Scattering theory II: continuation
What we learnt?

Scattering amplitude nuclear only

\[ f(\theta) = \frac{1}{2ik} \sum_{L=0}^{\infty} (2L+1)P_L(\cos \theta)(S_L - 1) \]

\[ \sigma(\theta) = \frac{d\sigma}{d\Omega} = \left| \frac{1}{2ik} \sum_{L=0}^{\infty} (2L+1)P_L(\cos \theta)(S_L - 1) \right|^2 \]

Coulomb+nuclear

\[ f_n(\theta) = \frac{1}{2ik} \sum_{L=0}^{\infty} (2L+1)P_L(\cos \theta)e^{2i\sigma_L(\eta)}(S_L^n - 1) \]

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

Integrated cross sections:

\[ \sigma_{cl} = \int_{0}^{2\pi} d\phi \int_{0}^{\pi} d\theta \sin \theta \sigma(\theta) \]

\[ = 2\pi \int_{0}^{\pi} d\theta \sin \theta |f(\theta)|^2 \]

\[ = \frac{\pi}{k^2} \sum_{L=0}^{\infty} (2L+1)|1 - S_L|^2 \]

\[ = \frac{4\pi}{k^2} \sum_{L=0}^{\infty} (2L+1)\sin^2 \delta_L, \]
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 $R_{\text{coul}}$

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

- real part weaker for neutrons than for protons

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

iso scalar and isovector components

- spin orbit term: couples spin and orbital motion
Box B.1 Fresco input for the elastic scattering of protons on $^{78}$Ni at several beam energies
elastic scattering in fresco

Which curve corresponds to highest energy?
Comments on homework (elastic scattering)

- $d\sigma_{el}/d\theta$ always forward peaked! Remember ratio to rutherford…
- optical potential is energy dependent
- relation of $R_r$ with diffraction pattern
- relation of $R_i$ and $L_{max}$ of absorption $S(L)$
- relation with $W$ and flux removal from elastic (absorption cross section)
  - are the results converged? Needs to be checked per energy
  - what were the difficulties in the analysis?
so far we have considered $p + t \rightarrow p' + t'$
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 $t$,

consider an exchange index

$$\varepsilon = +1 \text{ for boson-boson}$$
$$\varepsilon = -1 \text{ for fermion-fermion}$$

$$\hat{P}_p \Psi_{xJ_{tot}}^M (R_x, \xi_p, \xi_t) = \varepsilon \Psi_{xJ_{tot}}^M (-R_x, \xi_t, \xi_p)$$

$$\varepsilon = (-1)^{2I_p}$$
Direct and exchange amplitudes

- first identical spinless particles

\[ \psi_{\text{asym}}(\mathbf{R}) = A \left[ e^{ikz} + f(\theta) \frac{e^{ikR}}{R} \right] \]

- for two identical particles the wfn should be

\[ \Psi_{\varepsilon}^{\text{asym}}(\mathbf{R}) = \psi_{\text{asym}}(\mathbf{R}) + \varepsilon \psi_{\text{asym}}(-\mathbf{R}) \]

- scattered outgoing wave properly symmetrized should be:

\[ \Psi_{\varepsilon}^{\text{out}}(\mathbf{R}) = A[f(\theta) + \varepsilon f(\pi - \theta)] \frac{e^{ikR}}{R} = Af_{\varepsilon}(\theta) \frac{e^{ikR}}{R} \]
Direct and exchange amplitudes

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

- cross section for identical particle scattering

\[
\sigma(\theta) = |f_\varepsilon(\theta)|^2 = |f(\theta) + \varepsilon f(\pi - \theta)|^2 = |f(\theta)|^2 + |f(\pi - \theta)|^2 + 2\varepsilon \text{Re} f(\theta)^* f(\pi - \theta).
\]

- the partial wave expansion for the scattering amplitude is:

\[
f_\varepsilon(\theta) = \frac{1}{k} \sum_{L=0}^{\infty} (2L+1)P_L(\cos \theta) T_L[1 + \varepsilon (-1)^L].
\]

For bosons, odd partial waves do not contribute!
Even partial waves are doubled!
Direct and exchange with spin

- permutation best done in LS coupling:

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

- the partial wave expansion for the scattering amplitude is:

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

For S=0 odd partial waves do not contribute!
For S=1 even partial waves do not contribute!
Direct and exchange with spin

- characteristic interference patterns for different spin states!

