Resonance Theory

Basics

- Deals with the description of nucleus-nucleus interaction and aims at the prediction of the experimental structure of cross-sections
- Interaction model which treats the nucleus as a black box
  - Potential is unknown so models cannot predict accurately
  - Only care at what can be observed before and after a collision

R-matrix theory

- Introduced by Wigner and Eisenbud (1947)
- Requires no information about internal structure of the nucleus
- It is mathematically rigorous
  - Usually approximated
  - Most physical and appropriate of resonance framework
- Cross-sections are parametrized in terms of
  - Interaction radii & boundary condition
  - Resonance energy & widths
  - Quantum number (angular momentum, spin, …)

Why bother?

- Couldn’t we just use the measured data?
  - Too much information, too little understanding
    - x.s. vs energy would requires 100,000’s of experimental points
    - Angular distributions would require even more
  - Need for extrapolation
    - Different energies
    - Temperature changes
    - Geometry considerations (self-shielding, …)
    - Unstable or rare nuclides

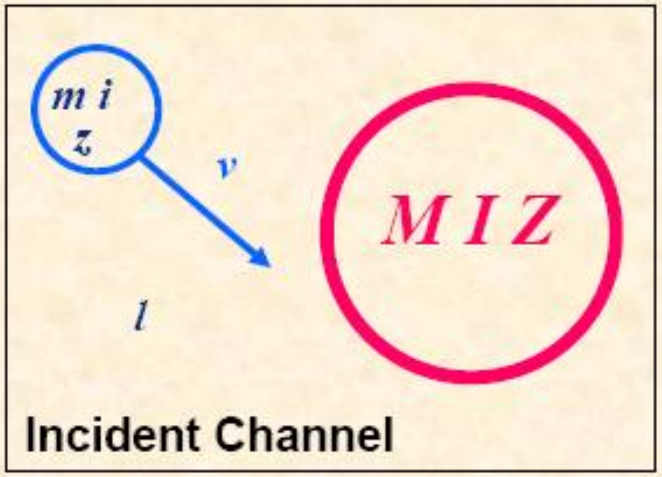
R-matrix theory Assumptions

- Applicability of non-relativistic quantum mechanics
- Unimportance of processes where more than two product nuclei are formed
- Unimportance of all processes of creation or destruction
- Existence of a finite radial distance beyond which no nuclear interaction occurs

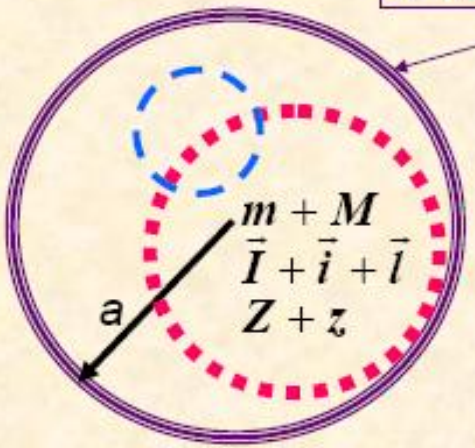
- Based on the notion that we can describe accurately what's far enough from the compound nucleus but not what's inside

Definition

- R-matrix is called a channel-channel matrix
- Channel
  - Designates a possible pair of nucleus and particle and the spin of the pair
  - Incoming channel (c)
  - Outgoing channel (c’)
  - Defined by pair of particles, mass, charge, spin
    - Many possible channels exist

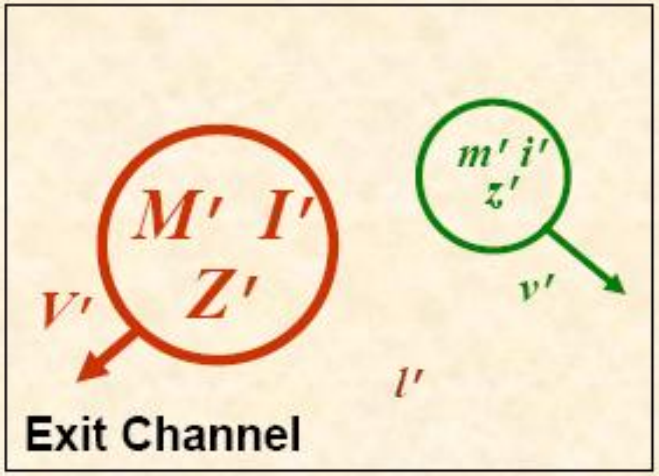


Compound Nucleus



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).

