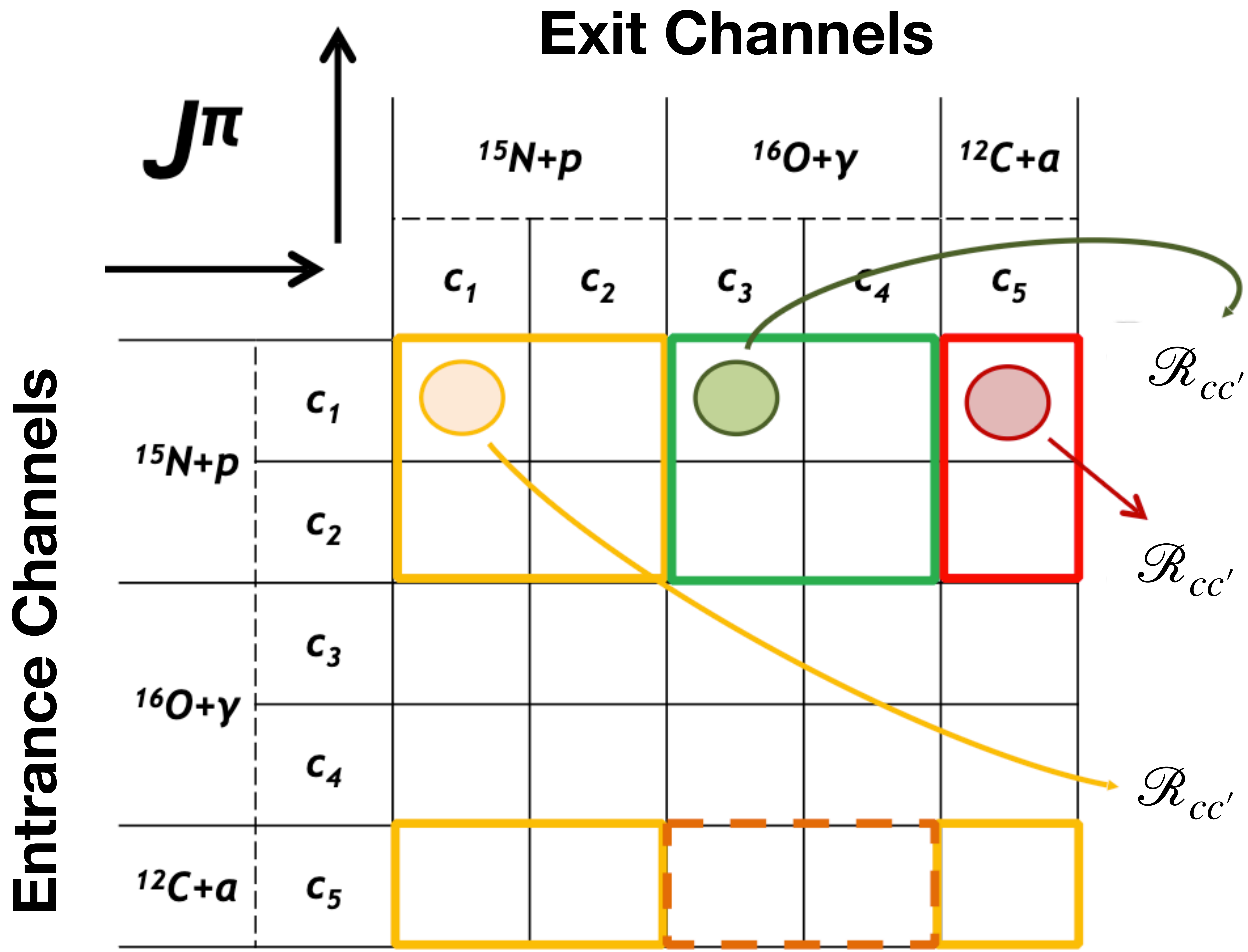


$$\mathcal{R}_{cc'} = \sum_{\lambda} \frac{\gamma_{\lambda c_3}\gamma_{\lambda c_1}}{E - E_\lambda}$$