![Graphs showing cross sections for different spin states](image)

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^{\text{exp}}(i) experimental data (\Delta \sigma \text{ standard deviation})

Measure of discrepancy
\[ \chi^2 = \sum_{i=1}^{N} \frac{(\sigma^{\text{th}}(i) - \sigma^{\text{exp}}(i))^2}{\Delta \sigma(i)^2}. \]

If theory agrees exactly with experiment \( \chi^2 = 0 \) (very unlikely!)
What is statistically reasonable \( \sigma^{\text{th}}(i) - \sigma^{\text{exp}}(i) \sim \Delta \sigma(i) \) 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)
\(\sigma^{\text{exp}}(i)\) experimental data (\(\Delta\sigma\) standard deviation)

Measure of discrepancy

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

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

What is statistically reasonable \(\sigma^{\text{th}}(i) - \sigma^{\text{exp}}(i) \sim \Delta \sigma(i)\) 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 \( \Delta \)

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

\[ E[X] = \int X f(x) dx \]
Chi2 and the covariance matrix

Probability that a data point $x_i$ with variance $\Delta_i^2$ 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:

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

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

$$\Delta = \prod_{i}^{N} \Delta_i$$

$$\chi^2 = \sum_{i}^{N} \frac{(x_i - y_i)^2}{\Delta_i^2}$$
Probability distribution for a set of correlated variables $\mathbf{x} = \{x_1, \ldots, x_N\}$ might no longer be normal

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

Symmetric covariance matrix

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

Diagonal terms are the standard deviations squared

Off diagonal depend on correlation coefficients

$$V_{ij} = \rho_{ij} \Delta_i \Delta_j$$
Chi2 and the covariance matrix

Probability that a data point $x_i$ with variance $\Delta_i^2$ 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:

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

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

$$\Delta = \prod_{i}^{N} \Delta_i$$

Using this we can generalize the Chi2 definition by:

$$\chi^2 = (x - y)^T V^{-1} (x - y)$$

$$= \sum_{ij=1}^{N} (x_i - y_i) [V^{-1}]_{ij} (x_j - y_j).$$
Chi2 distribution

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

\[ \chi^2 = \sum_{i=1}^{N} z_i^2 \]

\[ f(\chi^2) = \frac{1}{2\Gamma\left(\frac{N}{2}\right)} \left(\frac{\chi^2}{2}\right)^{\frac{N}{2}-1} e^{-\chi^2/2} \]

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

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

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

\[ z_i^2 = \frac{(x_i - y_i)^2}{\Delta_i^2} = \frac{(x_i - \mu_i)^2}{\Delta_i^2} \]

If \( z_i \) have normal distributions \( \chi^2 \) 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 minimum found for the set of parameters \( \{p_j^0\} \)

\[
\chi^2(p_1, \ldots, p_P) \approx \chi^2(p_1^0, \ldots, p_P^0) + \frac{1}{2} \sum_{m,n=1}^{P} H_{mn}(p_m - p_m^0)(p_n - p_n^0)
\]

\[
\equiv \chi^2(p^0) + \frac{1}{2}(p - p^0)^T H (p - p^0)
\]

Hesse matrix

\[
H_{mn} = \frac{\partial^2}{\partial p_m \partial p_n} \chi^2(p_1, \ldots, p_P)
\]

Covariance matrix

\[
(V^P)^{-1} = \frac{1}{2}H \quad \text{or} \quad V^P = 2H^{-1}.
\]

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

\[
P_{\text{tot}} = \frac{1}{(2\pi)^{N_2/2} \Delta} \exp \left[ -\frac{1}{4} \sum_{mn}^{P} (p_m - p_m^0)H_{mn}(p_n - p_n^0) \right]
\]
Allowed parameters within 1sigma

