SAMMY Workshop Part 4.1a

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Part 4.1a, Scattering Theory Equations

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Outline

- **Derivation for a simple case (no spin, no charge)**
  - ***U*** **in terms of** ***R***
  - **Cross section in terms of** ***U***
- **The general case**
  - **Cross section in terms of** ***U*** **for the general case**
  - ***U*** **in terms of** ***R***
- **Level-Level matrix**
  - **Relationship to Reich-Moore approximation**

Derivation of R-Matrix Equations

- **Start from Schrödinger's Equation for wave function (wf) ψ with complex potential**

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

- **where $V \leftrightarrow$ scattering and $W \leftrightarrow$ absorption**
- **Expand wf in usual fashion**

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

Derivation, cont.

- **Radial portion obeys**

$$u_l'' + \left[k^2 - \frac{2m}{\hbar^2}\left(V + iW\right) - \frac{l\left(l+1\right)}{r^2} \right] u_l = 0$$

where momentum k is given by $E = \dfrac{\hbar^2 k^2}{2m}$

- **Restriction:**

$|\psi|^2$ is finite

$$u_l\left(r = 0\right) = 0$$

Derivation, cont.

- **In external region *r* >*a***
  - **nuclear forces are zero (*V* = *W* = 0)**
  - **solution has the form** $u_l(r) = I_l(r) - U_l O_l(r)$

where

- I_l **is an incoming and** O_l **an outgoing free wave**
- U_l **is the scattering matrix or collision matrix, and**

$$|U_l|^2 = 1 \text{ for } W = 0$$

$$|U_l|^2 < 1 \text{ for } W \neq 0$$

- **Wanted: appropriate analytic form for** U_l

Derivation, cont.

- **In internal region *r* < *a***
  - **Define eigenvalues E_λ and eigenfunctions $w_{\lambda l}$ for wave equation with *W* = 0:**

$$w_{\lambda l}'' + \left[k_\lambda^{\,2} - \frac{2m}{\hbar^2} V - \frac{l(l+1)}{r^2} \right] w_{\lambda l} = 0$$

where

$$k_\lambda^2 = 2mE_\lambda / \hbar^2$$

with boundary conditions

$$w_{\lambda l}(r=0) = 0 \quad \text{and} \quad a \frac{w'_{\lambda l}(a)}{w_{\lambda l}(a)} = B_l$$

Derivation, cont.

- **Note "B_l is real" means "$w_{\lambda l}$ are real"**
- **Note also: eigenfunctions $w_{\lambda l}$ are orthonormal**
  - **proof is in SAMMY manual**
- **Expand true internal wf (for non-zero W) in terms of $w_{\lambda l}$**

$$u_l(r) = \sum_{\lambda} c_{\lambda l}\, w_{\lambda l}(r) \quad \text{for } r \le a$$

- **Substitute into radial Schrödinger equation, solve for coefficients, match the surface boundary conditions …**

Derivation, cont.

- **Do lots of algebra, …**
- **Ultimately, find this form for wf at boundary:**

$$u_l(a) = \left[a\,u'_l - u_l B_l\right]_{r=a} \sum_\lambda \frac{\gamma_{\lambda l}^2}{\left(E_\lambda - E + i\,\Gamma_{\lambda l}/2\right)}$$

with

$$\gamma_{\lambda l} \equiv \sqrt{\frac{\hbar^2 w_{\lambda l}^2(a)}{2m\,a}} \qquad \Gamma_{\lambda l} = \frac{2\int_0^a W\,u_l\,w_{\lambda l}\,dr}{\int_0^a u_l\,w_{\lambda l}\,dr}$$

Derivation, cont.

- **Setting** $R_l = \sum_\lambda \frac{\gamma_{\lambda l}^2}{\left(E_\lambda - E + i\Gamma_{\lambda l}/2\right)}$

  gives $u_l(a) = \left[a\,u'_l - u_l B_l\right]_{r=a} R_l$

- **Substituting** $u_l = I_l - U_l O_l$

  lets us rewrite as

$$I_l - U_l O_l = \left[a\left(I'_l - U_l O'_l\right) - B_l\left(I_l - U_l O_l\right)\right]$$

Derivation, cont.

- **Solving for U gives** $$U_l = e^{-2i\varphi}\frac{1-R_l\left(L_l^* - B_l\right)}{1-R_l\left(L_l - B_l\right)}$$

where L_l is given by $$L_l \equiv a\frac{O_l'(a)}{O_l(a)} \equiv S_l + iP_l$$

and $e^{-2i\varphi}$ by $$\frac{I_l}{O_l} = \frac{O_l^*}{O_l} = \frac{|O|e^{-i\varphi}}{|O|e^{i\varphi}} = e^{-2i\varphi}$$

- **QED** **(for particles without charge or spin)**
  - **Omitted details are in the SAMMY manual**

Relating *U* to cross section

- **External wf has the form** **(for a spinless particle)**

$$\psi(r,\theta) = e^{ikz} + \frac{e^{ikr}}{r} f(\theta)$$

in which

$$f(\theta) = \frac{1}{2ik} \sum_l (2l+1)\left[U_l - 1\right] P_l(\cos\theta)$$

- **Angular distribution is then** $\frac{d\sigma}{d\Omega} = \left|f(\theta)\right|^2$

Relating *U* to cross section, cont.

