Scattering theory II: continuation

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What we learnt?

Scattering amplitude nuclear only

$$f(\theta) = \frac{1}{2ik}\sum_{L=0}^{\infty}(2L+1)P_L(\cos\theta)(\mathbf{S}_L - 1)$$

$$\sigma(\theta) \equiv \frac{d\sigma}{d\Omega} = \left|\frac{1}{2ik}\sum_{L=0}^{\infty}(2L+1)P_L(\cos\theta)(\mathbf{S}_L - 1)\right|^2$$

Coulomb+nuclear

$$f_n(\theta) = \frac{1}{2ik}\sum_{L=0}^{\infty}(2L+1)P_L(\cos\theta)e^{2i\sigma_L(\eta)}(\mathbf{S}_L^n - 1)$$

$$\sigma_{nc}(\theta) = |f_c(\theta) + f_n(\theta)|^2 \equiv |f_{nc}(\theta)|^2$$

Integrated cross sections:

$$\begin{aligned}\sigma_{el} &= \int_0^{2\pi} d\phi \int_0^{\pi} d\theta \sin\theta\, \sigma(\theta) \\ &= 2\pi \int_0^{\pi} d\theta \sin\theta |f(\theta)|^2 \\ &= \frac{\pi}{k^2}\sum_{L=0}^{\infty}(2L+1)|1 - \mathbf{S}_L|^2 \\ &= \frac{4\pi}{k^2}\sum_{L=0}^{\infty}(2L+1)\sin^2\delta_L,\end{aligned}$$

$$\sigma_A = \frac{2}{\hbar v}\frac{4\pi}{k^2}\sum_L (2L+1)\int_0^{\infty}[-W(R)]\,|\chi_L(R)|^2\, dR$$

$$\sigma_R = \frac{\pi}{k^2}\sum_L (2L+1)(1 - |\mathbf{S}_L|^2)$$

Optical potentials

- obtained from:
  1) Fitting a single elastic scattering data set (local optical potential)
  2) Fitting many sets of elastic data at several energies on several targets (global optical potential)
  3) Theory (folding models – depend on density distribution)

- real parts get weak with beam energy (become repulsive at 300 MeV)
- imaginary terms dominate at the higher energies

- Coulomb interaction: uniform charge distribution with radius R_{coul}

$$V_{\mathrm{Coul}}(R) = Z_p Z e^2 \times \begin{cases} \left(\frac{3}{2} - \frac{R^2}{2R_{\mathrm{Coul}}^2}\right)\frac{1}{R_{\mathrm{Coul}}} & \text{for } R \leq R_{\mathrm{Coul}} \\ \frac{1}{R} & \text{for } R \geq R_{\mathrm{Coul}} \end{cases}$$

