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
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).

Inside $r > a$ we do not know what happens.
• 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 \( \Rightarrow \) incident, primed \( \Rightarrow \) exit):
    - \( i = \) intrinsic spin of incident particle = \( \frac{1}{2} \) for neutron \( +1 \) for neutron
    - \( I = \) spin of target nuclide = integer or \( \frac{1}{2} \) -integer \( \pi \)
    - \( l = \) relative orbital angular momentum (s, p, d, f, ...) \( (l = 0, 1, 2, 3, \ldots) \)
    - \( s = \) channel spin \( \vec{s} = \vec{l} + \vec{i} \) \( (+1) \ (\pi) \) \( (-1)^l \)
    - \( J = \) total spin for channel \( \vec{J} = \vec{s} + \vec{l} \) \( (+1) \ (\pi) \ (1)^l \)

- Required: conservation of spin and parity
  - (spin of incident channel = \( J^\pi = J' \ ^\pi' \) = 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

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<td>$b$</td>
<td>$c$</td>
<td>$a = b + c$</td>
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<td>0,1,2,3,4</td>
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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 $U$

$$\sigma = \left( \frac{\pi}{k^2} \right) \sin^2 \delta = \left( \frac{\pi}{k^2} \right) |1 - U| \ 2.$$  

- 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

\[
\psi(r, \cos \theta) = \sum_{l=0}^{\infty} \frac{\phi_l(r)}{r} P_l(\cos \theta)
\]
• In radial geometry, the moment is a solution of the following equation

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

\( (1) \)

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

\[
\phi_l(E,r) = \sum_{\lambda} A_{l\lambda} \phi_{l\lambda}(E,\lambda,r).
\]

– Eigenvectors are also solutions of the above equation
• Eigenvectors are also a solution of:

\[ (2) \begin{align*}
\frac{d^2}{dr^2} + \frac{2m}{\hbar^2} \left[ E_\lambda - V(r) - \frac{l(l+1)\hbar^2}{2mr^2} \right] \Phi_l(E_\lambda,r) &= 0.
\end{align*} \]

• 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 $r = a$

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

Where we can extract a definition of the R-matrix

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

Or more commonly

$$
R_i = \sum_\lambda \gamma_{\lambda i} \gamma_{\lambda i}, \quad \gamma_{\lambda i} = \sqrt{\frac{\hbar^2}{2ma} \phi_i(E_\lambda,a)}.
$$
- $\gamma_{\lambda l}$ is the reduced width amplitude for level $\lambda$ and angular momentum $l$
- $\lambda$ is the resonance
- $E_{\lambda}$ is the energy at the resonance peak
- $\gamma_{\lambda l}$'s and $E_{\lambda}$'s are unknown parameters and can be evaluated by observing measured cross-sections
  - $E_{\lambda}$ is the energy value at the peak
  - $\gamma_{\lambda l}$ is a measure of the width of the resonance at a certain amplitude for the nuclei at rest
    - Related to the more common $\Gamma$ 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/Disadvantages 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 condition

• 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)
  – $B_j$ 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

\[ \phi_i(r) = C_i \left[ \phi_i^{inc}(r) - U_i \phi_i^{out}(r) \right] \quad \text{for } r \geq a \]
• 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

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

\[ L_l^* = \left( \frac{r}{\phi_l^{out}} \frac{d\phi_l^{out}}{dr} \right)_{r=a} \]

\[ L_l = \left( \frac{r}{\phi_l^{inc}} \frac{d\phi_l^{inc}}{dr} \right)_{r=a} \]

• We get

\[ U_l = \left( \frac{\phi_l^{inc}}{\phi_l^{out}} \right)_{r=a} \frac{1 - (L_l^* - B_l)_{r=a}}{1 - (L_l - B_l)_{r=a}} R_l \]
General form

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

- 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

\[ A_{\mu\lambda}^{-1} = (E_\lambda - E) \delta_{\mu\lambda} - \sum_c (\gamma_{\mu c} L_{0 c} \gamma_{\lambda c}) \]
A-matrix

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

- 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

\[U_{cc'} = e^{-i(\Phi_c + \Phi_{c'})} \left[ \delta_{cc'} + 2i P_{c}^{1/2} \left( \sum_{\mu\lambda} \gamma_{\lambda c} A_{\lambda\mu} \gamma_{\mu c'} \right) P_{c'}^{1/2} \right].\]
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

\[ A_{\lambda \mu}^{-1} = (E_\lambda - E - \sum_c L_{0c} \gamma_{\lambda c}^2) \delta_{\lambda \mu} . \]

\[ U_{cc'} = e^{-i(\phi_c + \phi_{c'} - \frac{\pi}{2})} \sum_\lambda \frac{\Gamma^{1/2}_{\lambda c} \Gamma^{1/2}_{\mu c'}}{E_\lambda - E - \frac{i}{2} \Gamma_\lambda} , \]
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

\[
\sum_c \gamma_{\lambda c} L_{0c} \gamma_{\mu c} = \sum_{c \in \gamma} \gamma_{\lambda c} L_{0c} \gamma_{\mu c} + \sum_{c \in \gamma} \gamma_{\lambda c} L_{0c} \gamma_{\mu c}, \quad \sum_{c \in \gamma} \gamma_{\lambda c} L_{0c} \gamma_{\mu c} \approx \delta_{\mu \lambda} \sum_{c \in \gamma} L_{0c} \gamma_{\lambda c}^2 .
\]

\[
A^{-1}_{\lambda \mu} = (E_\lambda - E + \Delta_{\lambda \gamma} - i \frac{\Gamma_{\lambda \gamma}}{2}) \delta_{\lambda \mu} + \sum_{c \in \gamma} \gamma_{\lambda c} L_{0c} \gamma_{\mu c} .
\]
• 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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