This happens with argument of exp is $1/2$

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

Using the Taylor expansion this can be written as

$$\chi^2(p_1, \ldots, p_P) = \chi^2(p_1^0, \ldots, p_P^0) + 1$$
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:

\[ \sigma(\theta) = \left| \frac{1}{k} \sum_{L=0}^{\infty} (2L+1) P_L(\cos \theta) T_L \right|^2 \]

\[ = \frac{1}{k^2} \sum_{LL'} (2L+1)(2L'+1) P_L(\cos \theta) P_{L'}(\cos \theta) T_L^* T_{L'} . \]

\[ a_{\Lambda} = \frac{1}{k^2} \sum_{LL'} (2L+1)(2L'+1) \langle L0, L'0 | \Lambda 0 \rangle^2 T_L^* T_{L'} . \]
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 $V_{ws} = R_{ws}^2$)
    - Heavy nuclei (governed by tail of $V$)

$$ J = \int V(r) dr = 4\pi \int_0^\infty V(r)r^2 dr $$

$$ V(R) \approx -V_{ws}e^{-(R-R_{ws})/a_{ws}} = -V_{ws}e^{R_{ws}/a_{ws}}e^{-R/a_{ws}} $$
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)
Strategies 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
TALENT: theory for exploring nuclear reaction experiments

Introduction to sfresco
Antonio Moro
R-matrix method for solving equations: single channel

Solving the problem in a box $R=0,a$

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

Fixed logarithmic derivative
\[
\beta = \frac{d}{dR} \ln w(R) \equiv \frac{w'(R)}{w(R)} \quad R = a
\]

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
\[
R = \sum_{n=1}^{N} \frac{\hbar^2}{2\mu} \frac{w_n(a)^2}{\varepsilon_n - E}
\]

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

R-matrix in terms of reduced width amplitudes
\[
\gamma_n = \sqrt{\frac{\hbar^2}{2\mu}} \frac{w_n(a)}{\varepsilon_n - E}
\]

Once you have the R-matrix, you have the S-matrix
\[
S = \frac{H^- - aR(H'^- - \beta H^-)}{H^+ - aR(H'^+ - \beta H^+)}
\]
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.
Scattering theory III: integral forms
integral equations: green’s function methods

\[ \psi_\alpha(R) = \delta_{\alpha\alpha_i} F_\alpha(R) + \frac{2\mu_x}{\hbar^2} \int G^+(R, R') \Omega_\alpha(R') dR', \]

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:

\[ \psi_{\alpha\alpha_i}(R) = F_\alpha(R) \delta_{\alpha\alpha_i} + H_\alpha^+(R) T_{\alpha\alpha_i} \]

derive the relation for \( T \):

\[
T_{\alpha\alpha_i} = -\frac{2\mu_x}{\hbar^2 k_\alpha} \langle F_\alpha^* | \Omega_\alpha \rangle = -\frac{2\mu_x}{\hbar^2 k_\alpha} \langle F_\alpha(-) | \Omega_\alpha \rangle.
\]
Formal solutions to Scattering

Split the Hamiltonian in Free Hamiltonian and residual interaction

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

Free scattering equation: homogeneous

$$\int \phi_{k'}^*(r)\phi_k(r)\,dr = \delta(k - k')$$

$$\int \phi_k^*(r')\phi_k(r)\,dk = \delta(r - r')$$

General Scattering equation: inhomogeneous

$$(H_0 - E)\psi_k^\pm(r) = -V\psi_k^\pm(r)$$

Solution can be expressed as:

$$\psi_k^+(r) = \phi_k(r) + \frac{2\mu}{\hbar^2} \int G^+(r, r')V(r')\psi_k^+(r')\,dr'$$

Where the Green’s function is solution of:

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

$H = H_0 + V$

$H_0 = -\frac{\hbar^2}{2\mu}\nabla^2$
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 
\[ G^+(r, r') = \langle r|G^+|r' \rangle \]

