

Course 6: Theory for exploring nuclear reaction experiments

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Introduction to FRESCO/SFRESCO¹

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1 Some slides are taken from A.M.Moro, ISOLDE Nuclear Reaction and Nuclear Structure Course, 2014



What is FRESCO?

Fresco

Coupled Reaction Channels Calculations
www.fresco.org.uk

About Fresco

Fresco is a program developed by Ian Thompson over the period 1983 - 2006, to perform coupled-reaction channels calculations in nuclear physics. It uses Fortran 90 or Fortran 95 on Unix, Linux, Vax and Windows machines.



For

- Two body calculations
 - Elastic scattering (Optical potential)
 - Inelastic scattering (Coupled channel equations)
 - Capture
- Three body calculations
 - Breakup/Elastic scattering (CDCC)
 - Transfer (CDCC/DWBA)

What is FRESCO?

Fresco Input Examples

If a simple click on these files does not download them, then right-click and select 'download' or 'save as' or 'save link as'.

From Appendix B of the book:

		Input Files	Expected Output Files
B1	Elastic Scattering	B1-example-el.in	B1-example-el.out
B2	Inelastic Scattering	B2-example-inel2.in	B2-example-inel2.out
B3	Breakup (long form)	B3-example-br-long.in	B3-example-br-long.out
B4	Breakup (short form)	B4-example-br-short.in	B4-example-br-short.out
B5	Transfer	B5-example-tr.in	B5-example-tr.out
B6	Capture	B6-example-capture.in	B6-example-capture.out
B7		B7-p-cd.frin	B9-p-cd.out
B8	Parameter search	B8-p-cd.search	B9-p-cd-init.plot
B9		B9-p-cd.min	B9-p-cd-fit.plot

Note that there are some misprints in listing the inputs in the book. The above input files are those which do work: they give the output files.

From the Fresco distribution directory test/ :

	Reaction	Input Files	Expected Output Files
Transfer DWBA	$^{136}\text{Xe}(\text{t},\alpha)$	xeta	xeta.out
	$^{28}\text{Si}(^{19}\text{F},^{16}\text{O})$	f19xfs	f19xfs.out
Two-neutron transfers	$^{9}\text{Li}(\text{t},\text{p})^{11}\text{Li}$	li9tpss0	li9tpss0.out
Inelastic CC	$\alpha + ^{20}\text{Ne}^*$	lane20	lane20.out
	$^{16}\text{O} + ^{58}\text{Ni}^*$	on2	on2.out
	$^{11}\text{Be}^* + ^{197}\text{Au}$	be11	be11.out
CDCC	$^{11}\text{Be}^* + \alpha$	11be+He20ona1	11be+He20ona1.out
	$^{8}\text{B}^* + ^{58}\text{Ni}$	b8ex	b8ex.out
Adiabatic CDCC	$d^* + ^{208}\text{Pb}$	dexcc	dexcc.out
R-matrix solution	$d^* + ^{208}\text{Pb}$	dex	dex.out
CRC	$^{16}\text{O}^* + ^{208}\text{Pb}^*$	e8of49b	e8of49b.out
Capture	$p + ^7\text{Li}$	li7p-EM	li7p-EM.out
Search	$p + ^4\text{He}$ phase shifts	na.min na-all.search nalpha.frin	search-na-fit.plot
	$p + ^{112}\text{Cd}$ elastic scattering	ss.min ss.search p-cd.in	ss-fit.plot

Many inputs also have namelist forms in which the name ends in '-n', such as f19xfs-in.in.

The corresponding outputs are f19xfs-n.out, etc.

Renormalization used in Fresco

Plane wave

$$\langle \mathbf{r} | \mathbf{k} \rangle = e^{i\mathbf{k}\mathbf{r}}$$

momentum eigenstates

$$\langle \mathbf{k}' | \mathbf{k} \rangle = (2\pi)^3 \delta(\mathbf{k}' - \mathbf{k})$$

$$1 = \int d^3k | \mathbf{k} \rangle \frac{1}{(2\pi)^3} \langle \mathbf{k} |$$

coordinate eigenstates

$$\langle \mathbf{r}' | \mathbf{r} \rangle = \delta(\mathbf{r}' - \mathbf{r})$$

$$1 = \int dr^3 | \mathbf{r} \rangle \langle \mathbf{r} |$$

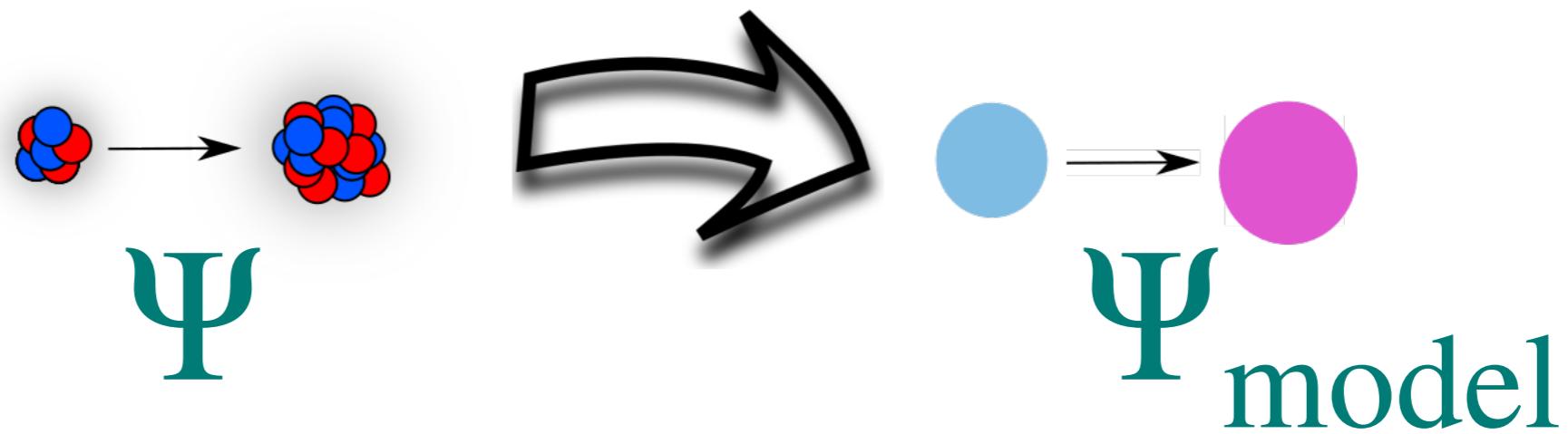
Asymptotic form

$$\psi^{\text{asym}}(R, \theta) = e^{ikz} + f(\theta) \frac{e^{ikR}}{R}$$

Partial wave expansion of scattering wave function

$$\psi(R, \theta) = \sum_{L=0}^{\infty} (2L+1) i^L P_L(\cos \theta) \frac{1}{kR} \chi_L(R)$$