- **Integrating over angle then gives the cross section as a function of energy**

$$\sigma = \frac{\pi}{k^2} \sum_l (2l+1) \left| U_l - 1 \right|^2$$

- **This holds for particles without charge or spin**
- **Next: equations for the general case**

σ in terms of *U* for the general case

- **Cross section from entrance channel *c* to exit channel *c'* (both with total angular momentum *J*)**

$$\sigma_{cc'} = \frac{\pi}{k_a^2} g_{J\alpha} \left| \delta_{cc'} - U_{cc'} \right|^2 \delta_{JJ'}$$

where

- ***U* is scattering matrix**
- **k_α = com momentum for the particles in channel c**

$$k_\alpha^2 = \frac{2m\, M^2}{(m+M)^2} E$$

σ in terms of *U*, cont.

- **where (continued)**
  - ***m*** **= projectile mass** **(neutron, perhaps)**
  - ***M*** **= nuclear mass**
  - ***E*** **= energy of incident neutron in the lab system**
  - g_c **is the spin statistical factor**

$$g_{J\alpha} = \frac{2J+1}{(2i+1)(2I+1)} = \frac{2J+1}{2(2I+1)}$$

σ in terms of *U*, cont.

- **Total cross section is the sum of all entrance channels *c*, all exit channels *c′*, and all angular momentum *J***

$$\sigma^{total} = \sum_{\substack{incident\\channels\\c}} \sum_{\substack{all\\channels\\c'}} \sum_{J} \frac{\pi}{k_\alpha^2} g_\alpha \left|\delta_{cc'} - U_{cc'}\right|^2$$

$$= \frac{\pi}{k_\alpha^2} \sum_{J} g_J \sum_{\substack{incident\\channels\\c}} \sum_{\substack{all\\channels\\c'}} \left(\delta_{cc'} - U_{cc'}^J \delta_{cc'} - U_{cc'}^* \delta_{cc'} + \left|U_{cc'}\right|^2\right)$$

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

σ in terms of *U*, cont.

- **Other cross sections are found similarly:**

$$\sigma^{elastic} = \frac{\pi}{k_\alpha^2} \sum_J g_J \sum_{\substack{c=incident \\ channel}} \left(1 - 2\,\mathrm{Re}\left(U_{cc}\right) + \sum_{\substack{c'=incident \\ channel}} \left| U_{cc'} \right|^2 \right)$$

and

$$\sigma_\alpha^{reaction} = \frac{\pi}{k_\alpha^2} \sum_J g_J \sum_{\substack{c=incident \\ channel}} \sum_{\substack{c'=reaction \\ channel}} \left| U_{cc'} \right|^2$$

where “reaction channels” include all channels that contribute to the particular interaction (reaction) of interest

U in terms of *R*

- **The scattering matrix *U* can be written as**

$$U_{cc'} = \Omega_c W_{cc'} \Omega_{c'}$$

with

$$\Omega_c = e^{-i\varphi_c}$$

Some equations are modified slightly for charged particles.

where

- l **= orbital angular momentum**
- **φ = potential phase shift**
- W **is given on next slide…**

U in terms of *R*, cont.

- **In matrix notation with indices suppressed, *W* is given by**

$$W = P^{1/2}(I - RL)^{-1}(I - RL^{*})P^{-1/2}$$

where

$$L = (S - B) + iP$$

and

- P **= penetrability**
- S **= shift factor**
- B **= arbitrary boundary constant at the channel radius** a_c
- I **= identity matrix**
- R **= R-matrix**

How to generate the pieces?

- **On next slide:**
  - **table of**
    - **penetrability (penetration factor) P**
    - **level shift factor S**
    - **potential scattering phase shift φ**
  - **for**
    - **orbital angular momentum l,**
    - **center of mass momentum k, and**
    - **channel radius a_c ,**
  - **with $\rho = ka_c$,**
  - **for non-Coulomb case**

l	P_l	S_l	φ_l
0	ρ	0	ρ
1	$\dfrac{\rho^3}{(1+\rho^2)}$	$\dfrac{-1}{(1+\rho^2)}$	$\rho - \tan^{-1}\rho$
2	$\dfrac{\rho^5}{(9+3\rho^2+\rho^4)}$	$-\dfrac{(18+3\rho^2)}{(9+3\rho^2+\rho^4)}$	$\rho - \tan^{-1}\left[\dfrac{3\rho}{(3-\rho^2)}\right]$
3	$\dfrac{\rho^7}{(225+45\rho^2+6\rho^4+\rho^6)}$	$\dfrac{-(675+90\rho^2+6\rho^4)}{(225+45\rho^2+6\rho^4+\rho^6)}$	$\rho - \tan^{-1}\left[\dfrac{\rho(15-\rho^2)}{(15-6\rho^2)}\right]$
4	$\dfrac{\rho^9}{(11025+1575\rho^2+135\rho^4+10\rho^6+\rho^8)}$	$\dfrac{-(44100+4725\rho^2+270\rho^4+10\rho^6)}{(11025+1575\rho^2+135\rho^4+10\rho^6+\rho^8)}$	$\rho - \tan^{-1}\left[\dfrac{\rho(105-10\rho^2)}{(105-45\rho^2+\rho^4)}\right]$
l	$\dfrac{\rho^2 P_{l-1}}{(l-S_{l-1})^2 + P_{l-1}^2}$	$\dfrac{\rho^2 (l-S_{l-1})}{(l-S_{l-1})^2 + P_{l-1}^2} - l$	$\varphi_{l-1} - \tan^{-1}\left(\dfrac{P_{l-1}}{l-S_{l-1}}\right)$

