Surrey MiniSchool: "Methods of Direct Nuclear Reactions"

Lecture notes

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Thursday 8th (14.00-15:30):
Distorted Wave Theories Use of perturbation theory for elastic scattering estimates using Born and DW Born approximation (to introduce ideas of T-matrix, rather than SE solution, methods) Nonelastic scattering using perturbation theory (DWBA).

Friday 9th (09.30-11.00):
Production of the Compound Nucleus: Fusion reactions, barrier penetration concepts, transmission coefficients, Bohr-Wheeler equation.

Decay of the Compound Nucleus: The Hauser-Feshbach theory.

Material in part from the forthcoming book *Nuclear Reactions for Astrophysics* by I.J. Thompson and F. Nunes, to be published in 2009 by Cambridge University Press.

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1 Perturbation Theory

1.1 Green's function methods

Integral solutions of inhomogeneous equations

Suppose the potential term in a Schrödinger equation is composed of two parts U_c and V. The solution

$$[T + U_c + V - E]\psi = 0 \tag{1}$$

can also be found by solving

$$\begin{aligned} [T + U_c - E]\psi &= -V\psi \\ \text{or } \psi &= [E - T - U_c]^{-1} V\psi \end{aligned} \tag{2}$$

This might not seem much of an advantage, since ψ is on both sides of the equation, but once this operator $G^+ = [E - T - U_c]^{-1}$ is found, we will be able to make different approximations for ψ in its two occurrences, and this will prove to be very useful.

If we write a source term as $\mathcal{S}(R) = V\psi(R)$, then we have to solve the inhomogeneous equation $[T(R) + U_c(R) - E]\psi(R) + \mathcal{S}(R) = 0$.

The outgoing-wave boundary conditions are

$$\psi(R) = \frac{\mathrm{i}}{2}(H^-(R) - H^+(R)\mathbf{S}) = F(R) + H^+(R)\mathbf{T} \ . \tag{3}$$

The $\mathbf{T}$ and $\mathbf{S}$ matrices are related by $\mathbf{S} = 1 + 2i\mathbf{T}$ since $H^\pm = G \pm \mathrm{i}F$.

Definition of $G^+(R, R')$

Let us use Green's function methods to find the outgoing solution of the linear equation

$$\left[\frac{d^2}{dR^2} - \frac{L(L+1)}{R^2} - \breve{U}_c(R) + k^2\right] \psi(R) = \frac{2\mu}{\hbar^2}\mathcal{S}(R) \ , \tag{4}$$

where $\breve{U}_c(R) \equiv \frac{2\mu}{\hbar^2}U_c(R)$.

The desired solution is a superposition of all the $G^+(R, R')$ with amplitudes corresponding to the magnitude of the source term at R', namely $\frac{2\mu}{\hbar^2}\mathcal{S}(R')$. This gives the wave function in terms of the integral expression

$$\psi(R) = F(R) + \frac{2\mu}{\hbar^2}\int G^+(R, R')\mathcal{S}(R')dR' \ , \tag{5}$$

where we have added in the homogeneous solution $F(R)$. This equation is often written more compactly in operator notation

$$\psi = F + \hat{G}^+\mathcal{S} \ , \tag{6}$$

where $\hat{G}^+$ is defined as the Green's integral operator that has the kernel function $2\mu/\hbar^2\, G^+(R,R')$, and where F is the homogeneous solution. Furthermore, because $\hat{G}^+\mathcal{S}$ is the solution ψ of the differential equation $[E-T]\psi = \mathcal{S}$ with T the kinetic energy operator, the Green's operator with the 'distorting' potential U_c can be written as

$$\hat{G}^+ = [E - T - U_c]^{-1} \tag{7}$$

with the specified outgoing boundary conditions. Eq. (6) can also be written as

$$\psi = F + [E - T - U_c]^{-1}\mathcal{S}\ . \tag{8}$$

We now specialise to U_c being the point Coulomb potential

$$U_c(R) = \frac{Z_1 Z_2 e^2}{R}\ . \tag{9}$$

To find $G^+(R,R')$

We know $F(R)$ and $H^+(R)$ as the the regular and irregular solutions of the Coulomb equation