Effective two body problem



Using the projection operator

$$\Psi_{\text{model}} = \mathcal{P}\Psi$$

$$\Psi = \mathcal{P}\Psi + \mathcal{Q}\Psi$$

$$\mathcal{P} + \mathcal{Q} = 1$$

$$\mathcal{P}^2 = \mathcal{P}$$

$$\mathcal{Q}^2 = \mathcal{Q}$$

$$\mathcal{P}\mathcal{Q} = \mathcal{Q}\mathcal{P} = 0$$

The Schrodinger equation becomes

$$(E - H)(\mathcal{P}\Psi + \mathcal{Q}\Psi) = 0$$

$$(E - \mathcal{P}H\mathcal{P})\mathcal{P}\Psi = (\mathcal{P}H\mathcal{Q})\mathcal{Q}\Psi$$

$$(E - \mathcal{Q}H\mathcal{Q})\mathcal{Q}\Psi = (\mathcal{Q}H\mathcal{P})\mathcal{P}\Psi$$

$$\mathcal{Q}\Psi = \frac{1}{E^{(+)} - \mathcal{Q}H\mathcal{Q}}(\mathcal{Q}H\mathcal{P})\mathcal{P}\Psi$$

$$(E - \mathcal{H})\mathcal{P}\Psi = 0$$

$$(E - \mathcal{H})\Psi_{\text{model}} = 0$$

$$\mathcal{H} = \mathcal{P}H\mathcal{P} + \mathcal{P}H\mathcal{Q}\frac{1}{E^{(+)} - \mathcal{Q}H\mathcal{Q}}\mathcal{Q}H\mathcal{P}$$

Effective interaction (optical potential)

Effective Hamiltonian

$$\mathcal{H} = \mathcal{P}H\mathcal{P} + \mathcal{P}H\mathcal{Q}\frac{1}{E^{(+)} - \mathcal{Q}H\mathcal{Q}}\mathcal{Q}H\mathcal{P}$$

The second term of \mathcal{H}

$$\Delta V(E) = H_{\mathcal{P}\mathcal{Q}}\frac{1}{E^{(+)} - H_{\mathcal{Q}\mathcal{Q}}}H_{\mathcal{Q}\mathcal{P}} \rightarrow \text{energy dependent}$$

By using the eigenstate:

$$(E_q - H_{\mathcal{Q}\mathcal{Q}})\Phi_q = 0$$

$$\Delta V = \sum_q \frac{H_{\mathcal{P}\mathcal{Q}}|\Phi_q\rangle\langle\Phi_q|Q\mathcal{P}}{E - E_q} + \int dE_q \frac{H_{\mathcal{P}\mathcal{Q}}|\Phi_q\rangle\langle\Phi_q|Q\mathcal{P}}{E^{(+)} - E_q} \rightarrow \text{nonlocal}$$

Mathematically,

$$\lim_{\epsilon \rightarrow 0} \frac{1}{E - E_q + i\epsilon} = \mathfrak{P}\left(\frac{1}{E - E_q}\right) - i\pi\delta(E - E_q)$$

Real part:

$$\Re \Delta V(E) = \sum_q \frac{H_{\mathcal{P}\mathcal{Q}}|\Phi_q\rangle\langle\Phi_q|Q\mathcal{P}}{E - E_q} + \mathfrak{P} \int dE_q \frac{H_{\mathcal{P}\mathcal{Q}}|\Phi_q\rangle\langle\Phi_q|Q\mathcal{P}}{E - E_q}$$

Imaginary part:

$$\Im \Delta V(E) = -\pi H_{\mathcal{P}\mathcal{Q}}|\Phi_q\rangle\langle\Phi_q|H_{\mathcal{Q}\mathcal{P}}$$

Dispersion relation:

$$\Re \Delta V(E) = \sum_q \frac{H_{\mathcal{P}\mathcal{Q}}|\Phi_q\rangle\langle\Phi_q|H_{\mathcal{Q}\mathcal{P}}}{E - E_q} - \frac{1}{\pi} \mathfrak{P} \int dE_q \frac{\Im \Delta V(E_q)}{E - E_q}$$

Elastic scattering with optical potential

Effective potential(local): $U(R) = U_c(R) + U_{nuc}(R)$

Coulomb potential: charge sphere distribution

$$U_c(R) = \begin{cases} \frac{Z_1 Z_2 e^2}{2R_c} \left(3 - \frac{R^2}{R_c^2}\right) & \text{if } R \leq R_c \\ \frac{Z_1 Z_2 e^2}{R} & \text{if } R \geq R_c \end{cases}$$

Nuclear potential (complex): Woods-Saxon parametrization

$$U_{\text{nuc}}(R) = V(r) + iW(r) = -\frac{V_0}{1 + \exp\left(\frac{R-R_0}{a_0}\right)} - i \frac{W_0}{1 + \exp\left(\frac{R-R_i}{a_i}\right)}$$