- Incoming channel (c)
  - We can control the incoming channel by the way we set up the experiment
    - Neutron energy
    - Target
- Outgoing channel (c’)
  - We can observe the outgoing channel with precise measurement

Total spin of the channel

- ***spin quantum numbers***
  - (Note unprimed → incident, primed → exit):

Each of these also has an associated parity.

  - i = intrinsic spin of incident particle = ½ for neutron — +1 for neutron
  - I = spin of target nuclide = integer or ½ -integer — π
  - l = relative orbital angular momentum (*s, p, d, f, ...*) (l = 0, 1, 2, 3,...)
  - s = channel spin $\vec{s} = \vec{I} + \vec{i}$ — (+1) (π) — $(-1)^l$
  - J = total spin for channel $\vec{J} = \vec{s} + \vec{l}$ — (+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

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

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

Cross-section

- In 22.101, you used the phase shift theory to determine an expression for the scattering cross-section
  - This expression can be defined in terms of the collision matrix U

$$\sigma = (\pi / k^2) \sin^2 \delta = (\pi / k^2) | 1 - U |^2.$$

  - Different relations between x.s and U exist for other interaction type

Goal of R-matrix

- Phase shift theory requires knowledge of the potential V(r)
  - Approximated by square well
- R-matrix theory builds a relationship between a matrix R that depends only on observable, measurable quantities and the collision matrix
  - Bypasses the need for the potential
  - Requires experimental data
- We will derive a simplistic case of a neutron interaction with no spin dependence

R-Matrix Derivation

- Start with the steady-state Schrödinger equation with a complex potential

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

  - Eigenvalue problem
- The wavefunction is expressed in the form of partial waves

$$\psi(r,\cos\theta)=\sum_{l=0}^{\infty}\frac{\varphi_l(r)}{r}P_l(\cos\theta)$$

- In radial geometry, the moment is a solution of the following equation

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

- Additionally, the moment can be represented by an expansion in terms of the eigenvectors of the solution

$$\phi_l(E,r)=\sum_{\lambda}A_{l\lambda}\phi_l(E_\lambda,r)\ .$$

  - Eigenvectors are also solutions of the above equation

- Eigenvectors are also a solution of:

(2) $$\left\{\frac{d^2}{dr^2}+\frac{2m}{\hbar^2}\left[E_\lambda - V(r) - \frac{l(l+1)\hbar^2}{2mr^2}\right]\right\}\phi_l(E_\lambda,r)=0 \ .$$

- Boundary conditions
  - Both equations must be finite at r = 0
  - Logarithmic derivative at nuclear surface is taken to be constant (where B_l is real)

$$\left[\frac{d\phi_l(E_\lambda,r)}{dr}\right]_{r=a} = a^{-1}B_l\phi_l(E_\lambda,a) \ ,$$

- The eigenvectors form a basis set, if normalized properly, they have the following property:

$$\int_0^a \phi_l(E_\lambda,r)\,\phi_l(E_{\lambda'},r)\,dr = \delta_{\lambda\lambda'} \ .$$