Optical potentials

o real part weaker for neutrons that for protons

$$V(R) = V_0(R) + \frac{1}{2} t_z \frac{N-Z}{A} V_T(R)$$

isoscalar and isovector components

o spin orbit term: couples spin and orbital motion

elastic scattering in fresco

```
p+Ni78 Coulomb and Nuclear;
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 &pot /
 &overlap /
 &coupling /
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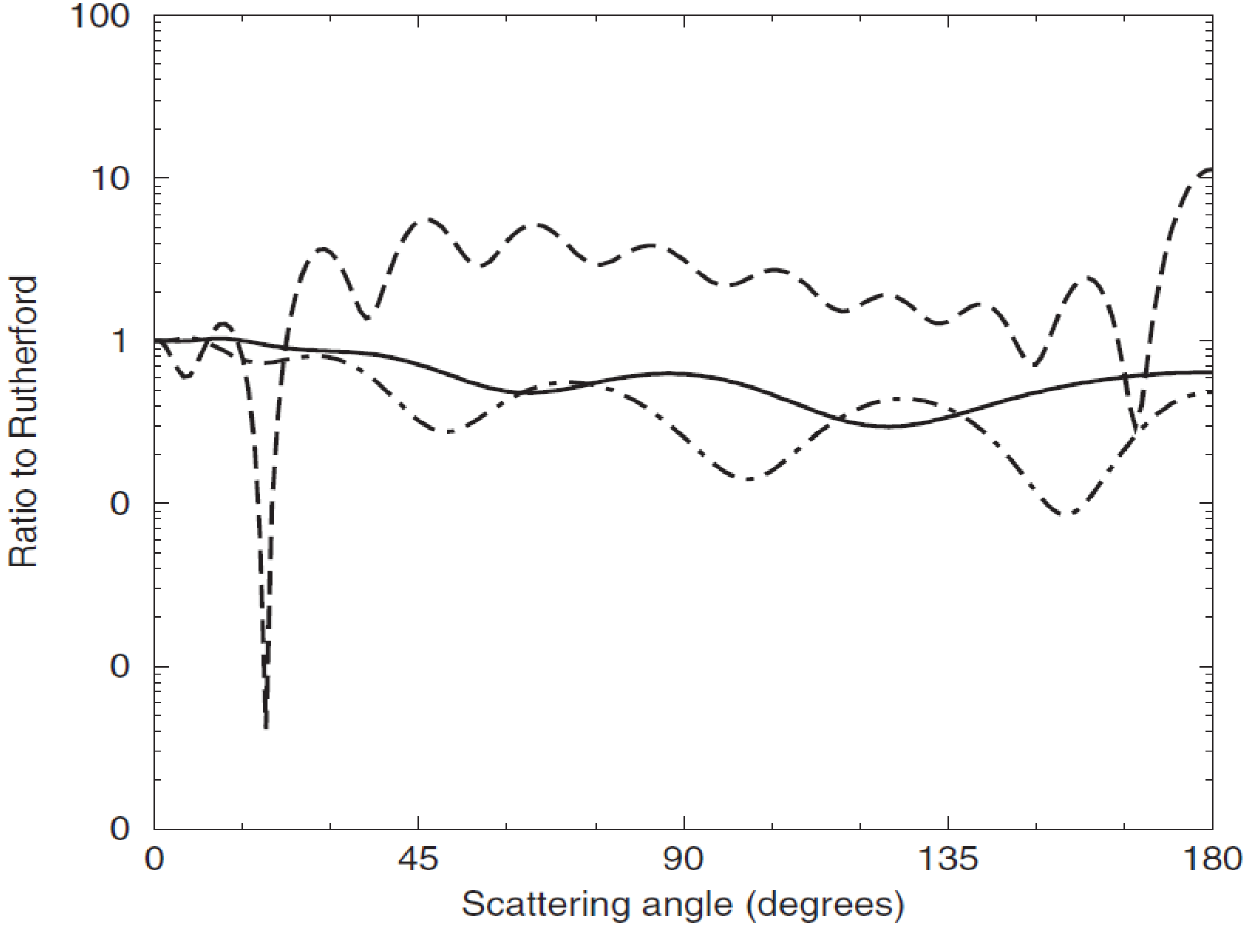
Box B.1 FRESCO **input for the elastic scattering of protons on ^{78}Ni at several beam energies**

elastic scattering in fresco



oWhich curve correponds to highest energy?

Comments on homework (elastic scattering)

o $d\sigma_{el}/d\theta$ always forward peaked! Remember ratio to rutherford...

o optical potential is energy dependent

orelation of R_r with diffraction pattern
o relation of R_i and L_{max} of absorption S(L)

o relation with W and flux removal from elastic (absorption cross section)

o are the results converged? Needs to be checked per energy
o what were the difficulties in the analysis?

Direct and exchange amplitudes

o so far we have considered p+t -> p' + t'

o now we need to consider:

(a) Scattering of identical fermions: $p = t$ of odd baryon number;

(b) Scattering of identical bosons: $p = t$ of even baryon number; and

(c) Exchange scattering: $p' = t$ and $t' = p$, and p is distinguishable from t,

o consider an exchange index

$$\begin{aligned} \varepsilon &= +1 \text{ for boson-boson} \\ \varepsilon &= -1 \text{ for fermion-fermion} \end{aligned}$$

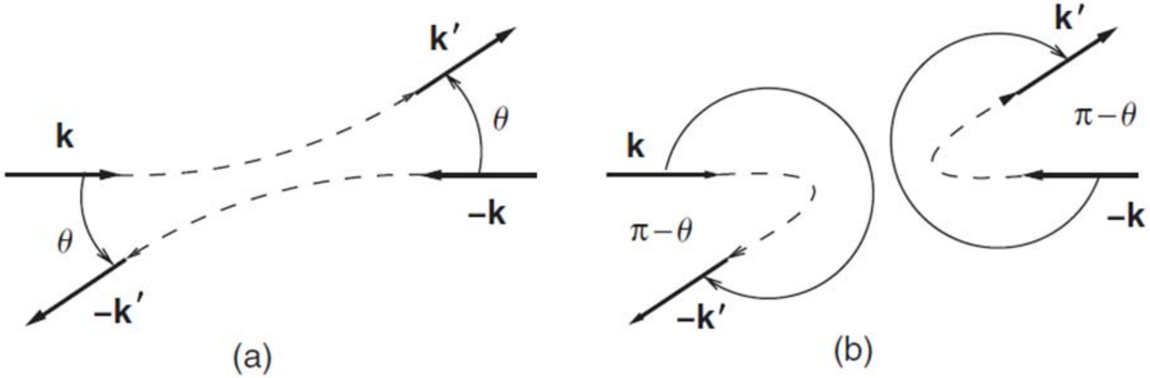
$$\hat{P}_{pt}\Psi^{M_{\text{tot}}}_{xJ_{\text{tot}}}(\mathbf{R}_x, \xi_p, \xi_t) = \varepsilon\Psi^{M_{\text{tot}}}_{xJ_{\text{tot}}}(-\mathbf{R}_x, \xi_t, \xi_p)$$

$$\varepsilon = (-1)^{2I_p}$$

Direct and exchange amplitudes

o first identical
spinless particles

$$\psi^{\mathrm{asym}}(\mathbf{R}) = A\left[\mathrm{e}^{\mathrm{i}kz} + f(\theta)\frac{\mathrm{e}^{\mathrm{i}kR}}{R}\right]$$



o for two identical particles the wfn should be

$$\Psi_{\varepsilon}^{\mathrm{asym}}(\mathbf{R}) = \psi^{\mathrm{asym}}(\mathbf{R}) + \varepsilon\,\psi^{\mathrm{asym}}(-\mathbf{R})$$

o scattered outgoing wave properly symmetrized should be:

$$\Psi_{\varepsilon}^{\mathrm{out}}(\mathbf{R}) = A[f(\theta) + \varepsilon f(\pi-\theta)]\frac{\mathrm{e}^{\mathrm{i}kR}}{R} \equiv A f_{\varepsilon}(\theta)\frac{\mathrm{e}^{\mathrm{i}kR}}{R}$$

Direct and exchange amplitudes

$$P_L(\cos(\pi - \theta)) = (-1)^L P_L(\cos\theta)$$

- cross section for identical particle scattering

$$\sigma(\theta) = |f_\varepsilon(\theta)|^2 = |f(\theta) + \varepsilon f(\pi - \theta)|^2$$
$$= |f(\theta)|^2 + |f(\pi - \theta)|^2 + 2\varepsilon \,\mathrm{Re}\, f(\theta)^* f(\pi - \theta).$$

- the partial wave expansion for the scattering amplitude is:

$$f_\varepsilon(\theta) = \frac{1}{k} \sum_{L=0}^{\infty} (2L+1) P_L(\cos\theta) \mathbf{T}_L [1 + \varepsilon(-1)^L],$$

For bosons, odd partial waves do not contribute!
Even partial waves are doubled!

Direct and exchange with spin

o permutation best done in LS coupling:

$$\hat{P}_{pt}|L(I_p,I_t)S;J_{\rm tot}x\rangle = (-1)^L(-1)^{S-I_p-I_t}|L(I_t,I_p)S;J_{\rm tot}x\rangle$$

o the partial wave expansion for the scattering amplitude is:

$$f_S(\theta) = \frac{1}{k}\sum_{L=0}^{\infty}(2L+1)P_L(\cos\theta)\mathbf{T}_L[1+\varepsilon(-1)^{L+S-I_p-I_t}]$$

$$= \frac{1}{k}\sum_{L=0}^{\infty}(2L+1)P_L(\cos\theta)\mathbf{T}_L[1+(-1)^{L+S}]$$

For S=0 odd partial waves do not contribute!
For S=1 even partial waves do not contribute!

Direct and exchange with spin

o characteristic interference patterns for different spin states!

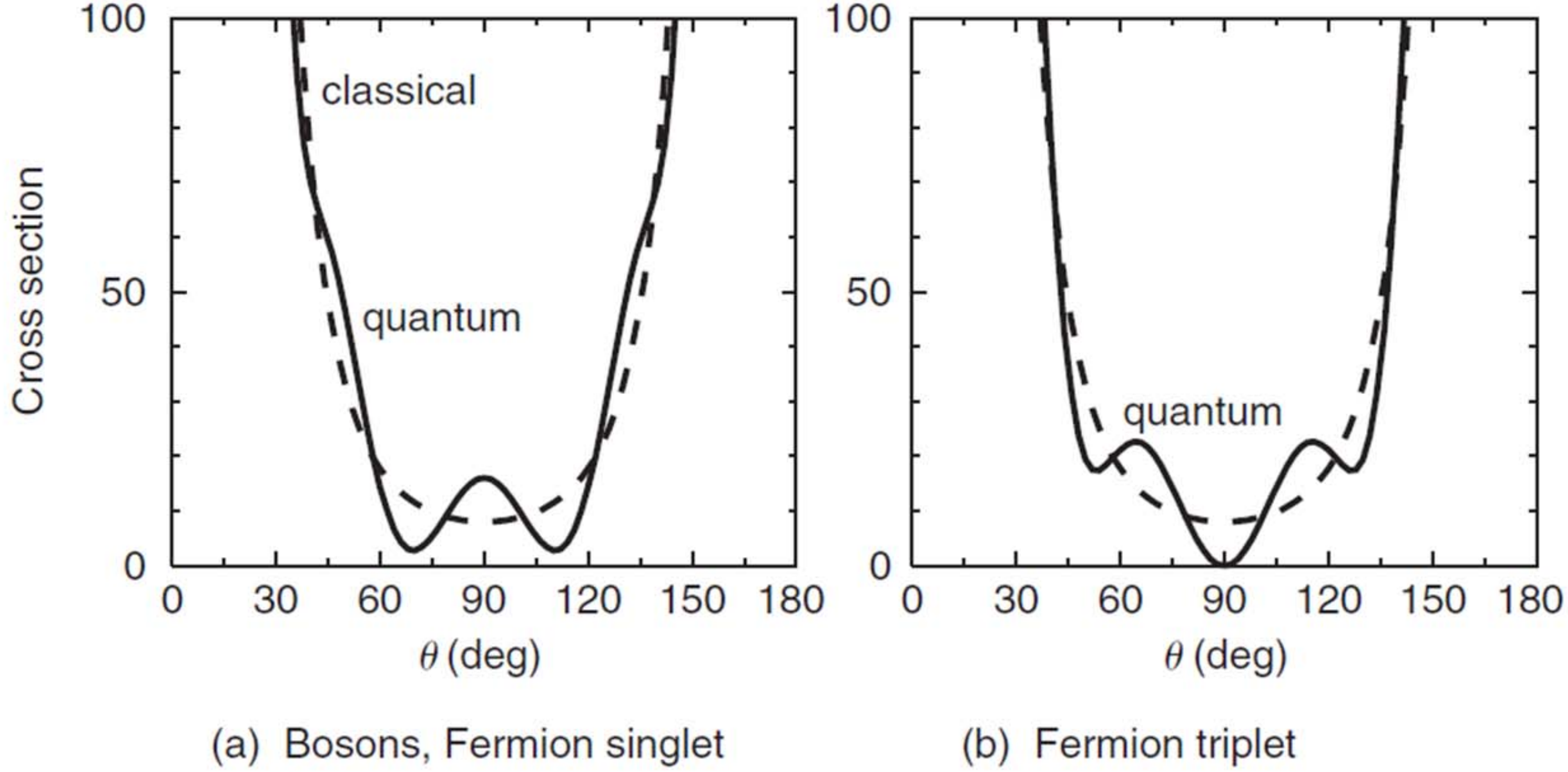


Fig. 3.9. Fermion singlet (a) and triplet (b) nucleon-nucleon scattering cross sections, assuming pure Coulomb scattering with $\eta = 5$. Case (a) also applies for boson scattering. The cross section is in units of $\eta^2/4k^2$.

Fitting data

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

Measure of discrepancy

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

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

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

If $\chi^2/N >> 1$ then theory needs improvement
If $\chi^2/N << 1$ errors have been overestimated

Fitting data (including an overall scale)

Comparing theory and experiment
$\{p_j, s\}$ inputs parameter set (s is overall scale)
$\sigma^{exp}(i)$ experimental data ($\Delta\sigma$ standard deviation)

Measure of discrepancy

$$\chi^2 = \frac{(s - E[s])^2}{\Delta s^2} + \sum_{i=1}^{N} \frac{(\sigma^{th}(i) - s\,\sigma^{exp}(i))^2}{\Delta\sigma(i)^2}$$

