SAMMY Workshop Part 4.1

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Part 4.1, Calculating cross sections

Updated July 2005

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U. S. DEPARTMENT OF ENERGY

1. Formalism for calculation of cross sections

Scattering Theory

- Also called: Collision Theory or R-Matrix Theory

- Definitive Paper:
  - Lane & Thomas, "R-Matrix Theory of Nuclear Reactions", *Reviews of Modern Physics* **30**, 257-353 (1958)
- Easier-reading Book:
  - Foderaro, *The Elements of Neutron Interaction Theory*, The MIT Press, Cambridge MA and London, England (1971)

- (There are many other resources on this topic)

Other valuable references:

- **F. H. Fröhner, "Applied Theory of Resolved and Unresolved Resonances," *Applied Nuclear Theory and Nuclear Model Calculations for Nuclear Technology Applications*, M.K. Mehta and J.J. Schmidt (eds.), World Scientific, Singapore (1989)**
  - **Work was initially presented at ICTP Winter Courses on Nuclear Physics and Reactors, 1978.**
  - **A comprehensive and useful guide to applied neutron resonance theory**
  - **A variety of topics — preparation of data, the various approximations to R-matrix theory, Doppler broadening, experimental complications, data-fitting procedures, statistical tests**

- **F. H. Fröhner, "Theory of Neutron Resonance Cross Sections for Safety Applications," KFK 5073, Kernforschungszentrum Karlsruhe (1992)**
  - **Review paper prepared for the "Workshop on Computation and Analysis of Nuclear Data Relevant to Nuclear Energy and Safety," held at the ICTP, Trieste, Italy, 10 Feb. - 13 March 1992**
  - **Updated version of the first paper... covers many of the same topics**

- **F. H. Fröhner, "Evaluation and Analysis of Nuclear Resonance Data," JEFF 18 (2000)**
  - **From the forward to this report – "describes in detail two elements necessary to perform a correct analysis of experimental data in the resonance energy range: the neutron-nucleus interaction theory in this energy range and the mathematical formalism of statistical inference."**

Scattering Theory…

- **Is mathematically rigorous (but usually approximated)**
- **Describes what is actually measured but not what happens inside the nucleus**
  - **(i.e. the neutron-nucleus interaction is not explicitly included)**
- **Parameterizes in terms of**
  - **interaction radii & boundary conditions**
  - **resonance energies & widths**
  - **quantum numbers**

Why parameterize the cross sections? Why not just use the measured data?

(for more details, see Frőhner's papers)

- **Too much information, too little understanding**
  - cross section vs energy ➔ ~100,000's of numbers
  - angular distributions have even more numbers
  - human minds seldom make sense of this many numbers!

- **Not enough information ➔ extrapolations are needed for practical applications**
  - other energies or energy regions
  - other experimental conditions:
    - temperature (Doppler broadening)
    - geometry (self-shielding calculations, multiple-scattering effects, etc.)
  - other nuclides (?)

Multilevel R-Matrix Theory

- **phenomenological**
  - **describes what is seen (i.e. the measured cross sections)**
  - **does not describe what is not seen (i.e. the underlying nuclear physics)**

- **mathematically correct**
  - **analytic, unitary, rigorous**

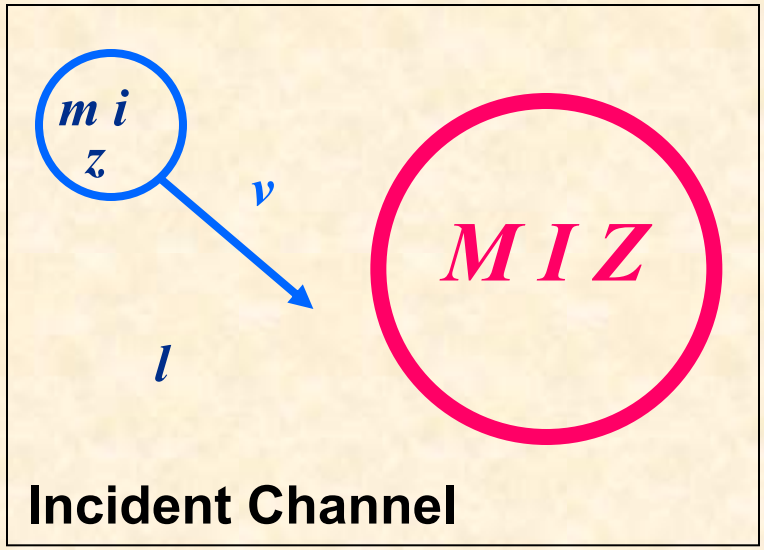
But is nearly always approximated in some fashion