  - They form an orthonormal basis set
- From this condition, the expansion coefficients can be defined as:

$$A_{l\lambda} = \int_0^a \phi_l(E_\lambda,r)\,\phi_l(E,r)\,dr \ .$$

- Our goal is to eliminate the potential V(r)
  - Multiply eq (1) by the eigenvector and multiply eq (2) by the moment
  - Subtract resulting equations
  - Integrate between 0 and a
  - Result: Gives an expression for $\phi_l(E_\lambda,r)\,\phi_l(E,r)$
    - Which can be used to find the expansion coefficients

$$A_{l\lambda} = \frac{\hbar^2}{2m}(E_\lambda - E)^{-1}\left[\phi_l(E_\lambda,r)\frac{d\phi_l(E,r)}{dr} - \phi_l(E,r)\frac{d\phi_l(E_\lambda,r)}{dr}\right]_{r=a}.$$

- We can now find an expression for the moment at r = a

$$\phi_l(E,a) = \frac{\hbar^2}{2ma}\sum_\lambda \left[\frac{\phi_l(E_\lambda,a)\phi_l(E_\lambda,a)}{E_\lambda - E}\right]\left[r\frac{d\phi_l(E,a)}{dr} - B_l\phi_l(E,r)\right]_{r=a} .$$

- Where we can extract a definition of the R-matrix

$$R_l = \frac{\hbar^2}{2ma}\sum_\lambda \left[\frac{\phi_l(E_\lambda,a)\phi_l(E_\lambda,a)}{E_\lambda - E}\right]$$

- Or more commonly

$$R_l = \sum_\lambda \frac{\gamma_{\lambda l}\gamma_{\lambda l}}{E_\lambda - E} , \qquad \gamma_{\lambda l} = \sqrt{\frac{\hbar^2}{2ma}}\,\phi_l(E_\lambda,a) .$$

- $\gamma_{\lambda I}$ is the reduced width amplitude for level λ and angular momentum *I*
- λ is the resonance
- E_λ is the energy at the resonance peak
- $\gamma_{\lambda I}$'s and E_λ's are unknown parameters and can be evaluated by observing measured cross-sections
  - E_λ is the energy value at the peak
  - $\gamma_{\lambda I}$ is a measure of the width of the resonance at a certain amplitude for the nuclei at rest
    - Related to the more common Γ through a matrix transform
    - Not easy to measure because of temperature effects (Doppler)
    - Usually inferred from the resonance integral

General Form

$$R_{cc'} = \sum_{\lambda} \frac{\gamma_{\lambda c}\,\gamma_{\lambda c'}}{E_\lambda - E} \ ,$$

$$\gamma_{\lambda c} = \sqrt{\frac{\hbar^2}{2m_c a_c}}\ \phi_c(E_\lambda, a_c) \ .$$

Advantages/Disadvatages of R-matrix theory

- Disadvantages
  - Matrix inversion is always required
  - Channel radii and boundary condition appear arbitrary
  - Difficult to accommodate direct reactions (i.e. potential scattering)
- Advantages
  - Channel radii and boundary condition have natural definitions which makes them appealing
  - Reduced width concept has an appealing relation to nuclear spectroscopy

Boundary conditon

- In the early days, there was much confusion in the choice of channel radii and boundary condition
  - This topic has been debated heavily over the last 40 years!
  - Early papers described their choice as arbitrary
  - Optical model has facilitated the choice of these parameters
- "Natural" choices exist
  - Described in more details in pdf R-matrix theory (2)
  - B_l must be kept real to preserve the nature of the eigenvalue problem
  - Choice of boundary condition is to set it equal to the shift function at some point in the energy interval of measurement.
    - Keep only real part of the logarithmic derivative of the outgoing wave
  - Matching radii usually selected based on square-well interaction

Relation with collision matrix

- We found an expression for the solution of the wavefunction that doesn't depend on the potential
  - Depends on R-matrix
  - R-matrix depends on experimentally measured data
- Total wave function in region outside nuclear potential interaction can be expressed as a linear combination of the incoming and outgoing waves

$$\phi_l(r) = C_l\left[\phi_l^{inc}(r) - U_l\phi_l^{out}(r)\right] \qquad \text{for } r \geq a\ ,$$

- From R-matrix analysis, we found

$$\phi_l(E,a) = \left[r \frac{d\phi_l(E_\lambda,a)}{dr} - B_l \phi_l(E,r) \right]_{r=a} R_l \ ,$$