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

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

Multivariate theory

Probability distribution for a set of random variables
(normal distribution)

$$f(x) = \frac{1}{\sqrt{2\pi}\,\Delta} \exp\left[-\frac{(x-\mu)^2}{2\Delta^2}\right]$$

Mean $\mu = E[x]$

Standard deviation Δ

$$\Delta^2 = E[(x-\mu)^2] = E[x^2] - 2\mu E[x] + \mu^2 = E[x^2] - \mu^2$$

$$E[X] \equiv \int X\, f(x) \mathrm{d}x$$

Chi2 and the covariance matrix

Probability that a data point x_i with variance Δ^2_i is correctly fitted by theory y_i

$$f_i(y_i) = \frac{1}{\sqrt{2\pi}\,\Delta_i} \exp\left[-\frac{(x_i - y_i)^2}{2\Delta_i^2}\right]$$

For many statistically independent points the joint probability is:

$$P_{\text{tot}} = (2\pi)^{-\frac{N}{2}} \Delta^{-1} \exp\left[-\frac{1}{2}\sum_{i=1}^{N} \frac{(x_i - y_i)^2}{\Delta_i^2}\right]$$

$$= (2\pi)^{-\frac{N}{2}} \Delta^{-1} \exp\left[-\frac{1}{2}\mathcal{X}^2\right],$$

$$\Delta = \prod_i^N \Delta_i$$

$$\mathcal{X}^2 = \sum_i^N \frac{(x_i - y_i)^2}{\Delta_i^2}$$

Multivariate theory (many correlated variables)

Probability distribution for a set of correlated variables $\underline{x}=\{x_1,\ldots,x_N\}$ might no longer be normal

$$f(\mathbf{x}) = (2\pi)^{-\frac{N}{2}} |\mathbf{V}|^{-\frac{1}{2}} \exp\left[-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu})^T \mathbf{V}^{-1} (\mathbf{x}-\boldsymbol{\mu})\right]$$

Symmetic covariance matrix

$$\mathbf{V}_{ij} = E[(x_i - \mu_i)(x_j - \mu_j)]$$

Diagonal terms are the standard deviations squared
Off diagonal depend on correlation coefficients

$$\mathbf{V}_{ij} = \rho_{ij} \Delta_i \Delta_j$$

Chi2 and the covariance matrix

Probability that a data point x_i with variance Δ^2_i is correctly fittend by theory y_i

$$f_i(y_i) = \frac{1}{\sqrt{2\pi}\,\Delta_i} \exp\left[-\frac{(x_i - y_i)^2}{2\Delta_i^2}\right]$$

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$$P_{\text{tot}} = (2\pi)^{-\frac{N}{2}} \Delta^{-1} \exp\left[-\frac{1}{2}\sum_{i=1}^{N} \frac{(x_i - y_i)^2}{\Delta_i^2}\right]$$

$$= (2\pi)^{-\frac{N}{2}} \Delta^{-1} \exp\left[-\frac{1}{2}\mathcal{X}^2\right],$$

$$\Delta = \prod_i^N \Delta_i \qquad \mathcal{X}^2 = \sum_i^N \frac{(x_i - y_i)^2}{\Delta_i^2}$$

Using this we can generalize the Chi2 definition by:

$$\mathcal{X}^2 = (\mathbf{x} - \mathbf{y})^T \mathbf{V}^{-1} (\mathbf{x} - \mathbf{y})$$

$$= \sum_{ij=1}^{N} (x_i - y_i)[\mathbf{V}^{-1}]_{ij}(x_j - y_j).$$

Chi2 distribution

Adding together N-squares of independent normal distributions z^2_i with zero mean and unit variance

$$\mathcal{X}^2 = \sum_{i=1}^{N} z_i^2$$

$$f(\mathcal{X}^2) = \frac{1}{2\Gamma(\frac{N}{2})} \left(\frac{\mathcal{X}^2}{2}\right)^{\frac{N}{2}-1} e^{-\mathcal{X}^2/2}$$

$$E[\mathcal{X}^2] = N; \quad V(\mathcal{X}^2) = 2N; \quad \sigma(\mathcal{X}^2) = \sqrt{2N}$$

For N>20 the Chi2 distribution becomes close to the normal distribution.

What is a perfect fit?

When theory predicts exactly the statistical mean of experiment

$$y_i = E[x_i] = \mu_i$$

$$z_i^2 = \frac{(x_i - y_i)^2}{\Delta_i^2} = \frac{(x_i - \mu_i)^2}{\Delta_i^2}$$ have zero means and unit variances

If z_i have normal distributions $\mathcal{X}^2 = \sum_i^N z_i^2$ follows ch2 distribution mean N and variance 2N

Thus our reasoning $\chi^2/N \sim 1$

Expanding chi2 around a minimum

Let us consider the expansion of chi2 around a mimimum found for the set of parameters $\{p_j^0\}$

$$\mathcal{X}^2(p_1,\ldots,p_P) \approx \mathcal{X}^2(p_1^0,\ldots,p_P^0) + \frac{1}{2}\sum_{m,n=1}^{P} \mathbf{H}_{mn}(p_m - p_m^0)(p_n - p_n^0)$$

$$\equiv \mathcal{X}^2(\mathbf{p}^0) + \frac{1}{2}(\mathbf{p}-\mathbf{p}^0)^T\,\mathbf{H}\,(\mathbf{p}-\mathbf{p}^0)$$

Hesse matrix

$$\mathbf{H}_{mn} = \frac{\partial^2}{\partial p_m \partial p_n}\mathcal{X}^2(p_1,\ldots,p_P)$$

Covariance matrix

$$(\mathbf{V}^{\mathrm{p}})^{-1} = \tfrac{1}{2}\mathbf{H} \quad \text{or} \quad \mathbf{V}^{\mathrm{p}} = 2\,\mathbf{H}^{-1}.$$

The fitting probability can be defined in terms of the Hesse matrix:

$$P_{\mathrm{tot}} = \frac{1}{(2\pi)^{\frac{N}{2}}\Delta} e^{-\frac{\mathcal{X}^2(\mathbf{p}^0)}{2}} \exp\left[-\frac{1}{4}\sum_{mn}^{P}(p_m - p_m^0)\mathbf{H}_{mn}(p_n - p_n^0)\right]$$

Allowed parameters within 1sigma

This happens with argument of exp is 1/2

$$\frac{1}{2}\sum_{mn}^{P}(p_m - p_m^0)\mathbf{H}_{mn}(p_n - p_n^0) = 1$$

Using the Taylor expansion this can be written as

$$\mathcal{X}^2(p_1, \ldots, p_P) = \mathcal{X}^2(p_1^0, \ldots, p_P^0) + 1$$

Ex: legendre polynomial fitting

Experimentalists have cross sections which they expand in legendre polynomials