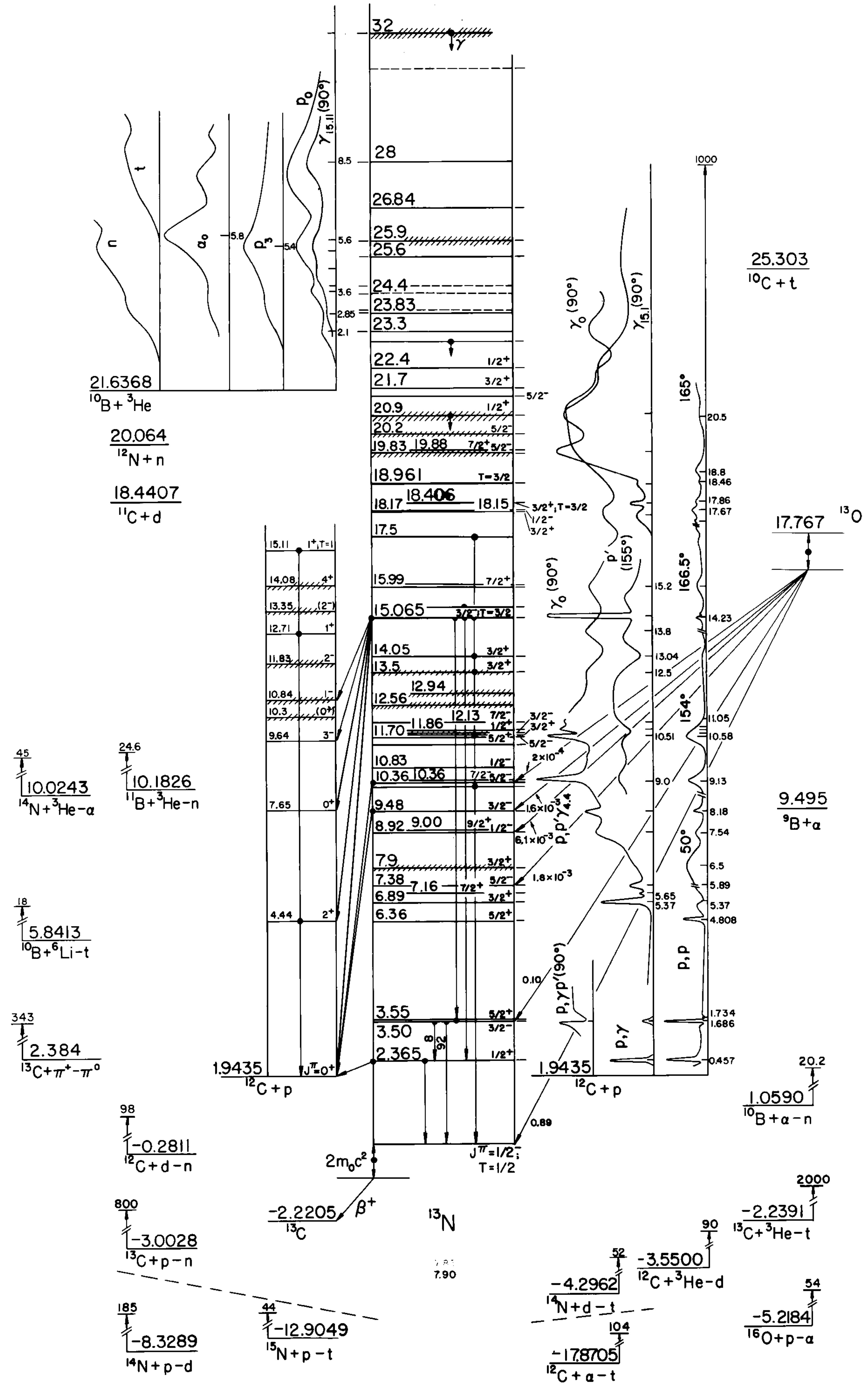
$$\mathcal{R}_{cc'} = \sum_{\lambda} \frac{\gamma_{\lambda c_5}\gamma_{\lambda c_1}}{E - E_\lambda}$$

$$\mathcal{R}_{cc'} = \sum_{\lambda} \frac{\gamma_{\lambda c_1}\gamma_{\lambda c_1}}{E - E_\lambda}$$