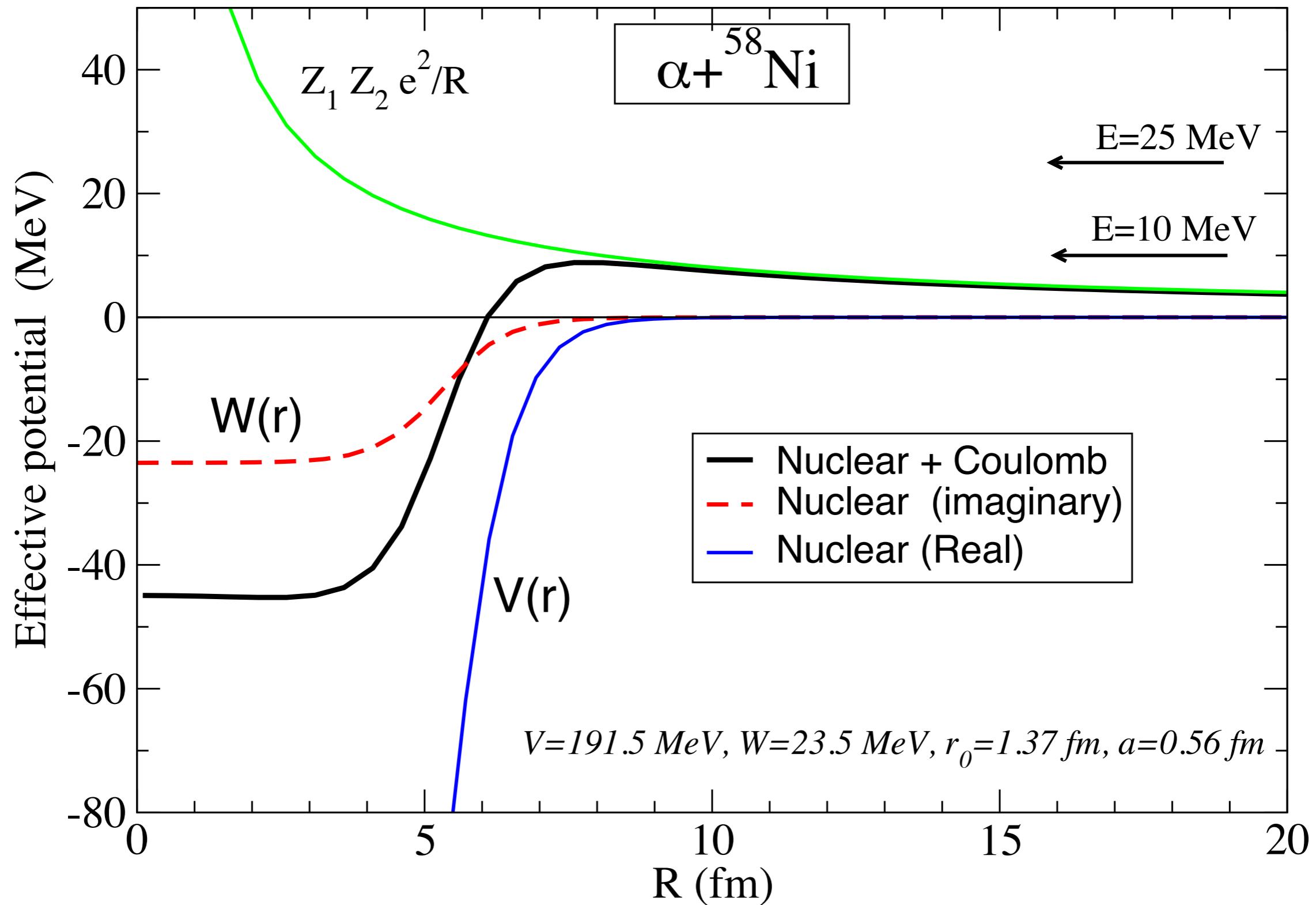
Typically $R_0 = r_0(A_T^{1/3} + A_P^{1/3})$

r_0 =reduced radius $r_0 \sim 1.1 - 1.4$ fm

A_T and A_P : mass number of projectile and target

Elastic scattering: effective potential

Take ${}^4\text{He} + {}^{58}\text{Ni}$ as an example



Partial wave decomposition and double differential equation

- Central potential $U = U(R)$:

$$\chi_0^{(+)}(\mathbf{K}, \mathbf{R}) = \frac{1}{KR} \sum_{\ell m} i^\ell (2\ell + 1) \chi_\ell(K, R) P_\ell(\cos \theta)$$

- $\chi_\ell(K, R)$ obtained from:

Complex

$$\left[-\frac{\hbar^2}{2\mu} \frac{d^2}{dR^2} + \frac{\hbar^2}{2\mu} \frac{\ell(\ell+1)}{R^2} + [U(R) - E_0] \right] \chi_\ell(K, R) = 0.$$

- Boundary condition:

$$\begin{aligned} \chi_\ell(K, R) &\rightarrow e^{i\sigma_\ell} [F_\ell(\eta, KR) + T_\ell H_\ell^{(+)}(\eta, KR)] \\ &= (i/2) e^{i\sigma_\ell} [H_\ell^{(-)}(\eta, KR) - S_\ell H_\ell^{(+)}(\eta, KR)] \end{aligned}$$

- ☞ $\sigma_\ell(\eta)$ =Coulomb phase shift
- ☞ $F_\ell(\eta, KR)$ =regular Coulomb wave
- ☞ $H_\ell^{(\pm)}(\eta, KR)$ =outgoing/ingoing Coulomb wave

Scattering amplitude and observables

Total scattering amplitude:

$$f(\theta) = f_C(\theta) + \frac{1}{2iK} \sum_{\ell} (2\ell + 1) e^{2i\sigma_{\ell}} (S_{\ell} - 1) P_{\ell}(\cos \theta)$$

☞ $f_C(\theta)$ is the amplitude for pure Coulomb:

$$\frac{d\sigma_R}{d\Omega} = |f_C(\theta)|^2 = \frac{\eta^2}{4K^2 \sin^4(\frac{1}{2}\theta)} = \left(\frac{Z_p Z_t e^2}{4E} \right)^2 \frac{1}{\sin^4(\frac{1}{2}\theta)}$$

Optical model calculations with fresco

Essential ingredients of an OM calculation:

- **Physical:**
 - Identify projectile and target (mass, spin, etc)
 - Incident energy
 - Parametrization of the optical potential
- **Numerical:**
 - Radial step for numerical integration (HCM in fresco)
 - Maximum radius R for integration (RMATCH)
 - Maximum angular momentum L . (JTMAX)

Example: ${}^4\text{He} + {}^{58}\text{Ni}$

Input example:

```
4he58ni_e10.in: 4He + 58Ni elastic scattering Ecm=10.0 MeV
NAMELIST
&FRESCO hcm=0.1 rmatch=25.0 jtmax=30
    thmin=1.0 thmax=180.0 thinc=2.0
    smats=2 xstabl=1
    elab=10.7 /
&PARTITION namep='ALPHA' massp=4 zp=2 namet='58Ni' masst=58 zt=28 nex=1 /
&STATES jp=0.0 bandp=1 ep=0.0 cpot=1 jt=0.0 bandt=1 et=0.0 /
&partition /
&POT kp=1 at=58 rc=1.4 /
&POT kp=1 type=1
    p1=191.5 p2=1.37 p3=0.56 p4=23.5 p5=1.37 p6=0.56 /
&pot /
&overlap /
&coupling /
```