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

\[ \psi^+_k = \phi_k + G^+ V (\phi_k + G^+ V \psi^+_k) \]
\[ = \phi_k + G^+ V \phi_k + G^+ V G^+ V (\phi_k + G^+ V \psi^+_k) \]
\[ = (1 + \sum_{n=1}^{\infty} (G^+ V)^n) \phi_k \]
Define a transition matrix (t-matrix) such that:

\[ \langle \phi_{k'} | t | \phi_k \rangle = \langle \phi_{k'} | V | \psi^+_k \rangle \]

Remember the Born series?

\[ \psi^+_k = \phi_k + G^+ V (\phi_k + G^+ V \psi^+_k) \]
\[ = \phi_k + G^+ V \phi_k + G^+ V G^+ V (\phi_k + G^+ V \psi^+_k) \]
\[ = \left(1 + \sum_{n=1}^{\infty} (G^+ V)^n \right) \phi_k \]

Multiply by: \( \langle \phi_{k'} | V \)

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

\[ t = V (1 + \sum_{n=1}^{\infty} (G^+ V)^n) \]
\[ t = V + V G^+ t \]

often used in few-body methods
Integral forms and T-matrix approach

\[ \psi = \phi + \hat{G}^+ \Omega \]

\[ = \phi + \hat{G}^+ V \psi, \]

\[ T = -\frac{2\mu}{\hbar^2 k} \langle \phi^{(-)} | V | \psi \rangle \equiv -\frac{2\mu}{\hbar^2 k} \int \phi(R) V(R) \psi(R) dR. \]

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

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

**Lippmann-Schwinger equation**

\( \phi \) is incoming free wave

(only non zero for elastic channel)

\( \psi \) is full wavefunction
two potential formula: definitions

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

<table>
<thead>
<tr>
<th>Free:</th>
<th>$[E - T] \phi = 0$</th>
<th>$\hat{G}_0^+ = [E - T]^{-1}$</th>
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two potential formula: derivation 1

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$$-\frac{\hbar^2 k}{2\mu} T^{(1+2)} = \int \phi(U_1 + U_2)\psi \ dR$$

$$= \int (\chi - \hat{G}_0^+ U_1 \chi)(U_1 + U_2)\psi \ dR$$

$$= \int \left[ \chi (U_1+U_2)\psi - (\hat{G}_0^+ U_1 \chi)(U_1+U_2)\psi \right] dR.$$
two potential formula: derivation 2

Free: \[ (E-T)\phi = 0 \quad \hat{G}_0^+ = (E-T)^{-1} \quad \phi = F \]

Distorted: \[ (E-T-U_1)\chi = 0 \quad \chi = \phi + \hat{G}_0^+ U_1 \chi \quad \chi \rightarrow \phi + T^{(1)} H^+ \]

Full: \[ (E-T-U_1-U_2)\psi = 0 \quad \psi = \phi + \hat{G}_0^+(U_1+U_2)\psi \quad \psi \rightarrow \phi + T^{(1+2)} H^+ \]

\[
-\frac{\hbar^2 k}{2\mu} T^{(1+2)} = \int \left[ \chi (U_1 + U_2)\psi - \chi U_1 \hat{G}_0^+ (U_1 + U_2)\psi \right] dR \\
= \int \left[ \chi (U_1 + U_2)\psi - \chi U_1 (\psi - \phi) \right] dR \\
= \int \left[ \phi U_1 \chi + \chi U_2 \psi \right] dR \\
= \langle \phi^{-}\rvert U_1 \rvert \chi \rangle + \langle \chi^{-}\rvert U_2 \rvert \psi \rangle.
\]
two potential formula: result

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\[
T^{(1+2)} = T^{(1)} + T^2(1)
\]

\[
T^2(1) = -\frac{2\mu}{\hbar^2 k} \int \chi U_2 \psi \ dR
\]

\[
T^{(1)}
\]
Born series

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

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

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

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

\[ T_{\text{PWBA}} = -\frac{2\mu}{\hbar^2 k} \langle \phi^(-) | U | \phi \rangle. \]

\[ T_{\text{PWBA}} = -\frac{2\mu}{\hbar^2 k} \int_0^\infty F_L(0, kR) U(R) F_L(0, kR) \, dR. \]

\[ f_{\text{PWBA}}(\theta) = -\frac{\mu}{2\pi \hbar^2} \int dR \, e^{-i\mathbf{q} \cdot \mathbf{R}} U(R) \]
two potential scattering: post