- We can then find that

$$U_l = \left(\frac{\phi_l^{inc}}{\phi_l^{out}} \right)_{r=a} \frac{1 - \left[\left(\frac{r}{\phi_l^{inc}} \frac{d\phi_l^{inc}}{dr} - B_l \right)_{r=a} \right] R_l}{1 - \left[\left(\frac{r}{\phi_l^{out}} \frac{d\phi_l^{out}}{dr} - B_l \right)_{r=a} \right] R_l} \ .$$

- Defining

$$L_l^* = \left(\frac{r}{\phi_l^{out}} \frac{d\phi_l^{out}}{dr} \right)_{r=a} . \qquad L_l = \left(\frac{r}{\phi_l^{inc}} \frac{d\phi_l^{inc}}{dr} \right)_{r=a} .$$

- We get

$$U_l = \left(\frac{\phi_l^{inc}}{\phi_l^{out}} \right)_{r=a} \frac{1 - (L_l^* - B_l)_{r=a} R_l}{1 - (L_l - B_l)_{r=a} R_l} .$$

General form

$$U = \rho^{1/2} \phi_{out}^{-1} [I - R(L - B)]^{-1} [I - R(\bar{L} - B)] \phi_{inc} \rho^{-1/2} \quad .$$

- No approximation has been made
  - Exact representation between U and R

Level matrix

- The R-matrix is fairly small but fairly complex to built
- Wigner introduced a clearer representation called the A-matrix whose elements correspond to energy levels
  - A is much larger
  - But its parameters are clearly defined
  - Summation is over incoming channels

$$A^{-1}_{\mu\lambda} = (E_\lambda - E)\,\delta_{\mu\lambda} - \sum_c (\gamma_{\mu c} L_{0c} \gamma_{\lambda c}) \ .$$

A-matrix

$$(A^{-1}) = \begin{pmatrix} E_1+\Delta_1-E-\frac{i}{2}\Gamma_1 & \Delta_{12}-\frac{i}{2}\Gamma_{12} & \Delta_{13}-\frac{i}{2}\Gamma_{13} & \cdot & \cdot \\ \Delta_{12}-\frac{i}{2}\Gamma_{12} & E_2+\Delta_2-E-\frac{i}{2}\Gamma_2 & \Delta_{23}-\frac{i}{2}\Gamma_{23} & \cdot & \cdot \\ \Delta_{13}-\frac{i}{2}\Gamma_{13} & \Delta_{23}-\frac{i}{2}\Gamma_{23} & E_3+\Delta_3-E-\frac{i}{2}\Gamma_3 & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & & \end{pmatrix}$$

- Very large
  - Corresponds to the total number of resonances
  - Symmetric matrix
  - Diagonal terms depend on each level independently
  - Off-diagonal terms are mixed terms that introduce the influence of different levels on each other

$$U_{cc'} = e^{-i(\phi_c+\phi_{c'})}\left[\delta_{cc'}+2i\,P_c^{1/2}\Big(\sum_{\mu\lambda}\gamma_{\lambda c}A_{\lambda\mu}\gamma_{\mu c'}\Big)P_{c'}^{1/2}\right].$$

Multi-level Breit Wigner

- Neglecting off-diagonal terms yields the Breit Wigner approximation
  - Analyzing a single level at a time yields the Single level Breit Wigner (SLBW) approximation
    - Works well if resonances are well spaced
    - Originally developed by Wigner based on an analogy to the dispersion of light
  - In some cases, off-diagonal terms matter

$$A^{-1}_{\lambda\mu} = (E_\lambda - E - \sum_c L_{0c}\gamma^2_{\lambda c})\,\delta_{\lambda\mu} \ . \qquad U_{cc'} = e^{-i(\phi_c + \phi_{c'} - \frac{\pi}{2})} \sum_\lambda \frac{\Gamma^{1/2}_{\lambda c}\,\Gamma^{1/2}_{\mu c'}}{E_\lambda - E - \frac{i}{2}\Gamma_\lambda} \ ,$$