Example: ${}^4\text{He} + {}^{58}\text{Ni}$

General variables

```
&FRESCO hcm=0.1 rmatch=25.0 jtmax=30
    thmin=1.00 thmax=180.00 thinc=2.00
    smats=2 xstabl=1
    elab=10.7 /
```

Mass partitions & states

```
&PARTITION namep='ALPHA' massp=4 zp=2 namet='58Ni' masst=58 zt=28
    nex=1 /
&STATES jp=0.0 bandp=1 ep=0.0 cpot=1 jt=0.0 bandt=1 et=0.0 /
&partition /
```

Potentials

```
&POT kp=1 itt=F at=58 rc=1.4 /
&POT kp=1 type=1
    p1=191.5 p2=1.37 p3=0.56 p4=23.5 p5=1.37 p6=0.56 /
&pot /
```

Example: ${}^4\text{He} + {}^{58}\text{Ni}$

Essential input variables: FRESCO namelist

```
&FRESCO hcm=0.1 rmatch=25.0 jtmax=30
    thmin=1.00 thmax=180.00 thinc=2.00
    smats=2 xstabl=1
    elab=10.7 /
```

- **hcm**: step for integration of radial equations.
- **rmatch**: matching radius (for $R > \text{RMATCH}$ asymptotic behaviour is assumed)
- **elab**: laboratory energy
- **jtmax**: maximum total angular momentum (projectile+target+relative)
- **smats**: trace variable
smats=2 → print elastic S-matrix
- **xstabl**: trace variable
xstabl=1 → print cross sections

Example: ${}^4\text{He} + {}^{58}\text{Ni}$

Essential input variables: partitions and states

```
&PARTITION namep='ALPHA' massp=4 zp=2 namet='58Ni' masst=58 zt=28
    nex=1 /
```

- **namep / namet**: projectile / target name
- **massp / masst**: projectile / target mass (amu)
- **zp / zt**: projectile / target charge
- **nex**: number of (pairs) of states in this partition

```
&STATES jp=0.0 bandp=1 ep=0.0 cpot=1 jt=0.0 bandt=1 et=0.0 /
```

- **jp / jt**: projectile / target spins
- **bandp / bandt**: projectile / target parities (± 1)
- **cpot**: index of potential for this pair of states.

Example: ${}^4\text{He} + {}^{58}\text{Ni}$

```
&POT kp=1 type=0 ap=0 at=58 rc=1.4 /
&POT kp=1 type=1 shape=0
    p1=191.5 p2=1.37 p3=0.56 p4=23.5 p5=1.37 p6=0.56 /
&pot /
```

- **kp**: index to identify this potential
- **ap**, **at**: projectile and target mass, for conversion from reduced to physical radii: $R = r(ap^{1/3} + at^{1/3})$
- **type**, **shape**: potential category and shape: \Rightarrow
 - **type=0**: Coulomb potential
shape=0: uniform charge sphere
 - **type=1**: volume nuclear potential
shape=0: Woods-Saxon shape
- **rc**: reduced radius for charge distribution
- **p1, p2, p3**: V_0, r_0, a_0 (real part)
- **p4, p5, p6**: W_0, r_i, a_i (imaginary part)

$$U_{\text{nuc}}(R) = V(r) + iW(r) = -\frac{V_0}{1 + \exp\left(\frac{R-R_0}{a_0}\right)} - i \frac{W_0}{1 + \exp\left(\frac{R-R_i}{a_i}\right)}$$

Tips from Fresco to solve the double differential equation

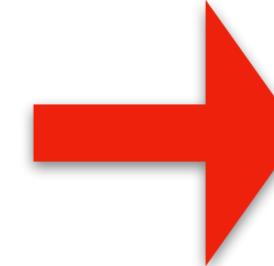
Boundary conditions

$$f_l(0) = 0$$

$$f_l(a) = \frac{i}{2} [H_L^-(\eta, ka) - S_L H_L^+(\eta, ka)]$$

$$f'_l(a) = \frac{i}{2} [H_L'^-(\eta, ka) - S_L H_L'^+(\eta, ka)]$$

complex potential

Choice of h $k(R) = \sqrt{2\mu(E - V(R))/\hbar^2}$ $\uparrow \longrightarrow h \downarrow$  $kh \leq 0.2$