$$\left[\frac{d^2}{dR^2} - \frac{L(L+1)}{R^2} - \breve{U}_c(R) + k^2\right]\left\{\begin{array}{c} F(R) \\ H^+(R) \end{array}\right\} = 0\ . \tag{10}$$

where $F(R)$ being regular means that $F(0)=0$, and $H(R)$ being irregular means that $H(0)\neq 0$.

Using standard derivations for second-order differential equations, the full Green's function is then

$$\begin{aligned} G^+(R,R') &= -\frac{1}{k}\left\{\begin{array}{l} H^+(R')F(R) \text{ for } R<R' \\ F(R')H^+(R) \text{ for } R>R' \end{array}\right. && (11)\\ &= -\frac{1}{k}F(R_<)H^+(R_>) && (12)\end{aligned}$$

where $R_< = \min(R,R')$ and $R_> = \max(R,R')$.

The solution of the original inhomogeneous equation is therefore

$$\psi(R) = -\frac{2\mu}{\hbar^2 k}\int F(R_<)H^+(R_>)\mathcal{S}(R')dR'\ . \tag{13}$$

At large distances $R>R'$, by construction $\psi(R)\to \mathsf{T}H^+(R)$, because of Eq. (3), so

$$\mathsf{T}H^+(R) = -\frac{2\mu}{\hbar^2 k}H^+(R)\int F(R')\mathcal{S}(R')dR'\ , \tag{14}$$

and we arrive at a very useful integral expression for the partial wave T matrix element:

$$\mathsf{T} = -\frac{2\mu}{\hbar^2 k}\int F(R')\mathcal{S}(R')dR'\ . \tag{15}$$

This may be rewritten in Dirac braket notation as

$$\begin{aligned} \mathsf{T} &= -\frac{2\mu}{\hbar^2 k}\langle F^*|\mathcal{S}\rangle && (16)\\ &= -\frac{2\mu}{\hbar^2 k}\langle F^{(-)}|\mathcal{S}\rangle\ . && (17)\end{aligned}$$

The complex conjugation in Eq. (16) is necessary to cancel the conjugation implicit in the matrix elements. The $^{(-)}$ superscript in the second form Eq. (17) is used to indicate the conjugate wave function F^* (though in our case, F^* and F are equal).

When $U_c(R) = 0$, the integral expression is called a *plane wave* $\mathbf{T}$ *matrix element*, and when $U_c(R)$ is the Coulomb distorting potential in the exit channel α, the integral becomes a *Coulomb distorted wave* $\mathbf{T}$ *matrix element*.

An *operator notation* is often used, so Eq. (5) can be written more compactly as

$$\begin{aligned} \psi &= \phi + \hat{G}^+ \mathcal{S} && (18) \\ &= \phi + \hat{G}^+ V \psi \ , && (19) \end{aligned}$$

using ϕ to refer to the homogeneous solution present only in the elastic channel, and using the operator definitions of Eq. (8), $\hat{G}^+ = [E - T]^{-1}$, with the + sign indicating outgoing boundary conditions of Eq. (3), and T the kinetic energy operator. The equation (19) is called a partial-wave *Lippmann-Schwinger equation*, and in this notation the $\mathbf{T}$-matrix (17) is the integral

$$\mathbf{T} = -\frac{2\mu}{\hbar^2 k} \langle \phi^{(-)} | V | \psi \rangle \equiv -\frac{2\mu}{\hbar^2 k} \int \phi(R) V(R) \psi(R) dR \ . \tag{20}$$

In a multichannel formulation, ψ and ϕ are interpreted as vectors (ϕ being only non-zero in the elastic channel), V as a matrix, and $\hat{G}^+$ is a matrix of integral operators.