Summary of the equations:

- **Cross sections were defined in terms of *U***
- ***U* is given by** $U_{cc'} = \Omega_c W_{cc'} \Omega_{c'}$

with $\Omega_c = e^{-i\varphi_c}$

$$W = P^{1/2}(I - RL)^{-1}(I - RL^*)P^{-1/2}$$

and $L = (S - B) + iP$

- **Finally, the R-matrix is given in terms of levels and channels:**

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

R-Matrix

- **This formula for the R-matrix is "exact"**

Note the infinite number of levels

$$R_{cc'} = \sum_{\lambda=1}^{\infty} \frac{\gamma_{\lambda c}\gamma_{\lambda c'}}{E_\lambda - E}$$

Denominator could be zero

- **This is *not* the formula used in SAMMY**

A-Matrix

- **The level-level matrix (A-matrix) is defined as**

$$A^{-1}_{\mu\lambda} = \left(E_\lambda - E\right)\delta_{\mu\lambda} - \sum_c \gamma_{\mu c}\, L_c\, \gamma_{\lambda c}$$

- **Simple algebra shows that *A* is related to *R* via**

$$\left[\left(I - RL\right)^{-1} R\right]_{cc''} = \sum_{\lambda\nu} \gamma_{\lambda c}\, A_{\lambda\nu} \gamma_{\nu c''}$$

- **Why use *R* not *A*?**
  - **Few channels, many levels ➔ *A* is much bigger**
- **So why talk about *A*?**

A-Matrix, cont.

- **Summation includes all channels…**

$$A^{-1}_{\mu\lambda} = \left(E_\lambda - E\right)\delta_{\mu\lambda} - \sum_{\substack{c = all \\ channels}} \gamma_{\mu c} L_c \gamma_{\lambda c}$$

- **Gamma channels**
  - **Do not interact very much**
  - **Can be treated "on average"**
- **Approximation: assume no level-level interference in the gamma channels**

A-Matrix, cont.

- **Assume no level-level interference in gamma channels –**

$$A^{-1}_{\mu\lambda} = \left(E_\lambda - E\right)\delta_{\mu\lambda} - \sum_{\substack{c = \text{gamma} \\ \text{channels}}} \gamma_{\mu c} L_c \gamma_{\lambda c} - \sum_{\substack{c = \text{non-} \\ \text{gamma} \\ \text{channels}}} \gamma_{\mu c} L_c \gamma_{\lambda c}$$

$$\approx \left(E_\lambda - E\right)\delta_{\mu\lambda} - \delta_{\mu\lambda} \sum_{\substack{c = \\ \text{gamma} \\ \text{channels}}} \gamma_{\lambda c} L_c \gamma_{\lambda c} - \sum_{\substack{c = \\ \text{particle} \\ \text{channels}}} \gamma_{\mu c} L_c \gamma_{\lambda c}$$

$$= \left(E_\lambda - E - \sum_{\substack{c = \\ \text{gamma} \\ \text{channels}}} L_c \gamma^2_{\lambda c} \right)\delta_{\mu\lambda} - \sum_{\substack{c = \\ \text{particle} \\ \text{channels}}} \gamma_{\mu c} L_c \gamma_{\lambda c}$$

A-Matrix, cont.

- **Note that $L = S - B + iP = i$ for gamma channels**

➔ $$A^{-1}_{\mu\lambda} \approx \left(E_\lambda - E - i\bar{\Gamma}_{\lambda\gamma}/2\right)\delta_{\mu\lambda} - \sum_{\substack{c = \\ \text{particle} \\ \text{channels}}} \gamma_{\mu c} L_c \gamma_{\lambda c}$$

in which we have set

$$\bar{\Gamma}_{\lambda\gamma} = 2 \sum_{\substack{c = \\ \text{gamma} \\ \text{channels}}} \gamma^2_{\lambda c}$$

A-Matrix, cont.

- **Translating that A-matrix into *R* gives the Reich-Moore formula**

$$R_{cc'} \approx \sum_{\lambda} \frac{\gamma_{\lambda c}\gamma_{\lambda c'}}{E_{\lambda} - E - i\bar{\Gamma}_{\lambda\gamma}/2}$$

Denominator could not be zero for real values of E

- **This *is* the formula used in SAMMY**