Starting point, for large centrifugal barrier $\frac{l(l+1)}{R}$

$$f_l(R) = 0, \quad \text{when } R < R_{min} \quad R_{min} = 2.0 * lh$$

$$f_l(R_{min} + h) = h^{(l+1)}$$

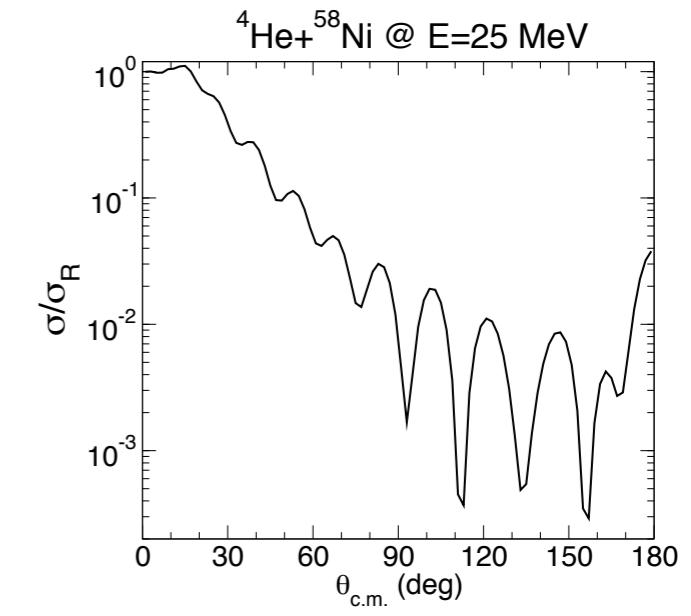
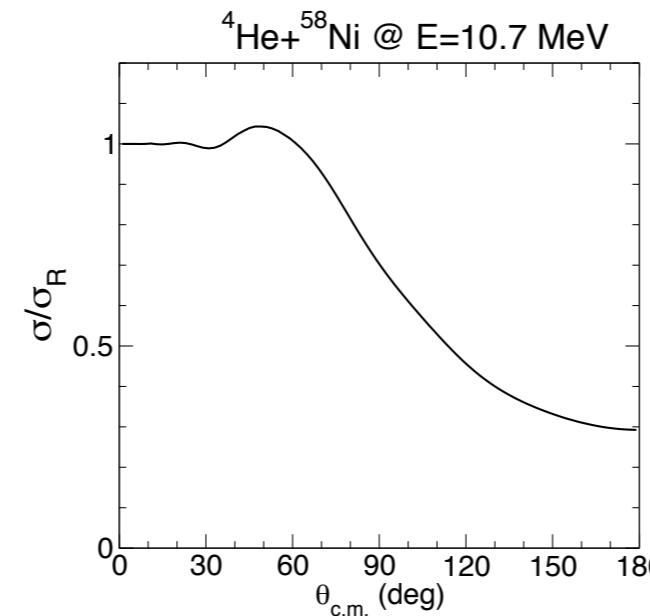
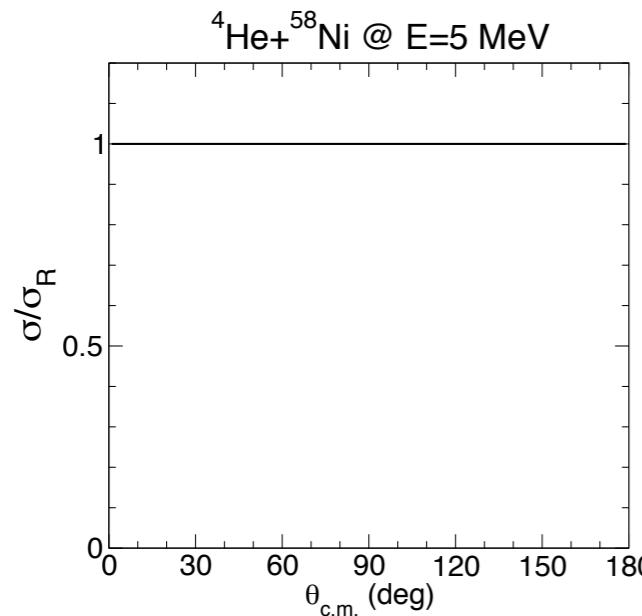
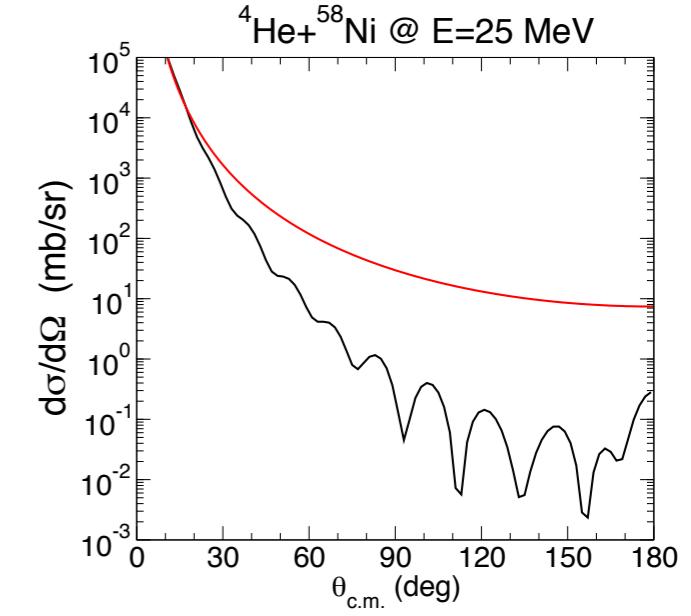
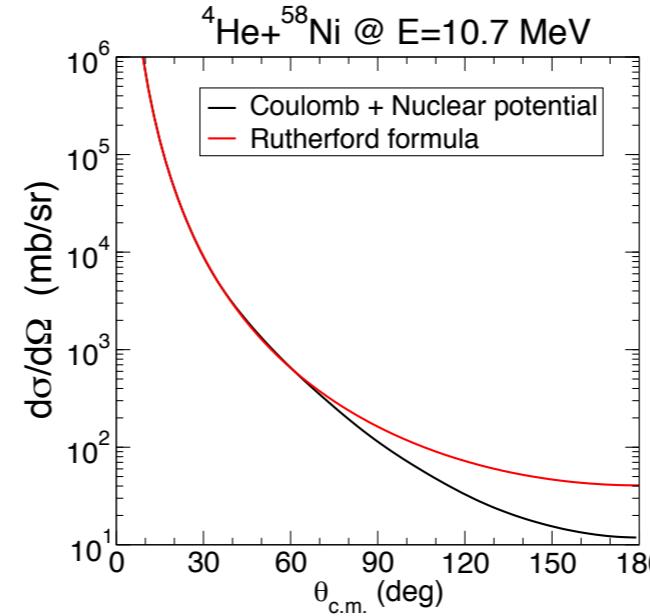
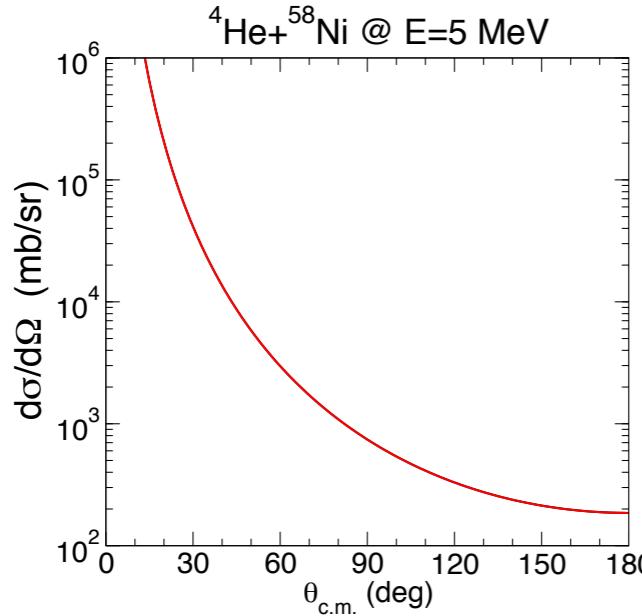
Method : enhanced numerov, more accurate for high-energy scattering with slowly varying potentials