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

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

If \( U_2 \) is weak we might expect the series to converge
two potential scattering: post and prior

\[ T^{(1+2)} = T^{(1)} - \frac{2\mu}{\hbar^2 k} \langle \chi^{(-)} \mid U_2 \mid \psi \rangle \]

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

If \( U_2 \) is weak we might expect the series to converge

\[ T^{(1+2)} = T^{(1)} - \frac{2\mu}{\hbar^2 k} \langle \psi^{(-)} \mid U_2 \mid \chi \rangle \]

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

\[ = T^{(1)}_{\alpha\alpha_i} - \frac{2\mu_\alpha}{\hbar^2 k_{\alpha\alpha_i}} \langle \psi^{(-)}_\alpha \mid U_2 \mid \chi^{(+)}_{\alpha\alpha_i} \rangle \] [prior].
distorted wave Born approximation (DWBA)

Born series is truncated after the first term

\[ T^{\text{DWBA}} = T^{(1)} - \frac{2\mu}{\hbar^2 k} \langle \chi^{(-)} | U_2 | \chi \rangle \]

\( U_2 \) appears to first order

There is similarly a second-order DWBA expression

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

\( U_2 \) appears to second order
multiple orders in DWBA

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

First order  

Second order  

All orders
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**

\[
V_{\text{DPP}} = V_{12} \hat{G}_2^+ V_{21}
\]

\[
V_{\text{DPP}} \psi_1 = V_{12} \hat{G}_2 V_{21} \psi_1 = V_{12}(R) \int_0^\infty G_2(R, R'; E_2) V_{21}(R') \psi(R') dR'
\]

Bare interaction

\[
U_1
\]
Fig. 1. $Q$-value diagram for one and two-neutron transfer the system $^6$He + $^{12}$C. The $Q$-value for the $^{14}$C ground state very positive and introduces a mismatch. For some transitions one- and two-step processes are indicated.
Multichannel definitions

- mass partitions \( x \)
- spins \( I_p \) and \( I_t \) and projections \( \mu_p \) and \( \mu_t \)

<table>
<thead>
<tr>
<th>'S basis'</th>
<th>Channel spin ( S )</th>
<th>( I_p + I_t = S )</th>
<th>( L + S = J_{\text{tot}} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>'J basis'</td>
<td>Projectile ( J )</td>
<td>( L + I_p = J_p )</td>
<td>( J_p + I_t = J_{\text{tot}} )</td>
</tr>
</tbody>
</table>
Multichannel wavefunction

- JJ couplings scheme

\[
\Psi_{xJ_{tot}}^{M_{tot}}(R_x, \xi_p, \xi_t) = \sum_{LIPJ_pI_lM_{\mu_pM_{\mu_l}}} \phi_{I_p\mu_p}^{xp}(\xi_p) \phi_{I_l\mu_l}^{xl}(\xi_t) i^L Y_L^M(\hat{R}_x) \frac{1}{R_x} \psi_{J_{tot}}^{J_{tot}}(R_x)
\]

\[
\langle LM, I_p\mu_p | J_pM_a, I_l\mu_l | J_{tot}M_{tot} \rangle
\]

\[
\equiv \sum_\alpha \left[ \left[ i^L Y_L(\hat{R}_x) \otimes \phi_{I_p}^{xp}(\xi_p) \right] J_p \otimes \phi_{I_l}^{xl}(\xi_t) \right]_{J_{tot}M_{tot}} \frac{1}{R_x} \psi_{\alpha}^{J_{tot}}(R_x)
\]