Reich Moore Formalism

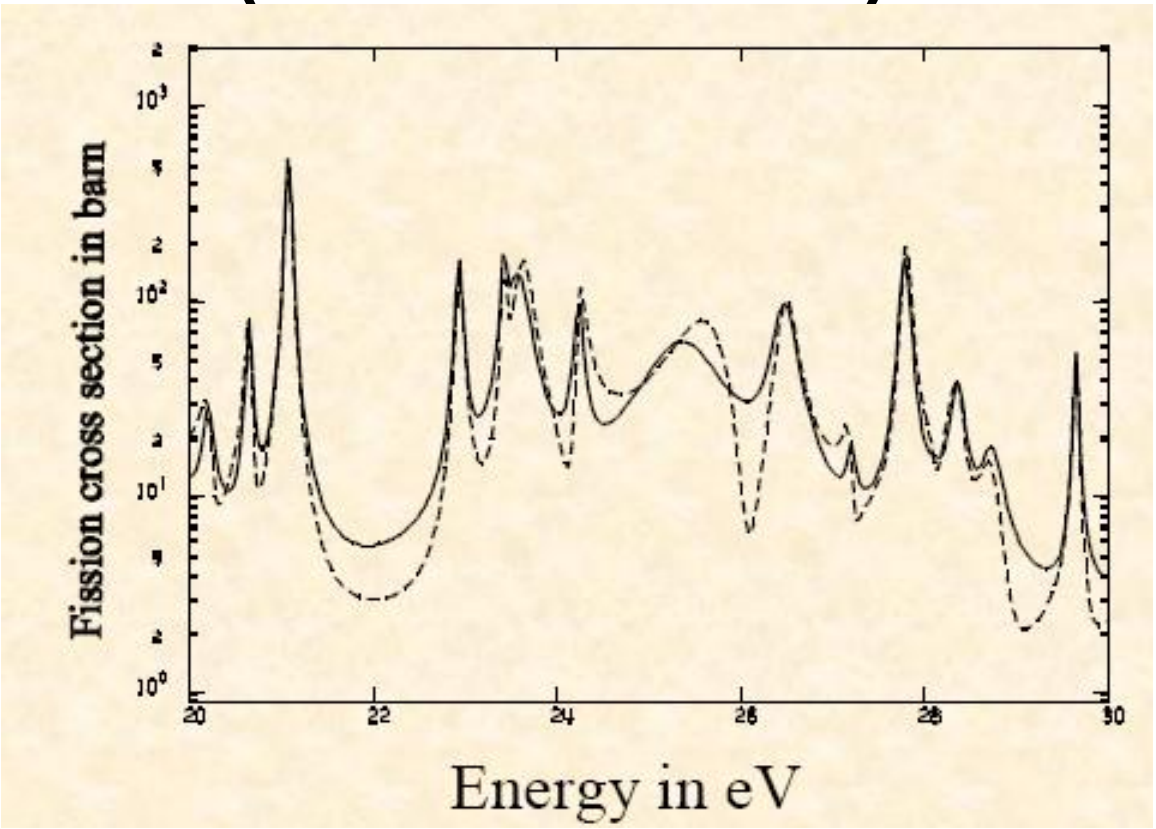
- Current method of choice
  - Keeps most off-diagonal terms
  - Neglects impact of gamma channels
    - Measurements have shown that fluctuations between gamma channels at different levels must be small

$$\sum_c \gamma_{\lambda c} L_{0c} \gamma_{\mu c} = \sum_{c \in \gamma} \gamma_{\lambda c} L_{0c} \gamma_{\mu c} + \sum_{c \notin \gamma} \gamma_{\lambda c} L_{0c} \gamma_{\mu c} \ , \qquad \sum_{c \in \gamma} \gamma_{\lambda c} L_{0c} \gamma_{\mu c} \approx \delta_{\mu\lambda} \sum_{c \in \gamma} L_{0c} \gamma_{\lambda c}^2 \ .$$

$$A_{\lambda\mu}^{-1} = (E_\lambda - E + \Delta_{\lambda\gamma} - \frac{i}{2}\Gamma_{\lambda\gamma})\,\delta_{\lambda\mu} + \sum_{c \notin \gamma} \gamma_{\lambda c} L_{0c} \gamma_{\mu c} \ ,$$