$$\sigma(\theta) = \sum_{\Lambda \geq 0} a_\Lambda P_\Lambda(\cos\theta)$$

We know more about the coefficients from reaction theory:

$$\sigma(\theta) = \left| \frac{1}{k} \sum_{L=0}^{\infty} (2L+1) P_L(\cos\theta) \mathbf{T}_L \right|^2$$

$$= \frac{1}{k^2} \sum_{LL'} (2L+1)(2L'+1) P_L(\cos\theta) P_{L'}(\cos\theta) \mathbf{T}_L^* \mathbf{T}_{L'}.$$

$$a_\Lambda = \frac{1}{k^2} \sum_{LL'} (2L+1)(2L'+1) \langle L0, L'0 | \Lambda 0 \rangle^2 \mathbf{T}_L^* \mathbf{T}_{L'}.$$

Ex: optical potential fits (optical model)

- Strongly non linear (fitting is done by iteration only)
- Need data at large scattering angles
- Spin orbit does not strongly affect elastic cross sections
  - Ambiguities:

❑low energy (phase equivalent potentials)

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

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

❑heavy nuclei (governed by tail of V)

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

Ex: multichannel fits

- Elastic : bare potential versus the optical potential
    - Can ignore dynamic polarization
    - Redo entire fitting in coupled channels
    - Switch off the backward coupling

- Inelastic scattering
    - First use first order theory
    - Then detail adjustment of optical potential
    - Plus non-linearities in deformation
    - Plus higher order effects

- Transfer
    - First 1step dwba (SF can be cleanly extracted)
    - Higher orders (other inelastic channels CCBA or other reaction channels CRC)

Stategies for chi2 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

Introduction to sfresco

Antonio Moro

R-matrix method for solving equations: single channel

Solving the problem in a box R=0,a

Basis states $$\left[-\frac{\hbar^2}{2\mu}\left(\frac{d^2}{dR^2} - \frac{L(L+1)}{R^2}\right) + V(R) - \varepsilon_n\right] w_n(R) = 0 \qquad \varepsilon_n,\ n = 1, 2, \ldots,$$

Fixed logarithmic derivative $$\beta = \frac{d}{dR} \ln w(R) \equiv \frac{w'(R)}{w(R)} \qquad R = a$$

4) Prove that w form an orthonormal basis inside box.

Solution expanded in the R-matrix basis $$\chi(R) = \sum_{n=1}^{N} A_n w_n(R)$$

Then Expansion coefficients can be defined by $$A_n = \int_0^a w_n(R)\chi(R)dR$$

Solving equations

After some manipulation:
$$\frac{\chi(a)}{\chi'(a)-\beta\chi(a)}=\sum_{n=1}^{N}\frac{\hbar^2}{2\mu}\frac{w_n(a)^2}{\varepsilon_n-E}$$

Generalized single-channel R-matrix
$$\mathbf{R}=\sum_{n=1}^{N}\frac{\hbar^2}{2\mu a}\frac{w_n(a)^2}{\varepsilon_n-E}$$

Once you have the R-matrix, you have the S-matrix
$$\mathbf{S}=\frac{H^- - a\mathbf{R}(H'^- - \beta H^-)}{H^+ - a\mathbf{R}(H'^+ - \beta H^+)}$$

Solution can be expressed as:
$$\chi(R)=\sum_{n=1}^{N}\frac{\hbar^2}{2\mu a}\frac{w_n(a)}{\varepsilon_n-E}[\chi'(a)-\beta\chi(a)]w_n(R)$$

R-matrix in terms of reduced width amplitudes
$$\gamma_n=\sqrt{\frac{\hbar^2}{2\mu a}}\,w_n(a)$$
$$\mathbf{R}=\sum_{n=1}^{N}\frac{\gamma_n^2}{\varepsilon_n-E}$$

R-matrix

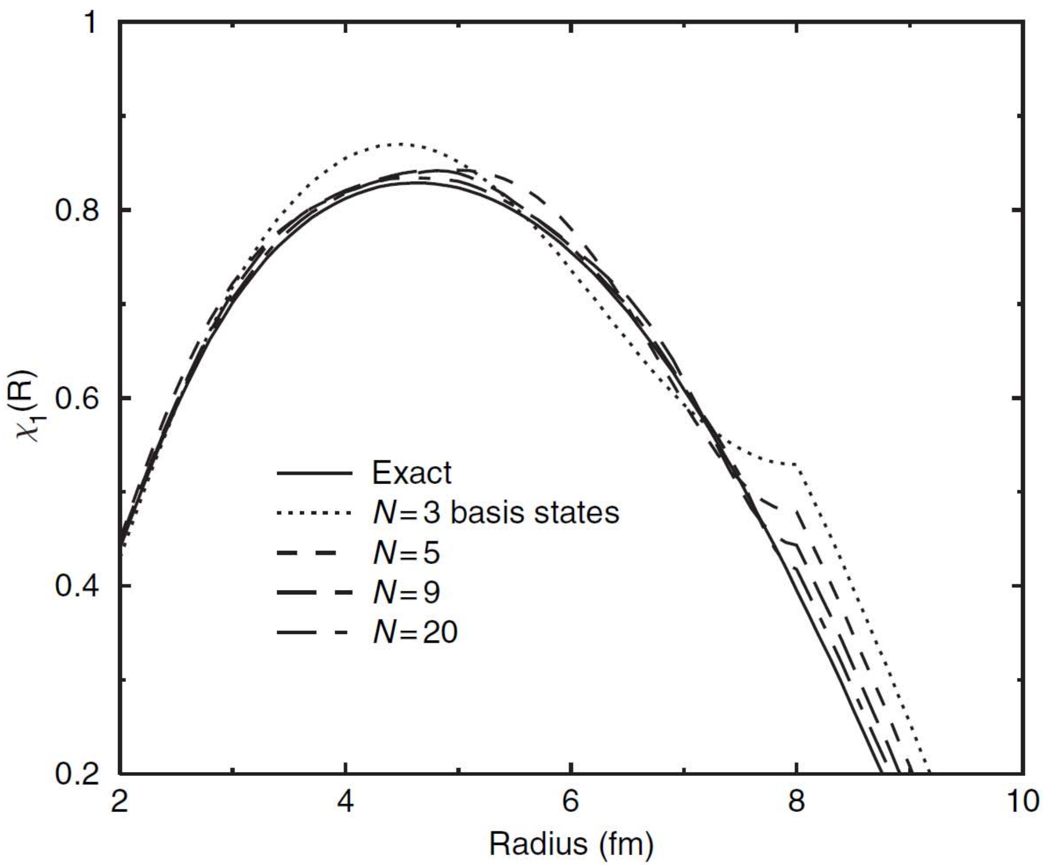

Fig. 6.1. Convergence of the one-channel scattering wave function with varying numbers of basis states, for $a = 8$ fm and $\beta = 0$. We plot the real part of $p_{1/2}$ neutron scattering wave function on ^{4}He at 5 MeV.

Much more on R-matrix in week 3!

Scattering theory III: integral forms

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integral equations: green's function methods

$$\psi_\alpha(R) = \delta_{\alpha\alpha_i} F_\alpha(R) + \frac{2\mu_x}{\hbar^2} \int G^+(R,R')\Omega_\alpha(R')\mathrm{d}R',$$

4) Work out the explicit form for G(R,R') in coordinate and momentum space
How do the boundary conditions come in?

5) Reminding yourself of the asymptotic form in terms:

$$\psi_{\alpha\alpha_i}(R) = F_\alpha(R)\delta_{\alpha\alpha_i} + H_\alpha^+(R)\mathbf{T}_{\alpha\alpha_i}$$

derive the relation for T:

$$\mathbf{T}_{\alpha\alpha_i} = -\frac{2\mu_x}{\hbar^2 k_\alpha}\langle F_\alpha^* | \Omega_\alpha\rangle$$
$$= -\frac{2\mu_x}{\hbar^2 k_\alpha}\langle F_\alpha^{(-)} | \Omega_\alpha\rangle.$$

Formal solutions to Scattering

Split the Hamiltonian in Free Hamiltonian and residual interaction

$$H = H_0 + V$$

- any other interaction can in principle be include in H_0
- V should be short range

$$H_0 = -\frac{\hbar^2}{2\mu}\nabla^2$$

Free scattering equation: homogeneous

$$(H_0 - E)\phi_{\mathbf{k}}(\mathbf{r}) = 0$$

$$\int \phi^*_{\mathbf{k}'}(\mathbf{r})\phi_{\mathbf{k}}(\mathbf{r})\, d\mathbf{r} = \delta(\mathbf{k} - \mathbf{k}')$$

$$\int \phi^*_{\mathbf{k}}(\mathbf{r}')\phi_{\mathbf{k}}(\mathbf{r})\, d\mathbf{k} = \delta(\mathbf{r} - \mathbf{r}')$$

General Scattering equation: inhomogeneous

$$(H_0 - E)\psi^{\pm}_{\mathbf{k}}(\mathbf{r}) = -V\psi^{\pm}_{\mathbf{k}}(\mathbf{r})$$