1.2 Two potential formula

If a channel potential is composed of two parts $U(R) = U_1(R) + U_2(R)$, then it is possible to use U_1 as the distorting potential, U_2 as the coupling interaction, and derive a $\mathbf{T}$ matrix integral expression for the scattering from their combined $U(R)$ potential. This will be useful when U_1 can be thought of as 'strong but easy' and U_2 as 'small but difficult', but first we derive an *exact* two-potential formula.

For each partial wave, let us define solutions ϕ for the free field, χ for U_1 only, and ψ for the full case, and use Eq. (19) to write down the corresponding Lippmann-Schwinger equations. Their asymptotic amplitudes will be derived from Eq. (20):

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

Then we can prove the *two potential formula*, that $\mathbf{T}^{(1+2)} = \mathbf{T}^{(1)} + \mathbf{T}^{2(1)}$, with an additional term

$$\mathbf{T}^{2(1)} = -\frac{2\mu}{\hbar^2 k} \int \chi U_2 \psi \ dR \equiv -\frac{2\mu}{\hbar^2 k} \langle \chi^{(-)} | U_2 | \psi \rangle \tag{21}$$

as the scattering $\mathbf{T}$ matrix contribution from coupling U_2, with U_1 appearing as a distorting potential in χ. This is valid for both real and complex potentials U_1, U_2. It uses the $^{(-)}$ superscript to indicate an additional complex conjugation for the left-hand wave function, as in Eq. (17). It is an exact equation.

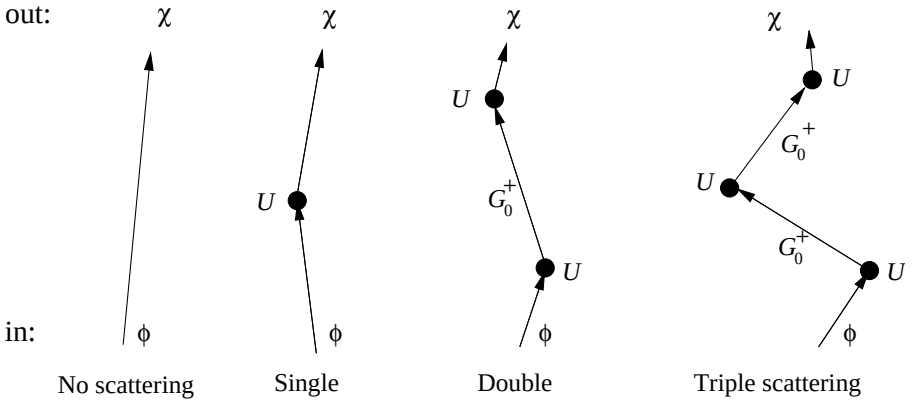

Figure 1: Illustrating the Born series (23) for the wave function χ, as a sum of a homogeneous term with single, double, and higher-order rescattering contributions to the outgoing wave χ.

The exact wave function ψ is the solution of the implicit equation

$$\psi = \chi + \hat{G}_1^+ U_2 \psi \ , \tag{22}$$

using $\hat{G}_1^+ = [E - T - U_1]^{-1}$ with outgoing wave boundary conditions. The first term χ represents the contribution present if $U_2 = 0$.

1.3 Born series and approximations

One-potential scattering

For a potential $U(R)$, solving the Lippmann-Schwinger equation $\chi = \phi + \hat{G}_0^+ U\chi$ provides an exact solution for the wave function χ for potential U. This however is an implicit equation, as χ appears on both the left and right sides. To find it explicitly, we would have to sum the iterated *Born series*:

$$\begin{aligned} \chi &= \phi + \hat{G}_0^+ U[\phi + \hat{G}_0^+ U[\phi + \hat{G}_0^+ U[\cdots]]] \\ &= \phi + \hat{G}_0^+ U\phi + \hat{G}_0^+ U\hat{G}_0^+ U\phi + \hat{G}_0^+ U\hat{G}_0^+ U\phi\hat{G}_0^+ U\phi + \cdots \ , \end{aligned} \tag{23}$$

from which the outgoing T matrix amplitude is

$$\mathsf{T} = -\frac{2\mu}{\hbar^2 k}\left[\langle\phi^{(-)}|U|\phi\rangle + \langle\phi^{(-)}|U\hat{G}_0^+ U|\phi\rangle + \cdots \right] . \tag{24}$$

The equation (23) may be illustrated by the figure 1, where each node of the graph is an action of the potential U and each line a propagation by $\hat{G}_0^+$.