Useful output in OM calculations

Useful output files:

- Main output file (stdout)
- **fort.201** : Elastic scattering angular distribution
 - `thmax > 0`: relative to Rutherford.
 - `thmax < 0`: absolute units (mb/sr).
- **fort.7**: Elastic S-matrix (real part, imaginary part, angular momentum)
- **fort.56**: Fusion (absorption), reaction and inelastic cross section for each angular momentum

Elastic scattering angular distribution



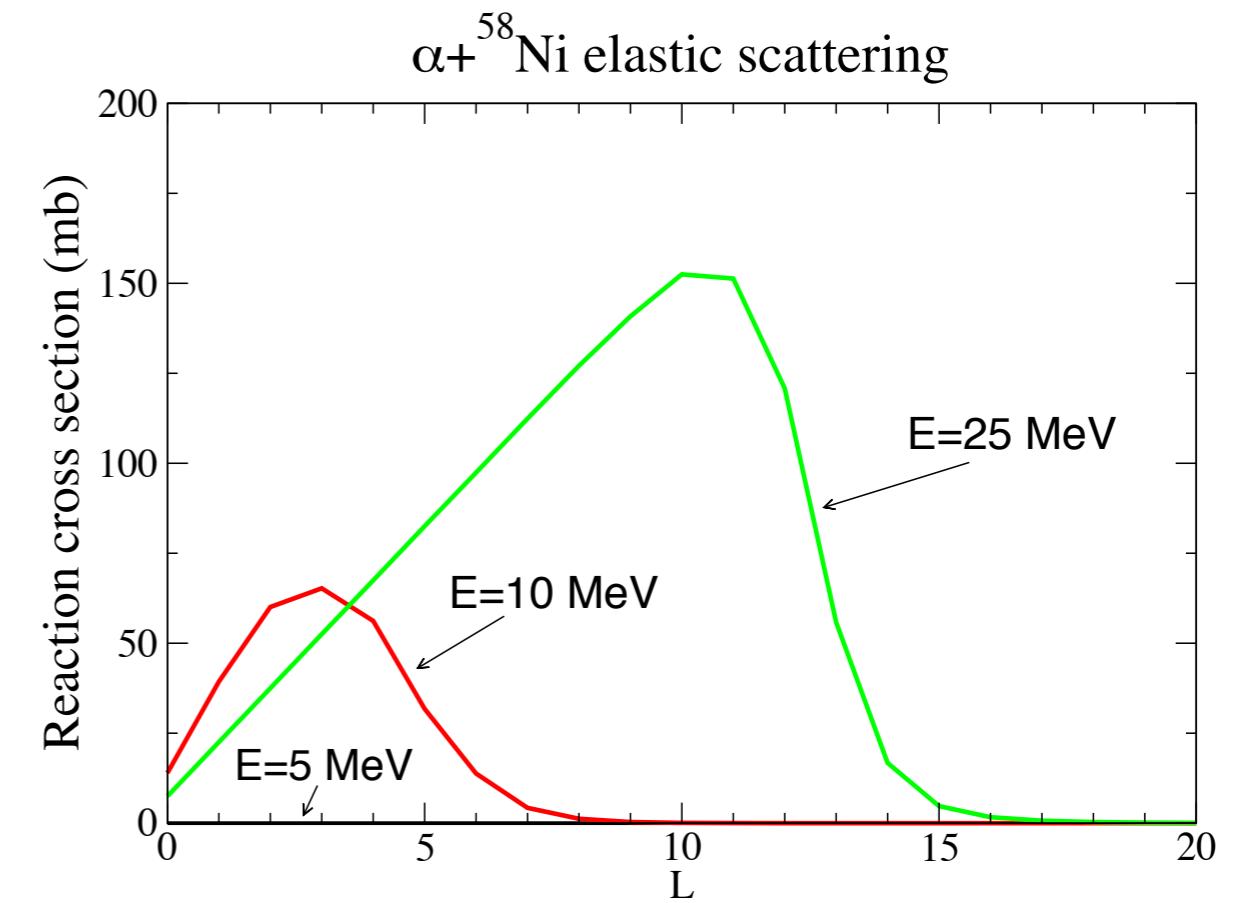
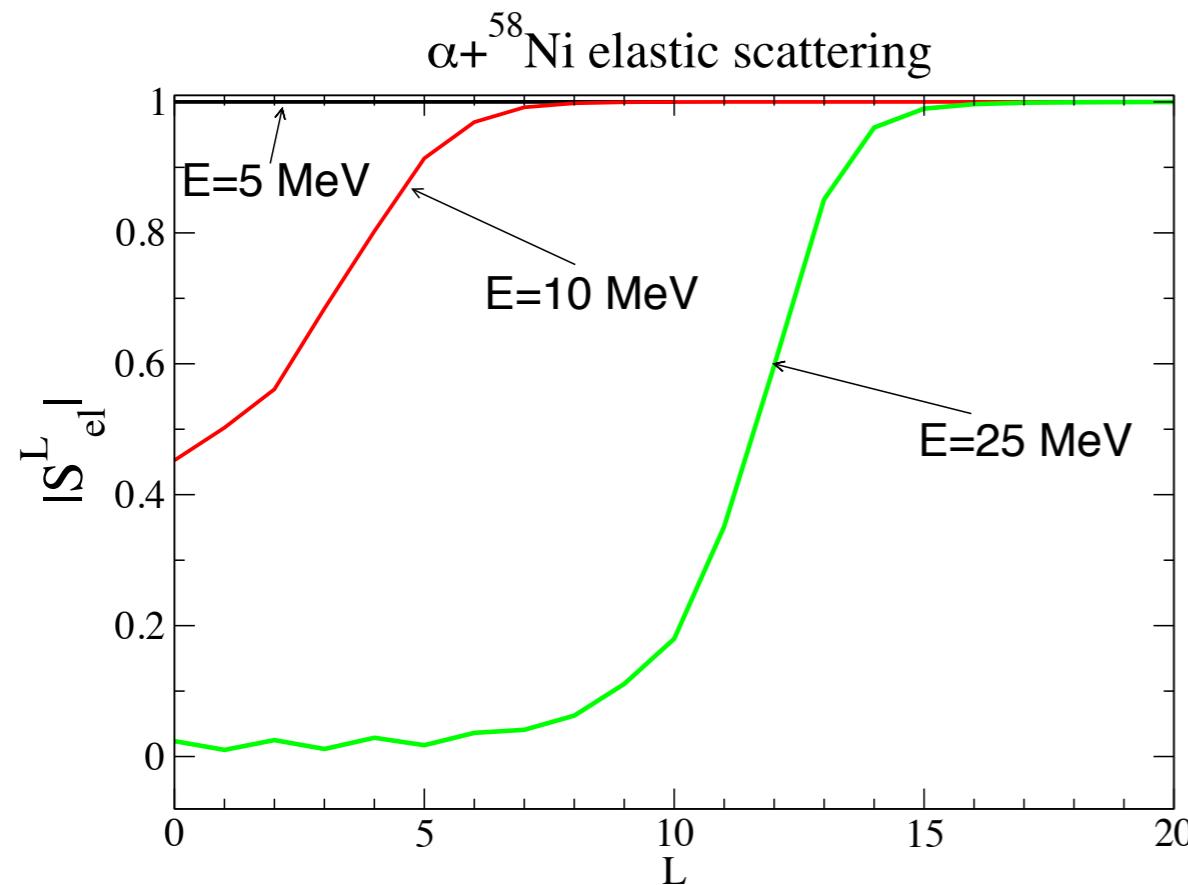
Rutherford scattering