Solution can be expressed as:

$$\psi^+_{\mathbf{k}}(\mathbf{r}) = \phi_{\mathbf{k}}(\mathbf{r}) + \frac{2\mu}{\hbar^2}\int G^+(\mathbf{r},\mathbf{r}')V(\mathbf{r}')\psi^+_{\mathbf{k}}(\mathbf{r}')\, d\mathbf{r}'$$

Where the Green's function is solution of:
with outgoing boundary conditions

$$(H_0 - E)G^+(\mathbf{r},\mathbf{r}') = -\frac{\hbar^2}{2\mu}\delta(\mathbf{r} - \mathbf{r}')$$

Wong, Introduction to Nuclear Physics, Wiley

Lippmann-Schwinger Equation

Rewriting in short form: $\psi_k^+ = \phi_k + G^+ V \psi_k^+$

where the Green's function operator is related to the Green's function by

$$G^+(\boldsymbol{r}, \boldsymbol{r}') = \langle \boldsymbol{r} | G^+ | \boldsymbol{r}' \rangle$$

The Green's function operator can be expressed by

$$G^+ = \lim_{\epsilon \to 0} \frac{1}{E - H_0 + i\epsilon}$$

Lippmann-Schwinger integral equation:

$$\psi_k^+ = \phi_k + \frac{1}{E - H_0 + i\epsilon} V \psi_k^+$$

equivalent to the differential form:

$$(E - H_0)\psi_k^+ = (E - H_0)\phi_k + V\psi_k^+$$

Born series expansion

$$\begin{aligned} \psi_k^+ &= \phi_k + G^+V(\phi_k + G^+V\psi_k^+) \\ &= \phi_k + G^+V\phi_k + G^+VG^+V(\phi_k + G^+V\psi_k^+) \\ &= \Big(1 + \sum_{n=1}^{\infty} (G^+V)^n\Big)\phi_k \end{aligned}$$

Wong, Introduction to Nuclear Physics, Wiley

Lippmann-Schwinger Equation

Define a transition matrix (t-matrix) such that: $\langle \phi_{\boldsymbol{k}'} | t | \phi_{\boldsymbol{k}} \rangle = \langle \phi_{\boldsymbol{k}'} | V | \psi_{\boldsymbol{k}}^{+} \rangle$

Remember the Born series?

$$\begin{aligned} \psi_{\boldsymbol{k}}^{+} &= \phi_{\boldsymbol{k}} + G^{+}V(\phi_{\boldsymbol{k}} + G^{+}V\psi_{\boldsymbol{k}}^{+}) \\ &= \phi_{\boldsymbol{k}} + G^{+}V\phi_{\boldsymbol{k}} + G^{+}VG^{+}V(\phi_{\boldsymbol{k}} + G^{+}V\psi_{\boldsymbol{k}}^{+}) \\ &= \left(1 + \sum_{n=1}^{\infty}(G^{+}V)^{n}\right)\phi_{\boldsymbol{k}} \end{aligned}$$

Multiply by: $\langle \phi_{\boldsymbol{k}'} | V$

and we can obtain an operator form of the equation in terms of the t-matrix

$$t = V\left(1 + \sum_{n=1}^{\infty}(G^{+}V)^{n}\right)$$

$$t = V + VG^{+}t$$

often used in few-body methods

Integral forms and T-matrix approach

$$\psi = \phi + \hat{G}^{+}\Omega$$
$$= \phi + \hat{G}^{+} V \psi ,$$

Lippmann-Schwinger equation

ϕ is incoming free wave
(only non zero for elastic channel)

ψ is full wavefunction

$$\mathbf{T} = -\frac{2\mu}{\hbar^2 k}\langle \phi^{(-)} | V | \psi \rangle \equiv -\frac{2\mu}{\hbar^2 k}\int \phi(R) V(R) \psi(R) \mathrm{d}R.$$

$$\mathbf{T}(\mathbf{k}', \mathbf{k}) = \langle \mathrm{e}^{\mathrm{i}\mathbf{k}' \cdot \mathbf{R}} | V | \Psi(\mathbf{R}; \mathbf{k}) \rangle .$$

$$f(\mathbf{k}'; \mathbf{k}) = -\frac{\mu}{2\pi\hbar^2}\mathbf{T}(\mathbf{k}', \mathbf{k})$$

two potential formula: definitions

Consider your potential can be split into two parts: $U=U_1+U_2$

Free:	$[E-T]\phi = 0$	$\hat{G}_0^+ = [E-T]^{-1}$	$\phi = F$
Distorted:	$[E-T-U_1]\chi = 0$	$\chi = \phi + \hat{G}_0^+ U_1 \chi$	$\chi \to \phi + \mathbf{T}^{(1)} H^+$
Full:	$[E-T-U_1-U_2]\psi = 0$	$\psi = \phi + \hat{G}_0^+ (U_1+U_2)\psi$	$\psi \to \phi + \mathbf{T}^{(1+2)} H^+$

two potential formula: derivation 1

Free:	$[E-T]\phi = 0$	$\hat{G}_0^+ = [E-T]^{-1}$	$\phi = F$
Distorted:	$[E-T-U_1]\chi = 0$	$\chi = \phi + \hat{G}_0^+ U_1 \chi$	$\chi \to \phi + \mathbf{T}^{(1)} H^+$
Full:	$[E-T-U_1-U_2]\psi = 0$	$\psi = \phi + \hat{G}_0^+ (U_1+U_2)\psi$	$\psi \to \phi + \mathbf{T}^{(1+2)} H^+$

$$-\frac{\hbar^2 k}{2\mu}\mathbf{T}^{(1+2)} = \int \phi(U_1+U_2)\psi \, \mathrm{d}R$$

$$= \int (\chi - \hat{G}_0^+ U_1 \chi)(U_1+U_2)\psi \, \mathrm{d}R$$

$$= \int \Big[\chi(U_1+U_2)\psi - (\hat{G}_0^+ U_1 \chi)(U_1+U_2)\psi\Big] \mathrm{d}R \, .$$

two potential formula: derivation 2

Free:	$[E-T]\phi = 0$	$\hat{G}_0^+ = [E-T]^{-1}$	$\phi = F$
Distorted:	$[E-T-U_1]\chi = 0$	$\chi = \phi + \hat{G}_0^+ U_1 \chi$	$\chi \to \phi + \mathbf{T}^{(1)} H^+$
Full:	$[E-T-U_1-U_2]\psi = 0$	$\psi = \phi + \hat{G}_0^+ (U_1+U_2)\psi$	$\psi \to \phi + \mathbf{T}^{(1+2)} H^+$

$$
\begin{aligned}
-\frac{\hbar^2 k}{2\mu}\mathbf{T}^{(1+2)} &= \int [\chi(U_1+U_2)\psi - \chi U_1 \hat{G}_0^+ (U_1+U_2)\psi]\,\mathrm{d}R \\
&= \int [\chi(U_1+U_2)\psi - \chi U_1(\psi - \phi)]\,\mathrm{d}R \\
&= \int [\phi U_1 \chi + \chi U_2 \psi]\,\mathrm{d}R \\
&= \langle \phi^{(-)}|U_1|\chi\rangle + \langle \chi^{(-)}|U_2|\psi\rangle.
\end{aligned}
$$

two potential formula: result

Free:	$[E-T]\phi = 0$	$\hat{G}_0^+ = [E-T]^{-1}$	$\phi = F$
Distorted:	$[E-T-U_1]\chi = 0$	$\chi = \phi + \hat{G}_0^+ U_1 \chi$	$\chi \to \phi + \mathbf{T}^{(1)} H^+$