If the potential $U(R)$ is *weak*, in the sense that we could treat it as a perturbation, then we might truncate these series and still achieve sufficient precision. The first term is called the *plane wave Born approximation* (PWBA):

$$\mathsf{T}^{\rm PWBA} = -\frac{2\mu}{\hbar^2 k}\langle\phi^{(-)}|U|\phi\rangle \ . \tag{25}$$

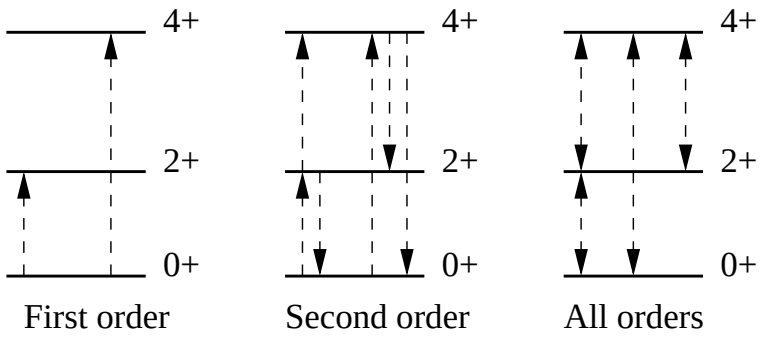

Figure 2: First, second and all-order couplings within a 0^+, 2^+ and 4^+ rotational band, starting from the ground state.

This partial wave PWBA, when written explicity with the radial wave functions, is

$$\mathsf{T}_L^{\rm PWBA} = -\frac{2\mu}{\hbar^2 k}\int_0^\infty F_L(0,kR)\; U(R)\; F_L(0,kR)\; dR\;. \tag{26}$$

Substituting these T matrix elements into

$$f(\theta) = \frac{1}{k}\sum_{L=0}^{\infty}(2L+1)P_L(\cos\theta)\mathsf{T}_L\;, \tag{27}$$

the three-dimensional form for the PWBA scattering amplitude is

$$f^{\rm PWBA}(\theta) = -\frac{\mu}{2\pi\hbar^2}\int d\mathbf{R}\;{\rm e}^{-i\mathbf{q}\cdot\mathbf{R}}\;U(\mathbf{R})\;, \tag{28}$$

where the momentum transfer $\mathbf{q} = \mathbf{k}' - \mathbf{k}$ so $q = 2k\sin\theta/2$. The PWBA amplitude is thus simply proportional to the Fourier transform of the potential. The PWBA is expected to be more accurate at very high energies when potentials are weak, such as in electron-nucleus scattering.

Two-potential scattering

From Eq. (21), the two-potential formula, the exact T matrix expression is again

$$\mathsf{T}^{(1+2)} = \mathsf{T}^{(1)} - \frac{2\mu}{\hbar^2 k}\langle\chi^{(-)}|U_2|\psi\rangle \tag{29}$$

where, from Eq. (22), the exact wave function is the solution of the implicit equation $\psi = \chi + \hat{G}_1 U_2\psi$. We may therefore again by iteration form a Born series

$$\mathsf{T}^{(1+2)} = \mathsf{T}^{(1)} - \frac{2\mu}{\hbar^2 k}\left[\langle\chi^{(-)}|U_2|\chi\rangle + \langle\chi^{(-)}|U_2\hat{G}_1U_2|\chi\rangle + \cdots\right]\;. \tag{30}$$

Post and prior T matrix integrals

The exact expression (29) is often called the *post* T *matrix integral* because the solution χ for the first potential U_1 is in the *post* or final channel. A mirror *prior* T *matrix integral* can also be derived where the χ is in the *prior* or entrance channel.