$^{12}C(p,\gamma)^{13}N$ - Example

	Reaction Channels		**Compound Nucleus**
$Q \sim 1.9$ MeV	$^{12}C + p$	⟶	^{13}N
$Q = 0$ MeV	$^{13}N + \gamma$	⟶	^{13}N

Possible reactions ?



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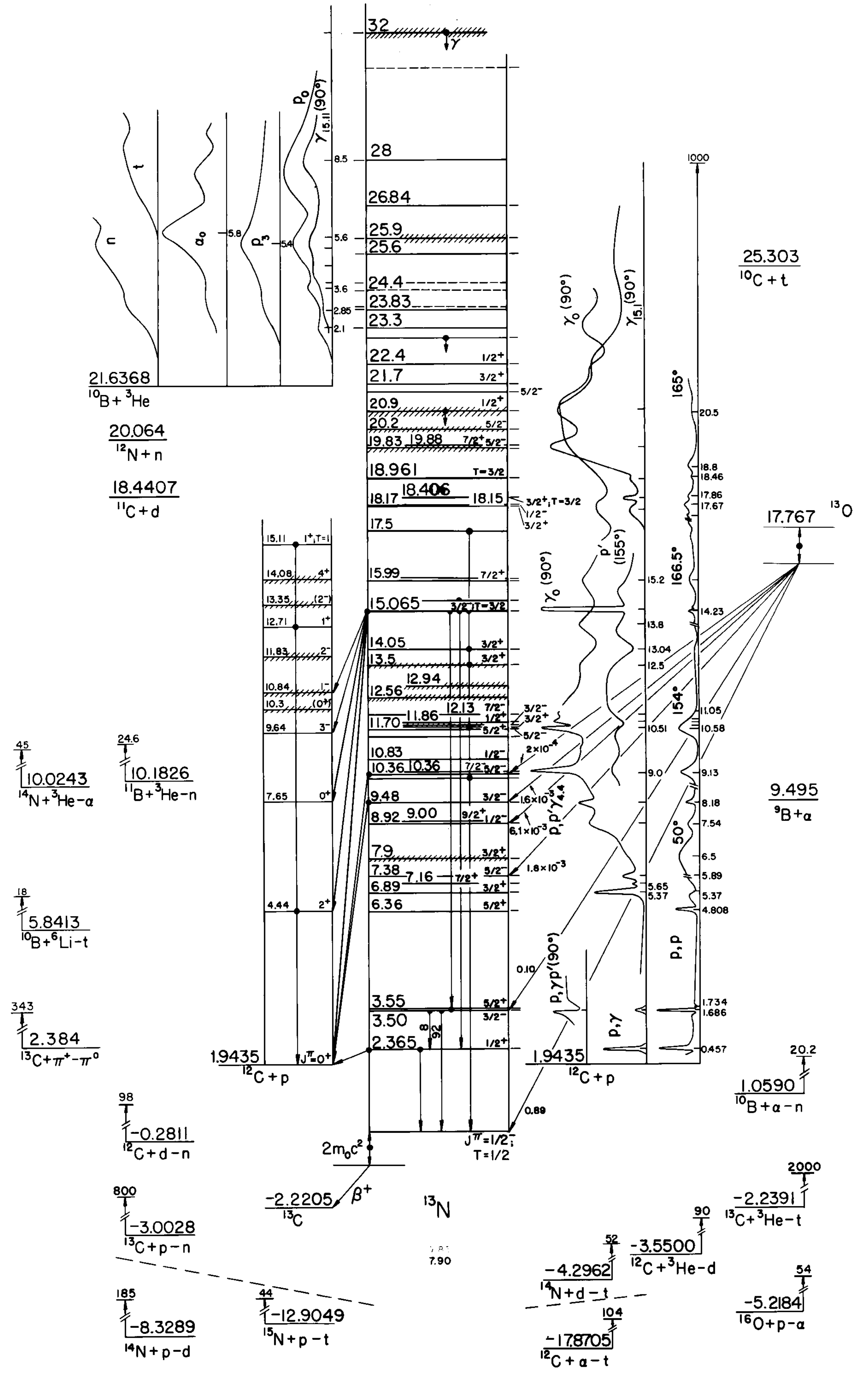
Possible reactions ?