Full:	$[E-T-U_1-U_2]\psi = 0$	$\psi = \phi + \hat{G}_0^+ (U_1+U_2)\psi$	$\psi \to \phi + \mathbf{T}^{(1+2)} H^+$

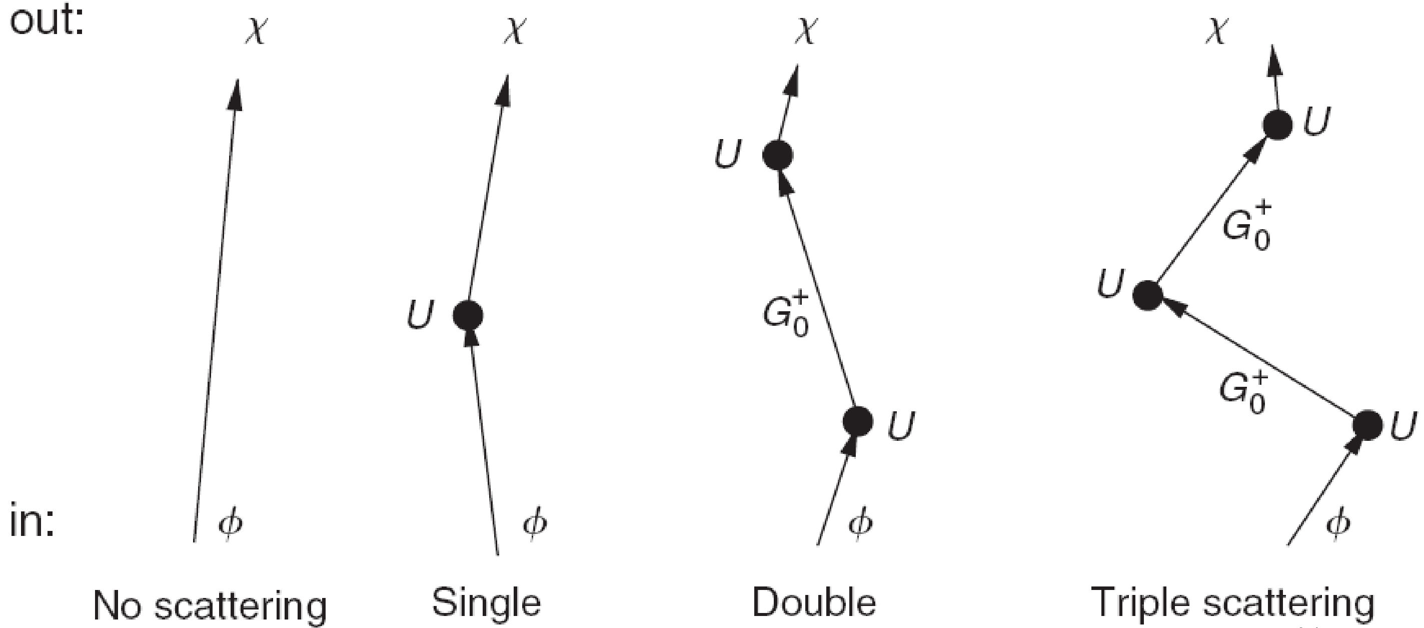
$$\mathbf{T}^{(1+2)} = \mathbf{T}^{(1)} + \mathbf{T}^{2(1)}$$

$$\mathbf{T}^{2(1)} = -\frac{2\mu}{\hbar^2 k} \int \chi U_2 \psi \, \mathrm{d}R$$

Born series

$$\chi = \phi + \hat{G}_0^+ U[\phi + \hat{G}_0^+ U[\phi + \hat{G}_0^+ U[\cdots]]]$$
$$= \phi + \hat{G}_0^+ U\phi + \hat{G}_0^+ U\hat{G}_0^+ U\phi + \hat{G}_0^+ U\hat{G}_0^+ U\phi\hat{G}_0^+ U\phi + \cdots,$$

$$\mathbf{T} = -\frac{2\mu}{\hbar^2 k}\left[\langle\phi^{(-)}|U|\phi\rangle + \langle\phi^{(-)}|U\hat{G}_0^+ U|\phi\rangle + \cdots\right].$$



plane wave Born approximation (PWBA)

NSCL

$$\mathbf{T} = -\frac{2\mu}{\hbar^2 k}\left[\langle\phi^{(-)}|U|\phi\rangle + \langle\phi^{(-)}|U\hat{G}_0^{+}U|\phi\rangle + \cdots\right].$$

$$\mathbf{T}^{\mathrm{PWBA}} = -\frac{2\mu}{\hbar^2 k}\langle\phi^{(-)}|U|\phi\rangle.$$

$$\mathbf{T}_L^{\mathrm{PWBA}} = -\frac{2\mu}{\hbar^2 k}\int_0^\infty F_L(0,kR)\, U(R)\, F_L(0,k_i R)\, \mathrm{d}R.$$

$$f^{\mathrm{PWBA}}(\theta) = -\frac{\mu}{2\pi\hbar^2}\int \mathrm{d}\mathbf{R}\, \mathrm{e}^{-i\mathbf{q}\cdot\mathbf{R}}\, U(\mathbf{R})$$

two potential scattering: post

$$\mathbf{T}^{(1+2)} = \mathbf{T}^{(1)} - \frac{2\mu}{\hbar^2 k}\langle\chi^{(-)}|U_2|\psi\rangle$$

post

$$\mathbf{T}^{(1+2)} = \mathbf{T}^{(1)} - \frac{2\mu}{\hbar^2 k}\left[\langle\chi^{(-)}|U_2|\chi\rangle + \langle\chi^{(-)}|U_2\hat{G}_1 U_2|\chi\rangle + \cdots\right].$$

If U_2 is weak we might expect the series to converge

two potential scattering: post and prior

$$\mathbf{T}^{(1+2)} = \mathbf{T}^{(1)} - \frac{2\mu}{\hbar^2 k} \langle \chi^{(-)} | U_2 | \psi \rangle$$

post

$$\mathbf{T}^{(1+2)} = \mathbf{T}^{(1)} - \frac{2\mu}{\hbar^2 k} \left[\langle \chi^{(-)} | U_2 | \chi \rangle + \langle \chi^{(-)} | U_2 \hat{G}_1 U_2 | \chi \rangle + \cdots \right].$$

If U_2 is weak we might expect the series to converge

$$\mathbf{T}^{(1+2)} = \mathbf{T}^{(1)} - \frac{2\mu}{\hbar^2 k} \langle \psi^{(-)} | U_2 | \chi \rangle.$$

prior

$$\mathbf{T}^{(1+2)}_{\alpha\alpha_i} = \mathbf{T}^{(1)}_{\alpha\alpha_i} - \frac{2\mu_\alpha}{\hbar^2 k_\alpha} \langle \chi^{(-)}_\alpha | U_2 | \psi^{(+)}_{\alpha_i} \rangle \quad \text{[post]},$$

$$= \mathbf{T}^{(1)}_{\alpha\alpha_i} - \frac{2\mu_\alpha}{\hbar^2 k_\alpha} \langle \psi^{(-)}_\alpha | U_2 | \chi^{(+)}_{\alpha_i} \rangle \quad \text{[prior]}.$$

distorted wave Born approximation (DWBA)

Born series is truncated after the first term

$$\mathbf{T}^{\mathrm{DWBA}} = \mathbf{T}^{(1)} - \frac{2\mu}{\hbar^2 k} \langle \chi^{(-)} | U_2 | \chi \rangle$$

U_2 appears to first order

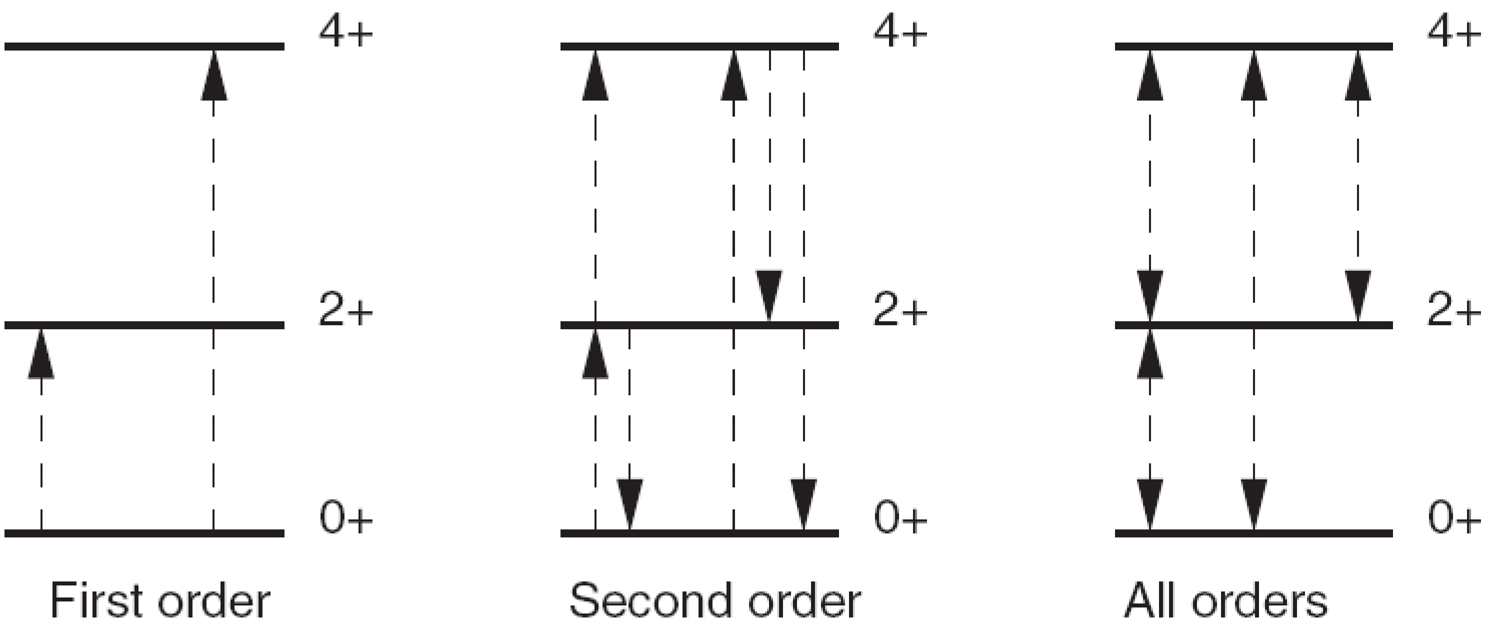
There is similarly a second-order DWBA expression

$$\mathbf{T}^{\mathrm{2nd-DWBA}}_{\alpha\alpha_i} = -\frac{2\mu_\alpha}{\hbar^2 k_\alpha} \left[\langle \chi^{(-)}_\alpha | U_2 | \chi_{\alpha_i} \rangle + \langle \chi^{(-)}_\alpha | U_2 \hat{G}^{+}_1 U_2 | \chi_{\alpha_i} \rangle \right].$$

U_2 appears to second order

multiple orders in DWBA

$$\mathbf{T}^{2\mathrm{nd}-\mathrm{DWBA}}_{\alpha\alpha_i} = -\frac{2\mu_\alpha}{\hbar^2 k_\alpha}\left[\langle\chi^{(-)}_\alpha|U_2|\chi_{\alpha_i}\rangle + \langle\chi^{(-)}_\alpha|U_2\hat{G}^+_1 U_2|\chi_{\alpha_i}\rangle\right].$$



Method for solving the problem

Differential equations:

- Direct integration methods (Numerov, Runge-Kutta)
- Iterative methods
- R-matrix methods
- Other expansion methods transforming the problem into a diagonalization problem (Expansion in Pseudo-states)

Integral equations:

- Iterative methods (smart starting point)
- Transform into matrix equations
- Multiple scattering expansion

Bare and effective interactions

Effects of neglected direct reaction channels: 2 channel example

$$[T_1 + U_1 - E_1]\psi_1(R) + V_{12}\psi_2(R) = 0$$

$$[T_2 + U_2 - E_2]\psi_2(R) + V_{21}\psi_1(R) = 0$$

Formally we can solve the second equation and replace it in the first:

$$[T_1 + U_1 + V_{12}\hat{G}_2^+ V_{21} - E_1]\psi_1(R) = 0.$$

Where an additional interaction has appeared to account for the effect of the second channel – this interaction is in general non-local and depends on E_2

Usually referred to as the **dynamic polarization potential**

$$V_{\mathrm{DPP}} = V_{12}\hat{G}_2^+ V_{21}$$

$$V_{\mathrm{DPP}}\psi_1 = V_{12}\hat{G}_2 V_{21}\psi_1$$

$$= V_{12}(R)\int_0^\infty G_2(R, R'; E_2)V_{21}(R')\psi(R')\mathrm{d}R'$$

Bare interaction U_1

multi-channels

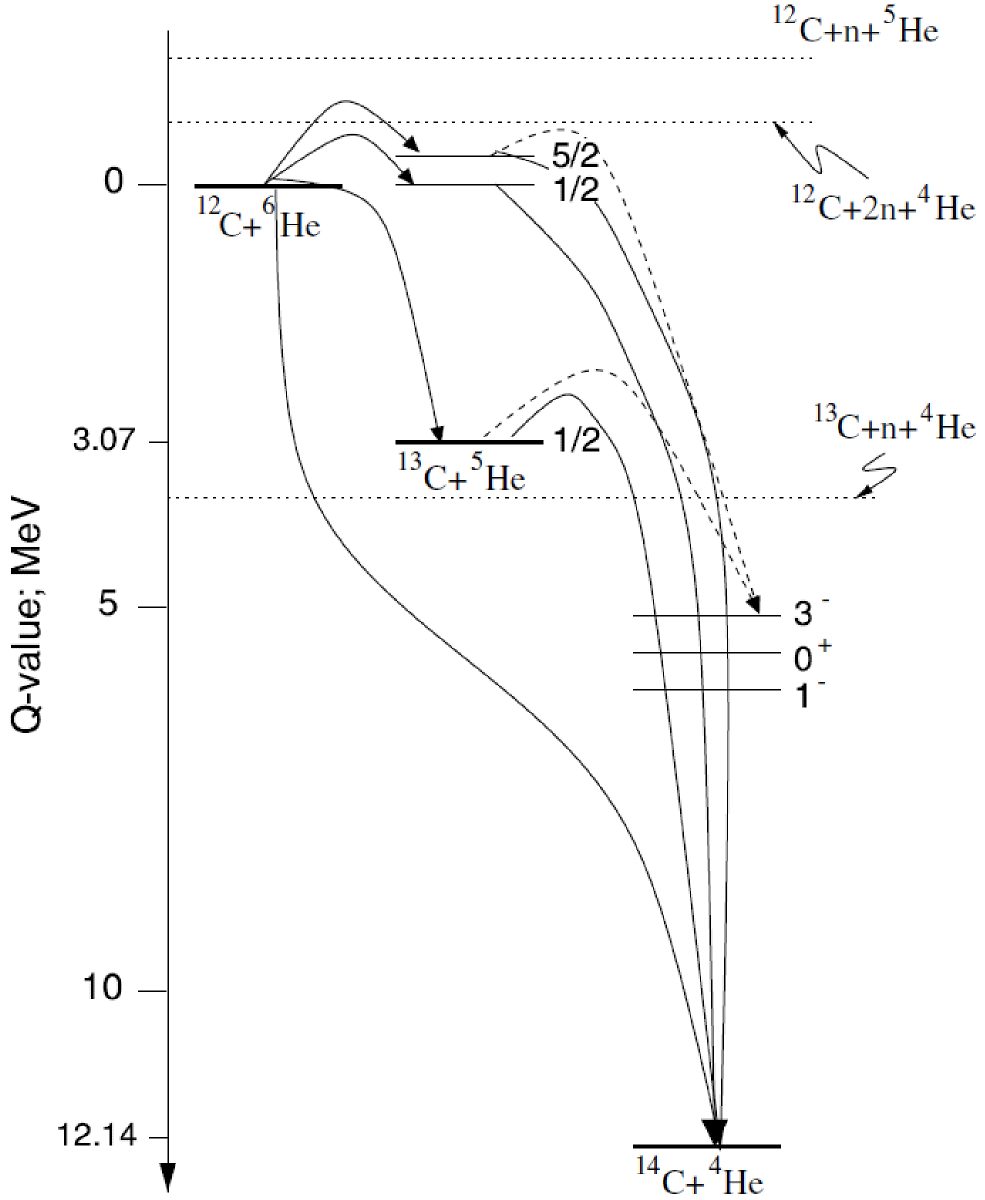


Fig. 1. Q-value diagram for one and two-neutron transfer the system $^6He + ^{12}C$. The Q-value for the ^{14}C ground state very positive and introduces a mismatch. For some transitio one- and two-step processes are indicated.

