

Fitting data (ch15)



Comparing theory and experiment
 $\{p_j\}$ inputs parameter set
 $\sigma^{\text{exp}}(i)$ experimental data ($\Delta\sigma$ standard deviation)

Measure of discrepancy

$$\chi^2 = \sum_{i=1}^N \frac{(\sigma^{\text{th}}(i) - \sigma^{\text{exp}}(i))^2}{\Delta\sigma(i)^2}.$$

If theory agrees exactly with experiment $\chi^2=0$ (very unlikely!)

What is statistically reasonable $\sigma^{\text{th}}(i) - \sigma^{\text{exp}}(i) \sim \Delta\sigma(i)$ so $\chi^2 \sim N$ (or $\chi^2/N \sim 1$)

If $\chi^2/N \gg 1$ then theory needs improvement

If $\chi^2/N \ll 1$ errors have been overestimated

Ex: optical potential fits (optical model)



- Strongly non linear (fitting is done by iteration only)
- Need data at large scattering angles
- Spin orbit affect T11 and not so much elastic cross sections
 - Ambiguities:
 - low energy (phase equivalent potentials)

- medium energy (volume integral $V_{ws}=R_{ws}^2$)

$$\mathcal{J} = \int V(\mathbf{r}) d\mathbf{r} = 4\pi \int_0^\infty V(r) r^2 dr$$

- heavy nuclei (governed by tail of V)

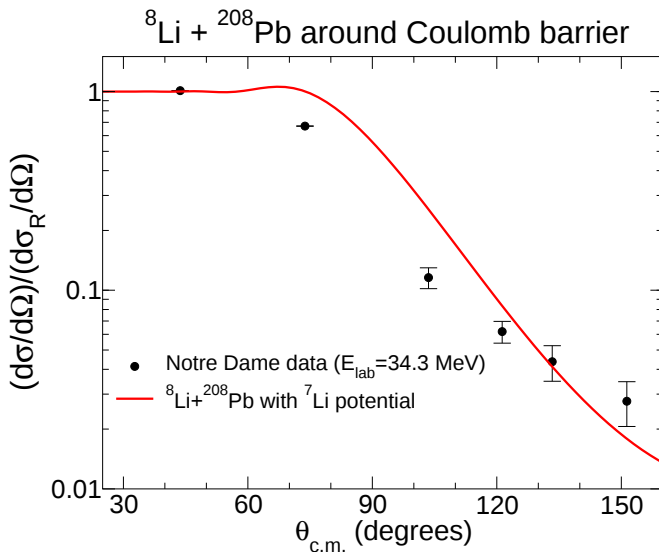
$$V(R) \approx -V_{ws} e^{-(R-R_{ws})/a_{ws}} = -V_{ws} e^{R_{ws}/a_{ws}} e^{-R/a_{ws}}$$

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

We need 3 input files:

- 1 FRESKO input file: [li8pb_e34.in](#)
- 2 MINUIT input file: [sfresco.in](#)
- 3 SEARCH input file: [search.in](#)

`sfresco.in  $\Rightarrow$  search.in  $\Rightarrow$  li8pb_e34.in`



FRESCO input file (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 /
```

Performing 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
```

Performing fits with SFRESCO (continued):

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
```

SEARCH input file (continued):

```
'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

SEARCH input file (continued):

```
&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).

```
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
(...)
```

Correlation matrix

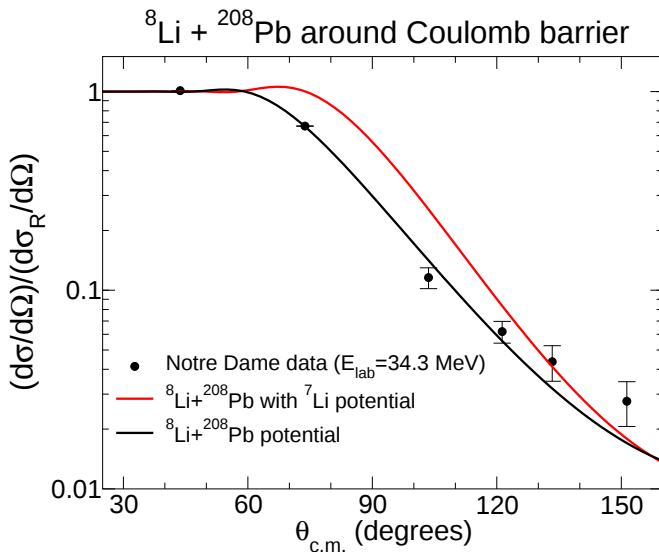
FRESCO input file (after fit)

```
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
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&PARTITION namep='Li-8' massp=8 zp=3 namet='Pb-208'
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&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=12.4 p2=1.3 p3=0.65 p4=60.3 p5=1.3 p6=0.65 /
&pot /
```



Strategies for χ^2 fitting



- Start with simplest data and simplest reaction model
(for example elastic and optical model)
- Restart from any intermediate stage
- If there are ambiguities, do grid searches and look at correlations in errors
- Artificially reduce error in data points if theory is having a hard time to get close in some region
- If minimum is found near the end of the range of a parameter, this is spurious – repeat with wider range
- Constrain with other experiments
- Two correlated variables : combine into one

Progressive improvement policy