Fresnel

Fraunhöfer

S-matrix

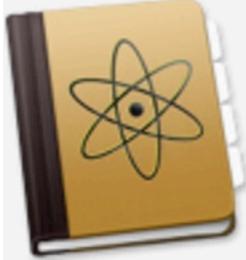
Elastic (nuclear) S-matrix (`fort.7`): $\chi_L^{el}(r) = I_L(r) - S_{el}^L O_L(r)$



\Rightarrow the number of partial waves required for convergence grows approximately as \sqrt{E}

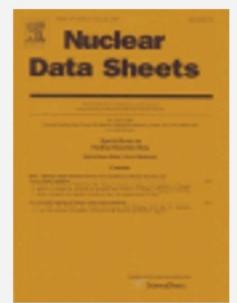
Useful database for nuclear reaction

Optical potential:



Reference Input Parameter Library (RIPL-3)

R. Capote, M. Herman, P. Oblozinsky, P.G. Young, S. Goriely, T. Belgya, A.V. Ignatyuk, A.J. Koning, S. Hilaire, V.A. Plujko, M. Avrigeanu, O. Bersillon, M.B. Chadwick, T. Fukahori, Zhigang Ge, Yinlu Han, S. Kailas, J. Kopecky, V.M. Maslov, G. Reffo, M. Sin, E.Sh. Soukhovitskii and P. Talou



Nuclear Data Sheets - Volume 110, Issue 12, December 2009, Pages 3107-3214

RIPL discrete levels database updated in August 2015 - it contains the correction for +X,.. levels

[Introduction](#) [MASSES](#) [LEVELS](#) [RESONANCES](#) [OPTICAL](#) [DENSITIES](#) [GAMMA](#) [FISSION](#) [CODES](#) [Contacts](#)

Experimental data:



Experimental Nuclear Reaction Data (EXFOR)
Database Version of 2019-06-03

⊕ Software Version of 2019-05-06

The EXFOR library contains an extensive compilation of experimental nuclear reaction data. Neutron reactions have been compiled systematically since the discovery of the neutron, while charged particle and photon reactions have been covered less extensively. [EXFOR Reference Paper: Nucl. Data Sheets 120\(2014\)272](#).

EXFOR Web database retrieval system provides: data search, output to various formats (incl.XML), plotting and comparison to ENDF, re-normalization old data to new standards, calculating data for inverse reactions and kinematics, constructing correlation matrices from partial uncertainties, etc. [EXFOR Web Database & Tools Paper: NIM A 888 \(2018\) 31](#).

The EXFOR database contains data from 22639 experiments (see [statistics](#) and recent database updates). Mirror-sites [⊕](#)

Fits with SFRESCO

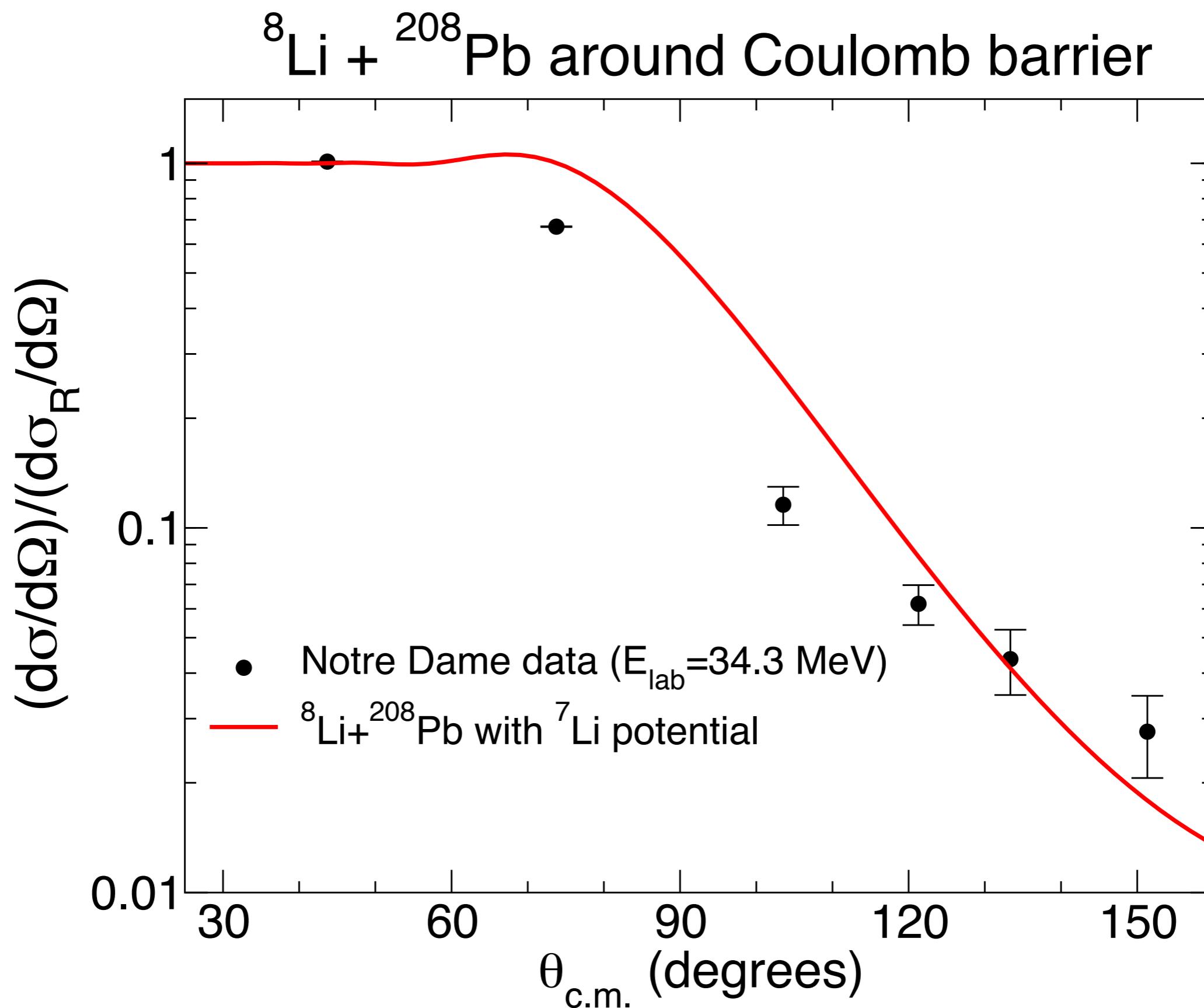
SFRESCO: Can be used together with FRESCO to do determine automatically optical model parameters by means of a χ^2 analysis of experimental angular distribution.