Multichannel definitions

- o mass partitions x
- o spins I_p and I_t and projections μ_p and μ_t

'S basis'	Channel spin S	$\mathbf{I}_p + \mathbf{I}_t = \mathbf{S}$	$\mathbf{L} + \mathbf{S} = \mathbf{J}_{\text{tot}}$
'J basis'	Projectile J	$\mathbf{L} + \mathbf{I}_p = \mathbf{J}_p$	$\mathbf{J}_p + \mathbf{I}_t = \mathbf{J}_{\text{tot}}$

Multichannel wavefunction

o JJ couplings scheme

$$\Psi^{M_{\rm tot}}_{xJ_{\rm tot}}(\mathbf{R}_x,\xi_p,\xi_t)$$

$$= \sum_{LI_pJ_pI_tM\,\mu_pM_a\mu_t} \phi^{xp}_{I_p\mu_p}(\xi_p)\phi^{xt}_{I_t\mu_t}(\xi_t)\mathrm{i}^L Y^M_L(\hat{\mathbf{R}}_x)\frac{1}{R_x}\psi^{J_{\rm tot}}_{\alpha}(R_x)$$

$$\langle LM\,,I_p\mu_p|J_pM_a\rangle\langle J_pM_a,I_t\mu_t|J_{\rm tot}M_{\rm tot}\rangle$$

$$\equiv \sum_{\alpha}\left[\left[\mathrm{i}^L Y_L(\hat{\mathbf{R}}_x)\otimes\phi^{xp}_{I_p}(\xi_p)\right]_{J_p}\otimes\phi^{xt}_{I_t}(\xi_t)\right]_{J_{\rm tot}M_{\rm tot}}\frac{1}{R_x}\psi^{J_{\rm tot}}_{\alpha}(R_x)$$

$$\equiv \sum_{\alpha}|xpt:(LI_p)J_p,I_t;J_{\rm tot}M_{\rm tot}\rangle\ \psi^{J_{\rm tot}}_{\alpha}(R_x)/R_x$$

$$\equiv \sum_{\alpha}|\alpha;J_{\rm tot}M_{\rm tot}\rangle\ \psi^{J_{\rm tot}}_{\alpha}(R_x)/R_x,$$

$$\{xpt,\ LI_pJ_pI_t\}$$

Multichannel wavefunction

o LS couplings scheme

$$\Psi^{M_{\rm tot}}_{xJ_{\rm tot}}(\mathbf{R}_x,\xi_p,\xi_t) = \sum_{LI_pSI_t}\left[\mathrm{i}^L Y_L(\hat{\mathbf{R}}_x)\otimes\left[\phi^{xp}_{I_p}(\xi_p)\otimes\phi^{xt}_{I_t}(\xi_t)\right]_S\right]_{J_{\rm tot}M_{\rm tot}}$$

$$\times\quad \psi^{J_{\rm tot}}_{\beta}(R_x)/R_x$$

$$\equiv \sum_{\beta}|xpt : L(I_p,I_t)S;J_{\rm tot}M_{\rm tot}\rangle\ \psi^{J_{\rm tot}}_{\beta}(R_x)/R_x$$

$$\equiv \sum_{\beta}|\beta;J_{\rm tot}M_{\rm tot}\rangle\ \psi^{J_{\rm tot}}_{\beta}(R_x)/R_x,$$

β is the set of quantum numbers $\{xpt,\ LI_pI_tS\}$

Multichannel wavefunction

o Spin coupling – transforming between LS and JJ

$$\langle \alpha | \beta \rangle = \sqrt{(2S+1)(2J_p+1)}\, W(LI_pJ_{\rm tot}I_t; J_pS).$$

Free field limit!

$$\Psi^{\mu_p\mu_t}_{xpt}(\mathbf{R}_x, \xi_p, \xi_t; \mathbf{k}_i) \stackrel{V=0}{\rightarrow} \mathrm{e}^{\mathrm{i}\mathbf{k}_i\cdot\mathbf{R}_x} \phi^{xp}_{I_p\mu_p}(\xi_p)\phi^{xt}_{I_t\mu_t}(\xi_t)$$

Multichannel wavefunction

o when the interaction is present

$$\Psi^{\mu_{p_i}\mu_{t_i}}_{x_i p_i t_i}(\mathbf{R}_x, \xi_p, \xi_t; \mathbf{k}_i) = \sum_{J_{\rm tot}M_{\rm tot}} \sum_{\alpha\alpha_i} |\alpha; J_{\rm tot}M_{\rm tot}\rangle \frac{\psi^{J_{\rm tot}}_{\alpha\alpha_i}(R_x)}{R_x} A^{J_{\rm tot}M_{\rm tot}}_{\mu_{p_i}\mu_{t_i}}(\alpha_i; \mathbf{k}_i)$$

where we define an 'incoming coefficient'

$$A^{J_{\rm tot}M_{\rm tot}}_{\mu_{p_i}\mu_{t_i}}(\alpha_i; \mathbf{k}_i) \equiv \frac{4\pi}{k_i} \sum_{M_i m_i} Y^{M_i}_{L_i}(\mathbf{k}_i)^* \langle L_i M_i, I_{p_i}\mu_{p_i}|J_{p_i} m_i\rangle \langle J_{p_i} m_i, I_{t_i}\mu_{t_i}|J_{\rm tot}M_{\rm tot}\rangle.$$

o parity of the full wavefunction $\pi = (-1)^L \pi_{xp}\pi_{xt}$

Multichannel S-matrix and T-matrix

o asymptotic behaviour in terms of S-matrix

$$\psi^{J_{\rm tot}\pi}_{\alpha\alpha_i}(R_x) = \frac{\rm i}{2}\left[H^-_{L_i}(\eta_\alpha, k_\alpha R_x)\,\delta_{\alpha\alpha_i} - H^+_L(\eta_\alpha, k_\alpha R_x)\,\mathbf{S}^{J_{\rm tot}\pi}_{\alpha\alpha_i}\right]$$

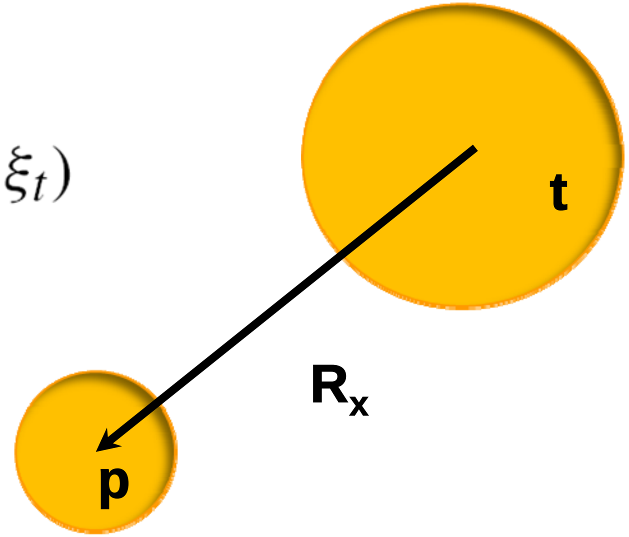
o asymptotic behaviour in terms of T-matrix

$$\psi^{J_{\rm tot}\pi}_{\alpha\alpha_i}(R_x) = F_{L_i}(\eta_\alpha, k_\alpha R_x)\,\delta_{\alpha\alpha_i} + H^+_L(\eta_\alpha, k_\alpha R_x)\,\mathbf{T}^{J_{\rm tot}\pi}_{\alpha\alpha_i}$$

$$\mathbf{S}_{\alpha\alpha_i} = \delta_{\alpha\alpha_i} + 2{\rm i}\mathbf{T}_{\alpha\alpha_i}$$

Multichannel coupled equations

$$H = H_{xp}(\xi_p) + H_{xt}(\xi_t) + \hat{T}_x(R_x) + \mathcal{V}_x(R_x, \xi_p, \xi_t)$$



$$H_{xp}(\xi_p)\phi_{I_p}^{xp}(\xi_p) = \epsilon_{xp}\phi_{I_p}^{xp}(\xi_p),$$

$$H_{xt}(\xi_t)\phi_{I_t}^{xt}(\xi_t) = \epsilon_{xt}\phi_{I_t}^{xt}(\xi_t),$$

$$\mathcal{V}_x(R_x, \xi_p, \xi_t) = \sum_{i\in p, j\in t} V_{ij}(\mathbf{r}_i - \mathbf{r}_j)$$

within the same partition, the Schrodinger equations becomes a coupled equation:

$$[\hat{T}_{xL}(R_x) - E_{xpt}]\psi_\alpha(R_x) + \sum_{\alpha'} \hat{V}_{\alpha\alpha'}^{\text{prior}}\psi_{\alpha'}(R_{x'}) = 0.$$

Multi-channel cross section

o For unpolarized beams, we have to sum over final m-states and average over initial states:

$$\sigma_{xpt}(\theta) = \frac{1}{(2I_{p_i}+1)(2I_{t_i}+1)} \sum_{\mu_p\mu_t,\mu_{p_i}\mu_{t_i}} \left| \tilde{f}^{xpt}_{\mu_p\mu_t,\mu_{p_i}\mu_{t_i}}(\theta) \right|^2$$

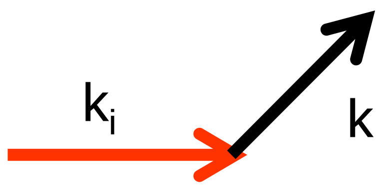
Multi-channel scattering amplitude