\[
\equiv \sum_\alpha \left| xpt : (LI_p)J_p, I_l ; J_{tot}M_{tot} \right\rangle \psi_{\alpha}^{J_{tot}}(R_x)/R_x
\]

\[
\equiv \sum_\alpha \left| \alpha ; J_{tot}M_{tot} \right\rangle \psi_{\alpha}^{J_{tot}}(R_x)/R_x,
\]

\[
\{xpt, LI_pJ_pI_l\}
\]
Multichannel wavefunction

- LS couplings scheme

\[
\psi_{xI_{i,t}}^{M_{i,t}}(R_x, \xi_p, \xi_I) = \sum_{LI_pS_I} \left[ i^L Y_L(\hat{R}_x) \otimes \left[ \phi_{I_p}^{xp}(\xi_p) \otimes \phi_{I_t}^{xi}(\xi_I) \right] \right]_{S_I} \psi_J^{M_{i,t}}(R_x)/R_x
\]

\[
\equiv \sum_{\beta} |xpt: L(I_p, I_t)S; J_{i,t}M_{i,t} \rangle \psi_{\beta}^{J_{i,t}}(R_x)/R_x
\]

\[
\equiv \sum_{\beta} |\beta; J_{i,t}M_{i,t} \rangle \psi_{\beta}^{J_{i,t}}(R_x)/R_x,
\]

\(\beta\) is the set of quantum numbers \{xpt, LI_pI_tS\}
Multichannel wavefunction

- Spin coupling – transforming between LS and JJ

\[
\langle \alpha | \beta \rangle = \sqrt{(2S+1)(2J_p+1)} \, W (L I_p J_{tot} I_t ; J_p S).
\]

Free field limit!

\[
\Psi_{\mu_p \mu_t}^{\xi_p \xi_t} (R_X, \xi_p, \xi_t ; k_i) \overset{V=0}{\rightarrow} e^{i k_i \cdot R_X} \phi_{I_p \mu_p}^{x_p} (\xi_p) \phi_{I_t \mu_t}^{x_t} (\xi_t)
\]
Multichannel wavefunction

- when the interaction is present

\[ \Psi_{\mu p_i \mu t_i}^{i} (R_x, \xi_p, \xi_t; k_i) = \sum_{J_{tot} M_{tot}} \sum_{\alpha \alpha_i} \left| \alpha; J_{tot} M_{tot} \right> \frac{\psi_{\alpha \alpha_i}^J (R_x)}{R_x} A_{\mu p_i \mu t_i}^{J_{tot} M_{tot}} (\alpha_i; k_i) \]

where we define an ‘incoming coefficient’

\[ A_{\mu p_i \mu t_i}^{J_{tot} M_{tot}} (\alpha_i; k_i) = \frac{4\pi}{k_i} \sum_{M_i m_i} Y_{Li}^M (k_i) \langle L_i M_i, I_{pi} \mu_{pi} | J_p m_i \rangle \langle J_p m_i, I_{ti} \mu_{ti} | J_{tot} M_{tot} \rangle. \]

- parity of the full wavefunction

\[ \pi = (-1)^L \pi_{xp} \pi_{xt} \]
Multichannel S-matrix and T-matrix

- asymptotic behaviour in terms of S-matrix

\[ \psi_{\alpha \alpha_i}^{J_{\text{tot}} \pi} (R_x) = \frac{i}{2} \left[ H_{L_i}^{-} (\eta_\alpha, k_\alpha R_x) \delta_{\alpha \alpha_i} - H_{L_i}^{+} (\eta_\alpha, k_\alpha R_x) S_{\alpha \alpha_i}^{J_{\text{tot}} \pi} \right] \]