We need 3 input files:

- ① FRESCO input file: `li8pb_e34.in`
- ② MINUIT input file: `sfresco.in`
- ③ SEARCH input file: `search.in`

`sfresco.in` \implies `search.in` \implies `li8pb_e34.in`

Before fit



Fresco input before fit

```
li8pb_e34.in
NAMELIST
&FRESCO hcm=0.05 rmatch=40.0 jtmax=60
    thmin=5.00 thmax=160.00 thinc=2.00
    smats=2 xstabl=1
    elab= 34.404 /
&PARTITION namep='Li-8' massp=8 zp=3 namet='Pb-208'
    masst=208 zt=82 qval=0.0000 pwf=T nex=1 /
&STATES jp=2.0 bandp=1 ep=0.000 cpot=1 jt=0.0
    bandt=1 et=0.000 fexch=F /
&partition /
&POT kp=1 ap=8 at=208 rc=1.25 /
&POT kp=1 type=1 itt=F p1=15.4 p2=1.3 p3=0.65 p4=13.2 p5=1.3 p6=0.65 /
&pot /
```

Fits with SFRESCO

- 1.- FRESCO input file: `li8pb_e34.in` (previous slide)
- 2.- MUNUIT input file: `sfresco.in`

```
search.in <---- file with search parameters
min
fix
migrad
end
q
show
plot
```

Fits with SFRESCO

3.- SEARCH input file: search.in

```
'li8pb_e34.in' 'li8pb_e34.out' 2 1

&variable kind=1 name='V' kp=1 pline=2 col=1 valmin=5.0 valmax=150.0 step=0.2/
&variable kind=1 name='W' kp=1 pline=2 col=4 valmin=5.0 valmax=100.0 step=0.2 /

&data type=0 iscale=2 idir=1 lab=F abserr=T/
43.7    1.01026 0.014
73.76   0.67003 0.014
103.537 0.11577 0.01394
121.296 0.06194 0.00778
133.351 0.04369 0.00888
151.332 0.02763 0.00701
&
```

```
sfresco < sfresco.in > sfresco.out
```

Fits with SFRESCO

```
'li8pb_e34.in' 'li8pb_e34.out' 2 1
```

input_file, output_file, nvariables, ndatasets

```
&variable kind=1 name='V' kp=1 pline=2 col=1 valmin=5.0 valmax=150.0 /
&variable kind=1 name='W' kp=1 pline=2 col=4 valmin=5.0 valmax=100.0 /
```

- **kind**: type of variable (1=potential)
- **kp**: potential index
- **pline=2**: potential component
- **col**: column (identifies parameter within component)
- **valmin-valmax**: constraints for this parameter

```
&POT kp=1 ap=8 at=208 rc=1.25 /
&POT kp=1 type=1 itt=F p1=15.4 p2=1.3 p3=0.65 p4=13.2 p5=1.3 p6=0.65 /
&pot /
```

Fits with SFRESCO

```
&data type=0 iscale=2 idir=1 abserr=T/  
43.7    1.01026  0.014  
73.76   0.67003  0.014  
(...)  
&
```

- **type**: type of observable (0= angular distribution for fixed energy)
- **iscale**: data units for absolute scale (2=mb/sr)
- **idir**: scale (1=ratio to Rutherford)
- **abserr**: specified errors are absolute (T) or relative (F).

output of SFRESCO

Var 1=V value 15.400000
 Var 2=W value 13.200000

Total ChiSq/N = 78.8745 from 78.874
 (...)

PARAMETER CORRELATION COEFFICIENTS

NO.	GLOBAL	1	2
1	0.62638	1.000	-0.626
2	0.62638	-0.626	1.000

(...)

Var 1=V value 12.440562, step 0.2000, error 4.4317
 Var 2=W value 60.305833, step 0.2000, error 4.9913

Angle	Datum	Abs. error	Theory	Chi
43.700	1.0103	0.14000E-01	0.99683	0.9199
73.760	0.67003	0.14000E-01	0.66383	0.1962
103.537	0.11577	0.13940E-01	0.14595	4.6878
121.296	0.61940E-01	0.77800E-02	0.59023E-01	0.1406
133.351	0.43690E-01	0.88800E-02	0.34596E-01	1.0489
151.332	0.27630E-01	0.70100E-02	0.18740E-01	1.6082

Total ChiSq/N = 1.4336 from 1.434
 (...)

After fit