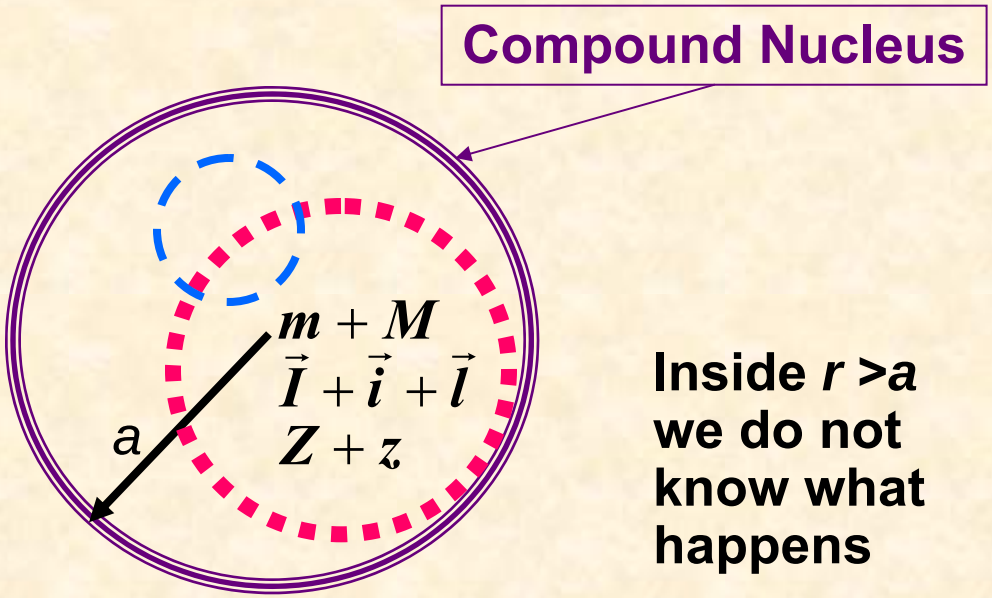
- **based on the following assumptions (re Lane & Thomas):**
  - **The applicability of nonrelativistic quantum mechanics**
  - **The absence or unimportance of all processes in which more than two product nuclei are formed**
  - **The absence or unimportance of all processes of creation or destruction**
  - **The existence of a finite radial separation beyond which no nuclear interactions occur**

Coulomb interaction is treated explicitly

Definitions of terms

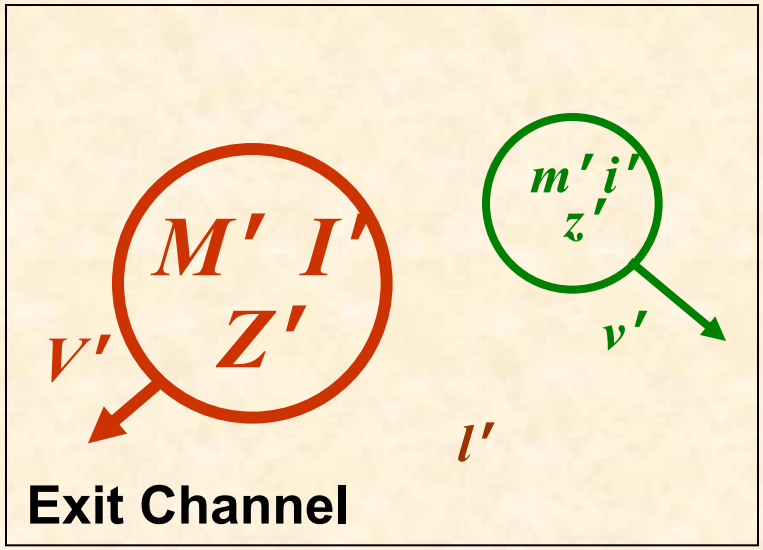
- ***Channel***
  - **pair of (incoming or outgoing) particles**
    - **info re interaction between those particles**
  - **illustrated on next slide**





Inside *r* >*a* we do not know what happens

Outside *r* >*a* there is no interaction
(except Coulomb)



Some channels can be both incident and exit. Others are exit only (e.g., fission fragments).