o We can obtain the scattering amplitude in terms of the T-matrix or the S-matrix:

$$\psi^{J_{\rm tot}\pi}_{\alpha\alpha_i}(R_x) \overset{R>R_n}{=} H^{+}_{L_\alpha}(\eta_\alpha, k_\alpha R_x)\,\mathbf{T}^{J_{\rm tot}\pi}_{\alpha\alpha_i} \to \mathrm{i}^{-L_\alpha}\,\mathrm{e}^{\mathrm{i}k_\alpha R_x}\,\mathbf{T}^{J_{\rm tot}\pi}_{\alpha\alpha_i}$$

$$\langle \phi^{xp}_{I_p\mu_p}(\xi_p)\,\phi^{xt}_{I_t\mu_t}(\xi_t)\,|\,\Psi^{\mu_{p_i}\mu_{t_i}}_{x_ip_it_i}(\mathbf{R}_x, \xi_p, \xi_t; \mathbf{k}_i)\rangle \overset{R_x>R_n}{=} f^{xpt}_{\mu_p\mu_t,\mu_{p_i}\mu_{t_i}}(\theta)\,\mathrm{e}^{\mathrm{i}k_\alpha R_x}/R_x$$

o From the two above equations one can derive



$$f^{xpt}_{\mu_p\mu_t,\mu_{p_i}\mu_{t_i}}(\theta) = \sum_{J_{\rm tot}\pi M_{\rm tot}} \sum_{\alpha\alpha_i} \mathrm{i}^{-L_\alpha}\langle \phi^{xp}_{I_p\mu_p}\phi^{xt}_{I_t\mu_t}|\alpha; J_{\rm tot}M_{\rm tot}\rangle \times A^{J_{\rm tot}M_{\rm tot}}_{\mu_{p_i}\mu_{t_i}}(\alpha_i; \mathbf{k}_i)\,\mathbf{T}^{J_{\rm tot}\pi}_{\alpha\alpha_i},$$

θ is the angle between k and k_i

Multi-channel scattering amplitude

o plugging in the definition of A and taking into account the Coulomb part:

$$\tilde{f}^{xpt}_{\mu_p\mu_t,\mu_{p_i}\mu_{t_i}}(\theta) = \delta_{\mu_p\mu_{p_i}}\delta_{\mu_t\mu_{t_i}}\delta_{xpt,x_ip_it_i} f_c(\theta) + \frac{4\pi}{k_i}\sum_{L_iLJ_{p_i}J_pm_imM_iJ_{\rm tot}} \langle L_iM_i, I_{p_i}\mu_{p_i}|J_{p_i}m_i\rangle \langle J_{p_i}m_i, I_{t_i}\mu_{t_i}|J_{\rm tot}M_{\rm tot}\rangle\langle LM, I_p\mu_p|J_pm\rangle\langle J_pm, I_t\mu_t|J_{\rm tot}M_{\rm tot}\rangle Y_L^M(\mathbf{k})Y_{L_i}^{M_i}(\mathbf{k}_i)\,\tilde{\mathbf{T}}^{J_{\rm tot}\pi}_{\alpha\alpha_i} e^{i[\sigma_L(\eta_\alpha)+\sigma_{L_i}(\eta_{\alpha_i})]}, \qquad (3.2.21)$$

o identically one can write the scattering amplitude in LS coupling.
o identically one can write the scattering amplitude in terms of S-matrix

$$\tilde{\mathbf{T}}^{J_{\rm tot}\pi}_{\alpha\alpha_i} = \frac{i}{2}[\delta_{\alpha\alpha_i} - \tilde{\mathbf{S}}^{J_{\rm tot}\pi}_{\alpha\alpha_i}]$$

Integrated channel cross section

o channel cross section

$$\sigma_{xpt}(\theta) = \frac{1}{(2I_{p_i}+1)(2I_{t_i}+1)} \sum_{\mu_p\mu_t,\mu_{p_i}\mu_{t_i}} \left| \tilde{f}^{xpt}_{\mu_p\mu_t,\mu_{p_i}\mu_{t_i}}(\theta) \right|^2$$

o total outgoing non-elastic cross section

$$\begin{aligned} \sigma_{xpt} &= 2\pi \int_0^\pi \mathrm{d}\theta \sin\theta \; \sigma_{xpt}(\theta) \\ &= \frac{\pi}{k_i^2} \frac{1}{(2I_{p_i}+1)(2I_{t_i}+1)} \sum_{J_{\mathrm{tot}}\pi LJ\alpha_i} (2J_{\mathrm{tot}}+1) |\tilde{\mathbf{S}}^{J_{\mathrm{tot}}\pi}_{\alpha\alpha_i}|^2 \\ &= \frac{\pi}{k_i^2} \sum_{J_{\mathrm{tot}}\pi LJ\alpha_i} g_{J_{\mathrm{tot}}} |\tilde{\mathbf{S}}^{J_{\mathrm{tot}}\pi}_{\alpha\alpha_i}|^2, \end{aligned}$$

Reaction cross section

o flux leaving the elastic channel (depends only on elastic S-matrix elements)

$$\sigma_R = \frac{\pi}{k_i^2} \frac{1}{(2I_{p_i}+1)(2I_{t_i}+1)} \sum_{J_{tot}\pi\alpha_i} (2J_{tot}+1)(1 - |\mathbf{S}^{J_{tot}\pi}_{\alpha_i\alpha_i}|^2)$$

$$= \frac{\pi}{k_i^2} \sum_{J_{tot}\pi\alpha_i} g_{J_{tot}} (1 - |\mathbf{S}^{J_{tot}\pi}_{\alpha_i\alpha_i}|^2), \text{ similarly.}$$

o the total cross section is elastic plus reaction cross sections

$$\sigma_{tot} = \sigma_R + \sigma_{el}$$

$$= \frac{2\pi}{k_i^2} \frac{1}{(2I_{p_i}+1)(2I_{t_i}+1)} \sum_{J_{tot}\pi\alpha_i} (2J_{tot}+1)[1 - \mathrm{Re}\,\mathbf{S}^{J_{tot}\pi}_{\alpha_i\alpha_i}]$$

o absorption cross section

$$\sigma_A = \sigma_R - \sum_{xpt \neq x_i p_i t_i} \sigma_{xpt}$$

Absorption cross section

o absorption cross section

$$\sigma_A = \sigma_R - \sum_{xpt \neq x_i p_i t_i} \sigma_{xpt}$$

o the absorption cross section depends on the imaginary part of the optical potential (W<0)

$$\sigma_A = \frac{2}{\hbar v_i} \frac{4\pi}{k_i^2} \sum_{J_{\text{tot}} \pi \alpha_i \alpha} \int_0^\infty [-W_\alpha(R_x)] \, |\psi_{\alpha \alpha_i}^{J_{\text{tot}} \pi}(R_x)|^2 \, \mathrm{d}R_x$$

detailed balance

Consequence of hermiticity: S-matrix is unitary

$$\sum_{\alpha} \tilde{\mathbf{S}}^{*}_{\alpha\alpha_i} \tilde{\mathbf{S}}_{\alpha\alpha'_i} = \delta_{\alpha_i\alpha'_i},$$

Even if the S-matrix is not unitary, it may be that:

$$|\tilde{\mathbf{S}}_{\alpha\alpha_i}|^2 = |\tilde{\mathbf{S}}_{\alpha_i\alpha}|^2,$$

3) Prove that above condition is sufficient for detailed balance:

$$\sigma_{x_ip_it_i:xpt} = \frac{k_i^2(2I_{p_i}+1)(2I_{t_i}+1)}{k^2(2I_p+1)(2I_t+1)}\sigma_{xpt:x_ip_it_i}.$$

$$\sigma_{xpt:x_ip_it_i} = \frac{\pi}{k_i^2}\frac{1}{(2I_{p_i}+1)(2I_{t_i}+1)}\sum_{J_{\rm tot}\pi\alpha\alpha_i}(2J_{\rm tot}+1)|\tilde{\mathbf{S}}^{J_{\rm tot}\pi}_{\alpha\alpha_i}|^2.$$