We may rewrite Eq. (30) as

$$\mathbf{T}^{(1+2)} = \mathbf{T}^{(1)} - \frac{2\mu}{\hbar^2 k}\left[\langle\chi^{(-)}| + \langle\chi^{(-)}|U_2\hat{G}_1 + \cdots\right] U_2|\chi\rangle \ , \tag{31}$$

and define the expression in the square brackets as $\langle\psi^{(-)}|$ where

$$\begin{aligned} \psi^{(-)} &= \chi^{(-)} + \hat{G}_1^- U_2^* \chi^{(-)} + \cdots \\ &= \chi^{(-)} + \hat{G}_1^- U_2^* \psi^{(-)} \ . \end{aligned} \tag{32}$$

The Green's function $\hat{G}_1^-$ is the complex conjugate of $\hat{G}_1^+$, and thus describes incoming boundary conditions. The wave function $\psi^{(-)}$ is thus *full* solution satisfying $[E - T - U_1 - U_2]\psi^{(-)} = 0$ but with incoming boundary conditions. This wave function appears now in the *prior* $\mathbf{T}$ *matrix integral*

$$\mathbf{T}^{(1+2)} = \mathbf{T}^{(1)} - \frac{2\mu}{\hbar^2 k}\langle\psi^{(-)}|U_2|\chi\rangle \ . \tag{33}$$

The wave functions on the kets of Eqs. (29) and (33) are often written with a (+) to remind that they are calculated with normal *outgoing* boundary conditions:

$$\mathbf{T}^{(1+2)} = \mathbf{T}^{(1)} - \frac{2\mu}{\hbar^2 k}\langle\chi^{(-)}|U_2|\psi^{(+)}\rangle = \mathbf{T}^{(1)} - \frac{2\mu}{\hbar^2 k}\langle\psi^{(-)}|U_2|\chi^{(+)}\rangle \ . \tag{34}$$

If furthermore we label the wave functions by the channels in which there is a boundary condition with a plane wave, the post and prior $\mathbf{T}$-matrix integrals for the reaction from entrance channel α_i to exit channel α are

$$\mathbf{T}^{(1+2)} = \mathbf{T}^{(1)} - \frac{2\mu}{\hbar^2 k}\langle\chi^{(-)}|U_2|\psi^{(+)}_{\alpha_i}\rangle = \mathbf{T}^{(1)} - \frac{2\mu}{\hbar^2 k}\langle\psi^{(-)}|U_2|\chi^{(+)}_{\alpha_i}\rangle. \tag{35}$$

Distorted wave Born approximation (DWBA)

If the series (30) is truncated after the first term, linear in U_2, then

$$\mathbf{T}^{\rm DWBA} = \mathbf{T}^{(1)} - \frac{2\mu}{\hbar^2 k}\langle\chi^{(-)}|U_2|\chi\rangle \tag{36}$$

is called the *Distorted Wave Born approximation* (DWBA), because it is a matrix element using wave functions $\chi(R)$ which include U_1 as a distorting potential. It is a *first order* DWBA because U_2 appears only linearly. It is particularly useful for exit channels where U_1 might be say a central optical potential that cannot by itself cause the transition. In this case $\mathbf{T}^{(1)} = 0$, and we have the convenient DWBA expression for the $\mathbf{T}$ matrix from incoming channel α_i to exit channel α:

$$\mathbf{T}^{\rm DWBA} = -\frac{2\mu}{\hbar^2 k}\langle\chi^{(-)}|U_2|\chi_{\alpha_i}\rangle \ . \tag{37}$$

Whether this DWBA is a good approximation depends on the size of U_2, as we see in Fig. 2.