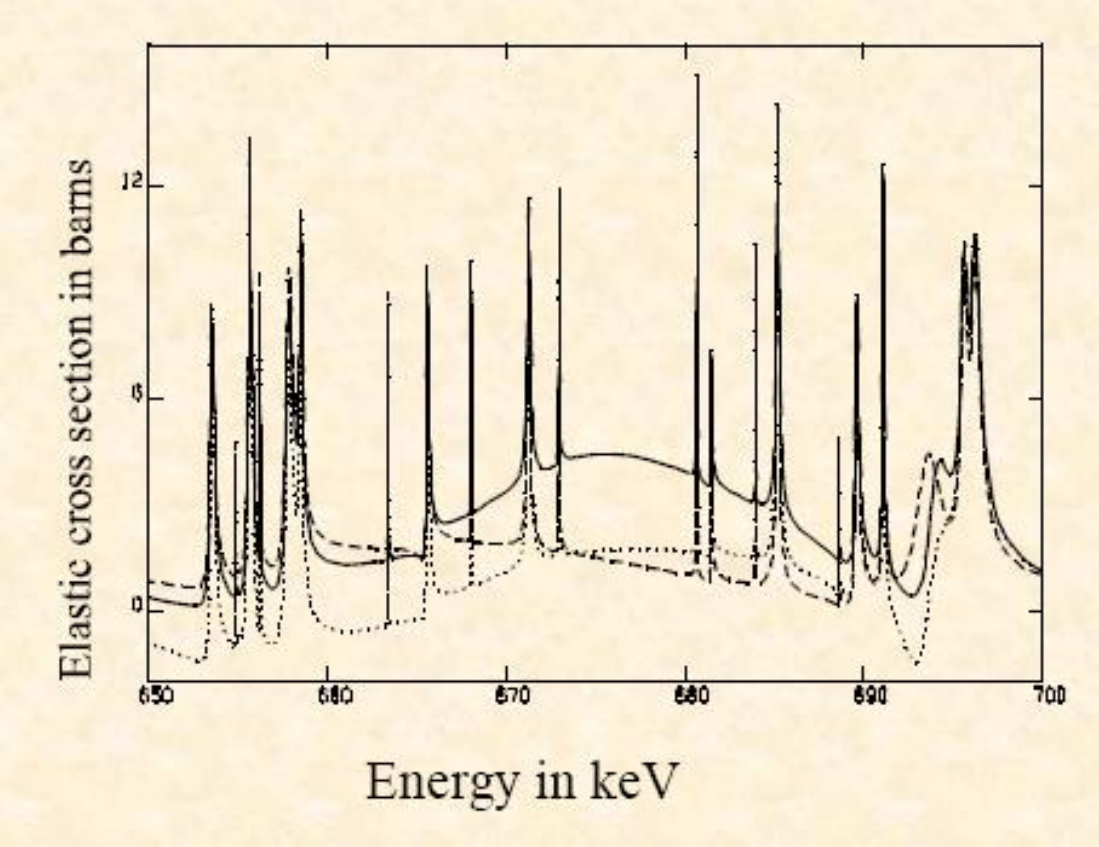
- MLBW is more restrictive than Reich Moore
  - Poor treatment of multi-channel effects
- SLBW is more restrictive than MLBW
  - Can give negative cross-section values

Reich Moore vs SLBW (U235 fission)



- Solid line : SLBW
- Dotted line : RM

Fe-56: RM, MLBW, SLBW



- Solid line: RM
- Dashed line: MLBW
- Dotted line: SLBW

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