- $^{12}C(p,\gamma)^{13}N$ Proton capture
- $^{12}C(p,p)^{12}C$ Elastic scattering
- $^{13}N(\gamma,p)^{12}C$ Photo dissociation



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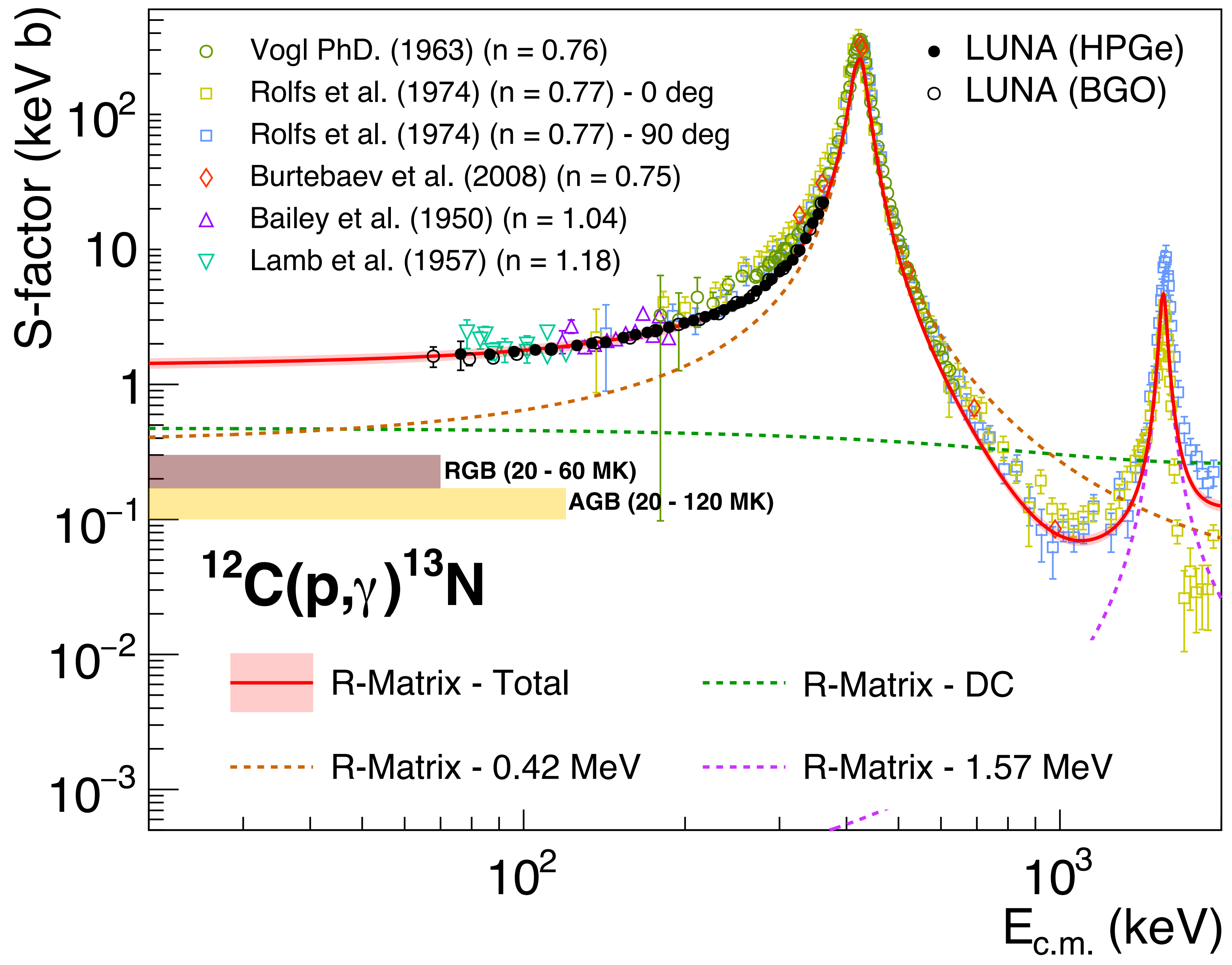