- asymptotic behaviour in terms of T-matrix

\[ \psi_{\alpha \alpha_i}^{J_{\text{tot}} \pi} (R_x) = F_{L_i} (\eta_\alpha, k_\alpha R_x) \delta_{\alpha \alpha_i} + H_{L_i}^{+} (\eta_\alpha, k_\alpha R_x) T_{\alpha \alpha_i}^{J_{\text{tot}} \pi} \]

\[ S_{\alpha \alpha_i} = \delta_{\alpha \alpha_i} + 2i T_{\alpha \alpha_i} \]
Multichannel coupled equations

\[ H = H_{xp}(\xi_p) + H_{xt}(\xi_t) + \hat{T}_x (R_x) + V_x (R_x, \xi_p, \xi_t) \]

\[ H_{xp}(\xi_p) \phi_{xp}^{\xi_p} (\xi_p) = \epsilon_{xp} \phi_{xp}^{\xi_p} (\xi_p), \]

\[ H_{xt}(\xi_t) \phi_{xt}^{\xi_t} (\xi_t) = \epsilon_{xt} \phi_{xt}^{\xi_t} (\xi_t), \]

\[ V_x (R_x, \xi_p, \xi_t) = \sum_{i \in p, j \in t} V_{ij}(r_i - r_j) \]

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

\[ [\hat{T}_{XL} (R_x) - E_{xp} t] \psi_\alpha (R_x) + \sum_{\alpha'} \hat{V}_{\alpha \alpha'}^{prior} \psi_{\alpha'} (R_x') = 0. \]
For unpolarized beams, we have to sum over final m-states and average over initial states:

\[
\sigma_{xpt}(\theta) = \frac{1}{(2I_{p_i}+1)(2I_{t_i}+1)} \sum_{\mu_p \mu_{t_i}, \mu_{p_i} \mu_{t_i}} \left| \tilde{f}_{xpt}^{\mu_p \mu_{t_i}, \mu_{p_i} \mu_{t_i}}(\theta) \right|^2
\]
We can obtain the scattering amplitude in terms of the T-matrix or the S-matrix:

\[
\psi_{J_{tot}^\pi}^{\alpha \alpha_i}(R_x) \stackrel{R \geq R_n}{=} H_+^{L_\alpha}(\eta_\alpha, k_\alpha R_x) T_{J_{tot}^\pi}^{\alpha \alpha_i} \rightarrow i^{-L_\alpha} e^{ik_\alpha R_x} T_{J_{tot}^\pi}^{\alpha \alpha_i} 
\]

\[
\langle \phi_{I_p\mu_p}^{xp}(\xi_p) \phi_{I_t\mu_t}^{xt}(\xi_t) | \Psi_{x_i p_{i t_i}}^{\mu_p \mu_t}(R_x, \xi_p, \xi_t; k_i) \rangle \stackrel{R \geq R_n}{=} f_{\mu_p \mu_t, \mu_p \mu_t}(\theta) e^{ik_\alpha R_x/R_x} 
\]

From the two above equations one can derive

\[
f_{\mu_p \mu_t, \mu_p \mu_t}(\theta) = \sum_{J_{tot}} \sum_{\alpha \alpha_i} i^{-L_\alpha} \langle \phi_{I_p\mu_p}^{xp} \phi_{I_t\mu_t}^{xt} | \alpha; J_{tot} M_{tot} \rangle 
\times A_{\mu_p \mu_t, \mu_p \mu_t}(\alpha_i; k_i) T_{J_{tot}^\pi}^{\alpha \alpha_i} 
\]

\(\theta\) is the angle between \(k\) and \(k_i\)
Multi-channel scattering amplitude

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

\[
\tilde{f}_{\mu_p\mu_i,\mu_i\mu_i}(\theta) = \delta_{\mu_p\mu_i} \delta_{\mu_i\mu_i} \delta_{x_{p+i} x_{i+p}} f_{c}(\theta)
\]

\[
+ \frac{4\pi}{k_i} \sum_{L_i M_i J_i p_m i m M_i J_{tot}} \langle L_i M_i, I_i \mu_i | J_{tot} M_{tot} \rangle \langle L M, I_p \mu_p | J_p m \rangle \langle J_p m, I_t \mu_t | J_{tot} M_{tot} \rangle
\]

\[
Y_{L_i}^{M_i}(k_i) Y_{L_i}^{M_i}(k_i) \quad \tilde{T}_{\alpha \alpha_i}^{J_{tot} \pi} \quad e^{i[\sigma_L(\eta_\alpha) + \sigma_L(\eta_{\alpha_i})]}, \quad (3.2.21)
\]