Definitions of terms

- ***Channel***
  - **pair of (incoming or outgoing) particles, defined by *mass*, *charge*, and *spin quantum numbers***
- ***Mass***
  - **atomic mass of the particles**
  - **neutron mass = 1.008665 amu**
  - ***amu* = atomic mass unit, from Nuclear Wallet Cards:**

```
= 1.49241909 × 10-3 erg   = 7.51300563 × 1012 /cm
= 9.3149432 × 108 eV      = 1.0809478 × 1013 K
= 2.25234242 × 1023 / sec = 1.6605402 × 10-24 g
```

- ***Charge* = *Z* for nuclide, 0 for neutron, 1 for proton**
- **Spin quantum numbers** **(see next page)**

Definitions of terms, continued

- ***spin quantum numbers***
  - (Note unprimed ➔ incident, primed ➔ exit):
  - i = intrinsic spin of incident particle = ½ for neutron
  - I = spin of target nuclide = integer or ½ -integer
  - l = relative orbital angular momentum (*s, p, d, f*, ...) (l = 0, 1, 2, 3,...)
  - s = channel spin $\vec{s} = \vec{I} + \vec{i}$
  - J = total spin for channel $\vec{J} = \vec{s} + \vec{l}$

Each of these also has an associated parity.

+1 for neutron

π

$(-1)^l$

(+1) (π)

(+1) (π) $(-1)^l$

- **Required: conservation of spin and parity**
  - (spin of incident channel = J^{π} = $J'^{\pi'}$ = spin of exit channel)

Angular momentum addition rules

(for those unfamiliar with vector algebra)

If vector spin $\vec{a}$ is given by

$$\vec{a} = \vec{b} + \vec{c}$$

then *a* (the magnitude of $\vec{a}$) is within the limits

$$|b - c| \le a \le b + c$$

and *a* is either integer

(if *b* and *c* are both integer or both half-integer)

or half-integer

(if one of *b* and *c* is integer and the other half-integer)

Table shows angular momentum summations for 0, 1/2, 1, 3/2, and 2

b	*c*	*a = b + c*
0	0	0
0	1/2	1/2
0	1	1
0	3/2	3/2
0	2	2
1/2	1/2	0,1
1/2	1	1/2,3/2
1/2	3/2	1,2
1/2	2	3/2,5/2
1	1	0,1,2
1	3/2	1/2,3/2,5/2
1	2	1,2,3
3/2	3/2	0,1,2,3
3/2	2	1/2,3/2,5/2,7/2
2	2	0,1,2,3,4

Multilevel R-matrix theory

$$\sigma^{total} = \frac{2\pi}{k^2} \sum_J g_J \sum_{\substack{incident \\ channels\ c}} \left(1 - \mathrm{Re}\left(U_{cc}^{J^\pi}\right)\right)$$

(There are similar equations for other cross section types)

Scattering matrix

$$U_{cc'}^J = \Omega_l W_{cc'}^J \Omega_{l'} \qquad \Omega_l = e^{-i\varphi_l}$$

$$W = P^{1/2}\left(I - RL\right)^{-1}\left(I - RL^*\right)P^{-1/2} \qquad L = \left(S - B\right) + iP$$

R-matrix

$$R_{cc'} = \sum_\lambda \frac{\gamma_{\lambda c}\gamma_{\lambda c'}}{E_\lambda - E - i\Gamma_\lambda^\gamma} \qquad \Gamma_{\lambda c} = 2P_l\left(\gamma_{\lambda c}\right)^2$$

Resonance parameters (values are needed in R-matrix codes)

Multilevel R-matrix theory, continued

$$R_{cc'} = \sum_{\lambda} \frac{\gamma_{\lambda c}\, \gamma_{\lambda c'}}{E_{\lambda} - E - i\Gamma_{\lambda}^{\gamma}/2}$$

The presence of capture width in denominator is what makes Reich-Moore different from "full" R-matrix.

Multilevel R-matrix theory, continued

- **Complete list of definitions, equations, derivations, etc., are available**
  - **in the SAMMY users' manual**
  - **in extended lecture notes**