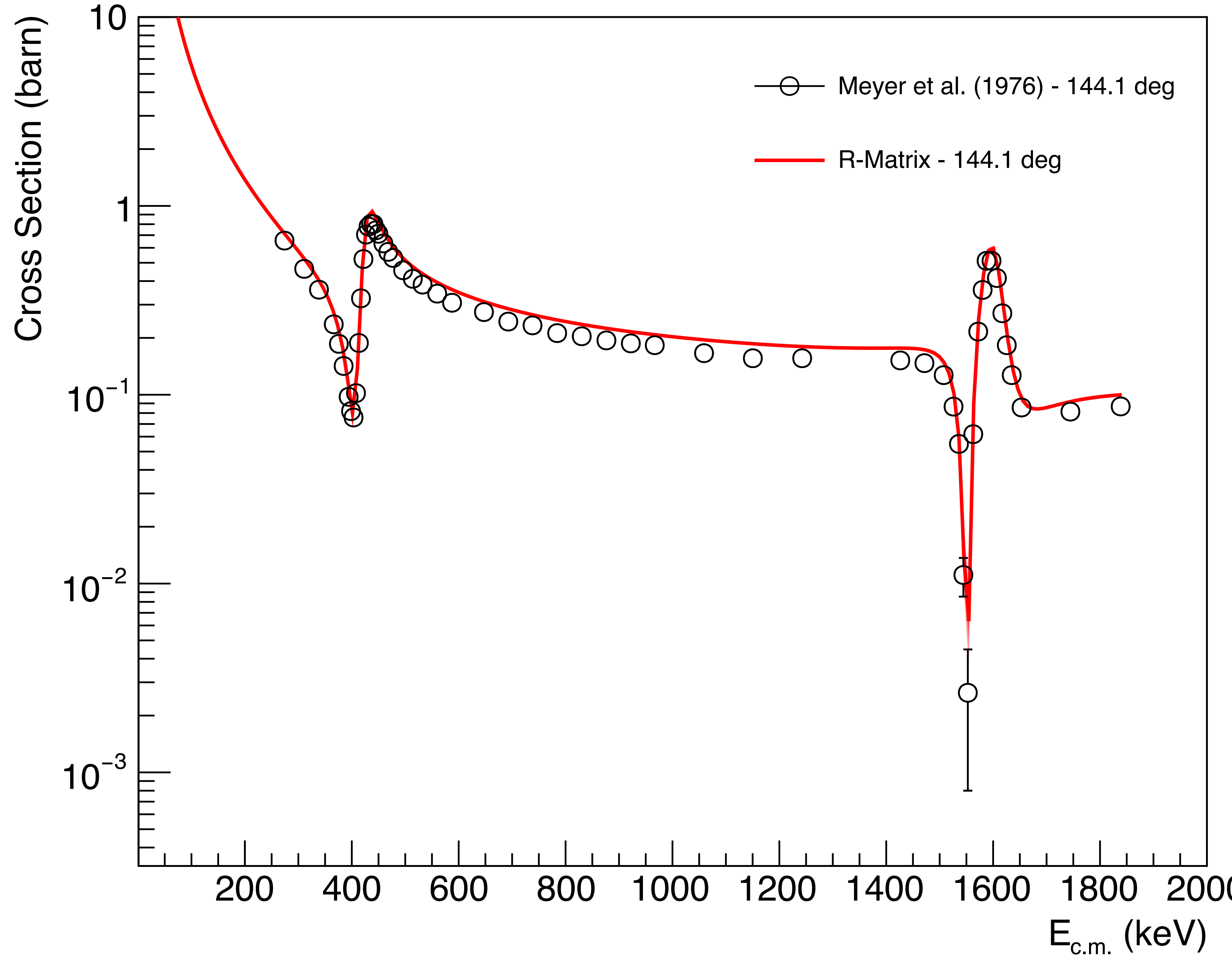
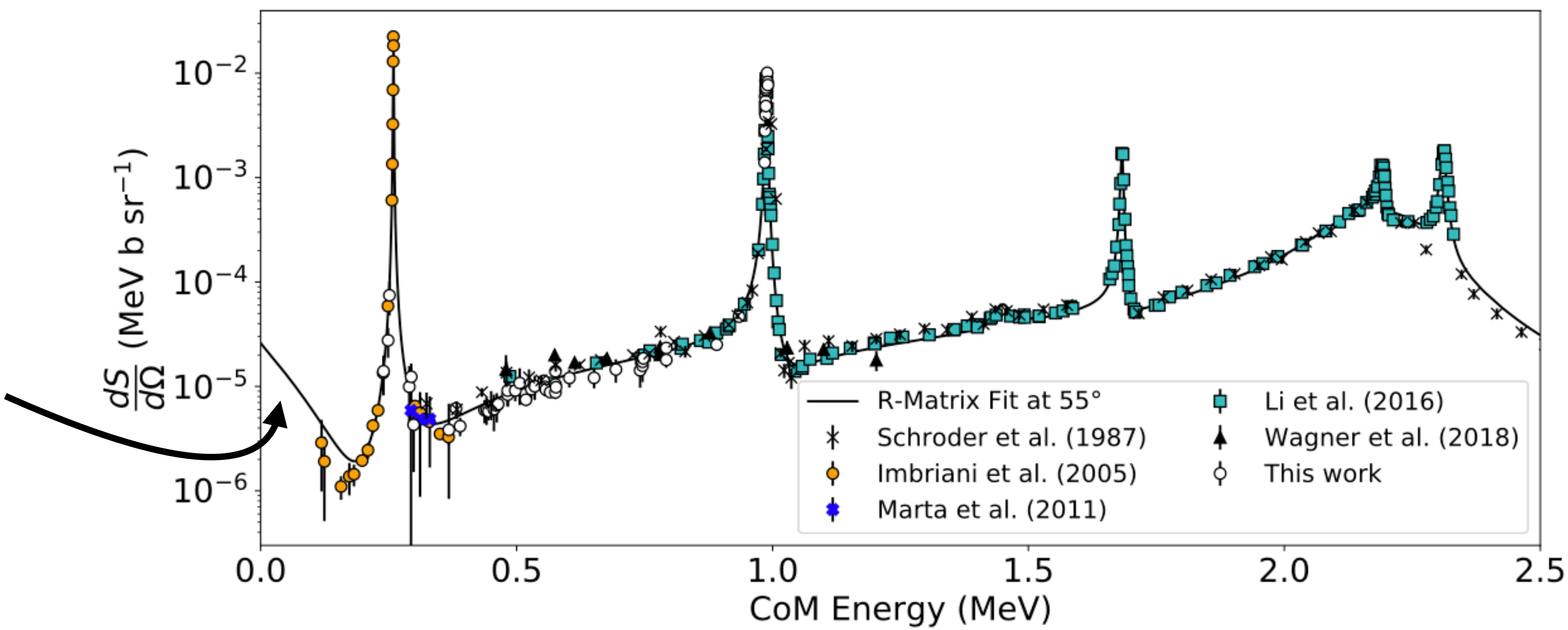