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

\[
\tilde{T}_{\alpha \alpha_i}^{J_{tot} \pi} = \frac{i}{2} \left[ \delta_{\alpha \alpha_i} - \tilde{S}_{\alpha \alpha_i}^{J_{tot} \pi} \right]
\]
Integrated channel cross section

- Channel cross section

\[
\sigma_{xpt}(\theta) = \frac{1}{(2I_{p_i}+1)(2I_{t_i}+1)} \sum_{\mu_p \mu_{t_1, \mu_p; \mu_{t_i}}} \left| \tilde{f}_{\mu_p \mu_{t_1, \mu_p; \mu_{t_i}}}^{xpt}(\theta) \right|^2
\]

- Total outgoing non-elastic cross section

\[
\sigma_{xpt} = 2\pi \int_0^\pi d\theta \sin \theta \sigma_{xpt}(\theta)
\]

\[
= \frac{\pi}{k_i^2} \frac{1}{(2I_{p_i}+1)(2I_{t_i}+1)} \sum_{J_{tot \pi L J_{al}}(2J_{tot}+1)} |\tilde{S}_{\alpha \alpha_i}^{J_{tot \pi}}|^2
\]

\[
= \frac{\pi}{k_i^2} \sum_{J_{tot \pi L J_{al}}} g_{J_{tot}} |\tilde{S}_{\alpha \alpha_i}^{J_{tot \pi}}|^2
\]
Reaction cross section

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

\[ \sigma_R = \frac{\pi}{k_i^2} \frac{1}{(2I_{p_i}+1)(2I_{l_i}+1)} \sum_{J_{tot} \pi \alpha_i} (2J_{tot}+1)(1 - |S_{\alpha_i \alpha_i}^{J_{tot} \pi}|^2) \]

\[ = \frac{\pi}{k_i^2} \sum_{J_{tot} \pi \alpha_i} g_{J_{tot}} (1 - |S_{\alpha_i \alpha_i}^{J_{tot} \pi}|^2), \text{ similarly.} \]

- the total cross section is elastic plus reaction cross sections

\[ \sigma_{tot} = \sigma_R + \sigma_{el} \]

\[ = \frac{2\pi}{k_i^2} \frac{1}{(2I_{p_i}+1)(2I_{l_i}+1)} \sum_{J_{tot} \pi \alpha_i} (2J_{tot}+1)[1 - \text{Re}S_{\alpha_i \alpha_i}^{J_{tot} \pi}] \]

- absorption cross section

\[ \sigma_A = \sigma_R - \sum_{xpt \neq x_ip_i} \sigma_{xpt} \]
Absorption cross section

- absorption cross section

\[ \sigma_A = \sigma_R - \sum_{xpt \neq xip\pi i} \sigma_{xpt} \]

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

\[ \sigma_A = \frac{2}{\hbar v_i} \frac{4\pi}{k_i^2} \sum_{J_{tot}, \pi, \alpha_i, \alpha} \int_0^\infty \left[ -W_\alpha(R_x) \right] |\psi_{J_{tot}, \pi, \alpha_i, \alpha} (R_x)|^2 dR_x \]
Consequence of hermiticity: S-matrix is unitary

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

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

\[ |\tilde{S}_{\alpha \alpha_i}|^2 = |\tilde{S}_{\alpha_i \alpha}|^2, \]

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

\[ \sigma_{xip;ti:xpt} = \frac{k_i^2 (2I_{p_i}+1)(2I_{t_i}+1)}{k^2 (2I_{p}+1)(2I_{t}+1)} \sigma_{xpt:xip;ti}. \]

\[ \sigma_{xpt:xip;ti} = \frac{\pi}{k_i^2 (2I_{p_i}+1)(2I_{t_i}+1)} \sum_{J_{tot} \alpha \alpha_i} (2J_{tot}+1) |\tilde{S}_{\alpha \alpha_i}^{J_{tot} \pi}|^2. \]