$^{12}C(p,p)^{12}C$



$^{14}N(p,\gamma)^{15}O$ - Example

Sub-threshold state at **6.79 MeV** dominates the cross section at **astrophysical energies**



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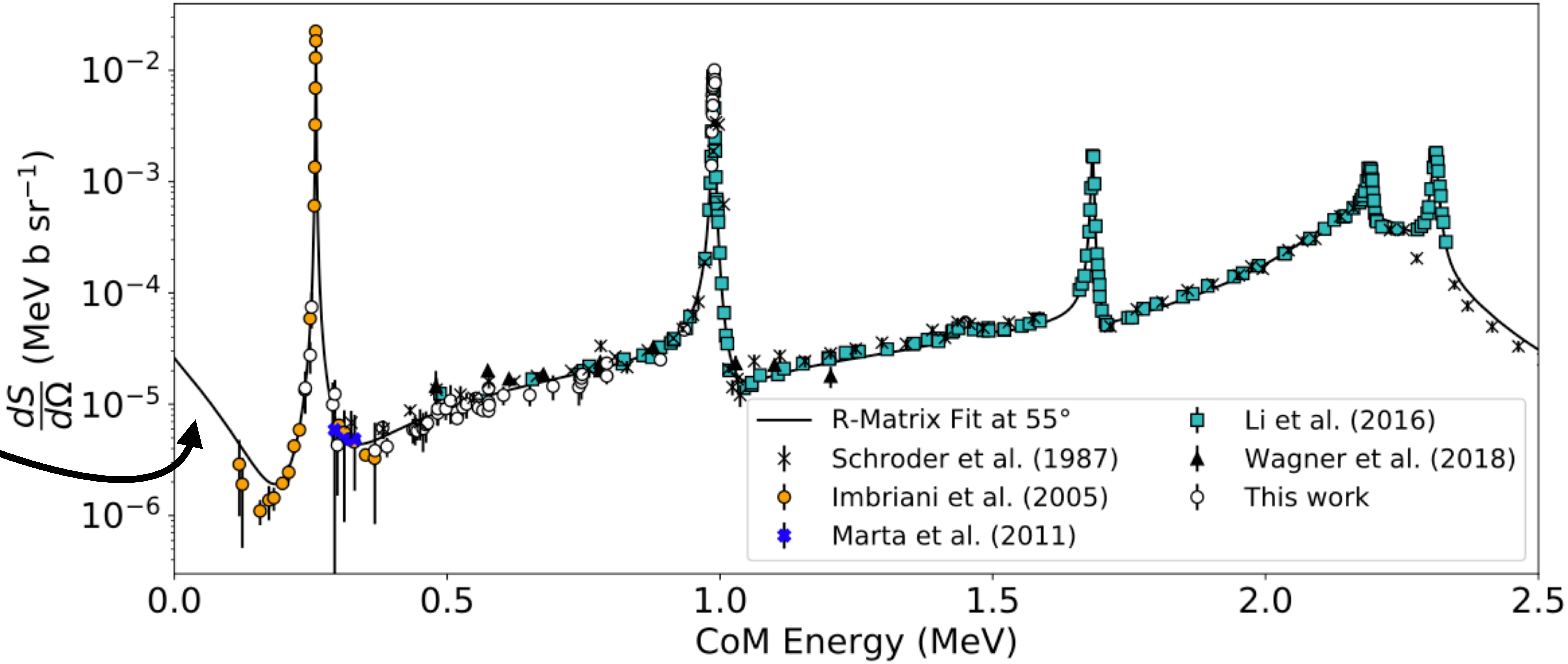

Idea: measure the 6.79 MeV **lifetime**

AZURE2 Code

- Originally developed by **R.E. Azuma** and published in 2010
- **AZURE2** publicly available from 2012 at azure.nd.edu
- State-of-the-art code for performing **R-matrix evaluations in nuclear astrophysics community**
- Designed for **charged particle reactions** with focus on extrapolations to low energies
- Simultaneous **multiple exit and entrance channel** fits