3

Scattering theory

In order to find the cross sections for reactions in terms of the interactions between the reacting nuclei, we have to solve the Schrödinger equation for the wave function of quantum mechanics. Scattering theory tells us how to find these wave functions for the positive (scattering) energies that are needed. We start with the simplest case of finite spherical real potentials between two interacting nuclei in section 3.1, and use a partial wave analysis to derive expressions for the elastic scattering cross sections. We then progressively generalise the analysis to allow for long-ranged Coulomb potentials, and also complex-valued optical potentials. Section 3.2 presents the quantum mechanical methods to handle multiple kinds of reaction outcomes, each outcome being described by its own set of partial-wave *channels*, and section 3.3 then describes how multi-channel methods may be reformulated using integral expressions instead of sets of coupled differential equations. We end the chapter by showing in section 3.4 how the Pauli Principle requires us to describe sets identical particles, and by showing in section 3.5 how Maxwell's equations for electromagnetic field may, in the one-photon approximation, be combined with the Schrödinger equation for the nucleons. Then we can describe photo-nuclear reactions such as photo-capture and disintegration in a uniform framework.

3.1 Elastic scattering from spherical potentials

When the potential between two interacting nuclei does not depend on their relative orientiation, we say that this potential is spherical. In that case, the only reaction that can occur is elastic scattering, which we now proceed to calculate using the method of expansion in partial waves.

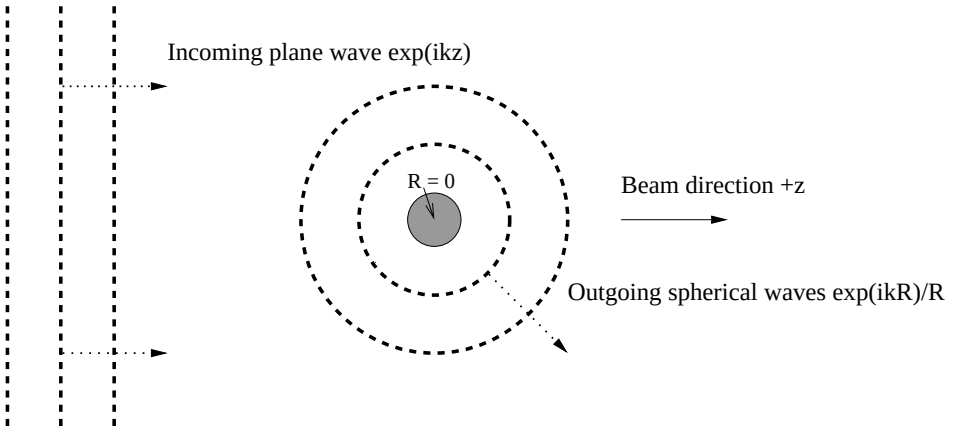

Fig. 3.1. A plane wave in the $+z$ direction incident on a spherical target, giving rise to spherically-outgoing scattering waves

3.1.1 Partial wave scattering from a finite spherical potential

We start our development of scattering theory by finding the elastic scattering from a potential $V(\mathbf{R})$ that is spherically symmetric and so can be written as $V(R)$. Finite potentials will be dealt with first: those for which $V(R) = 0$ for $R \geq R_n$, where R_n is the finite range of the potential. This excludes Coulomb potentials, which will be dealt with later.

We will examine the solutions at positive energy of the time-independent Schrödinger equation with this potential, and show how to find the scattering amplitude $f(\theta, \phi)$ and hence the differential cross section $\sigma(\theta, \phi) = |f(\theta, \phi)|^2$ for elastic scattering. We will use a decomposition in partial waves L=0, 1, $\cdots$, and the spherical nature of the potential will mean that each partial wave function can be found separately.

The time-independent Schrödinger equation for the relative motion with c.m. energy E, from Eq. (2.3.18), is

$$[\hat{T} + V - E]\psi(R, \theta, \phi) = 0 \ , \tag{3.1.1}$$

using polar coordinates (θ, ϕ) such that $z = R\cos\theta$, $x = R\sin\theta\cos\phi$ and $y = R\sin\theta\sin\phi$. In Eq. (3.1.1), the kinetic energy operator $\hat{T}$ uses the reduced mass μ, and is

$$\begin{aligned} \hat{T} &= -\frac{\hbar^2}{2\mu}\nabla_R^2 \\ &= \frac{1}{2\mu}\left[-\frac{\hbar^2}{R^2}\frac{\partial}{\partial R}\left(R^2\frac{\partial}{\partial R}\right) + \frac{\hat{L}^2}{R^2}\right] \ , \end{aligned} \tag{3.1.2}$$

with $\hat{L}^2$ being the squared angular momentum operator

$$\hat{L}^2 = -\hbar^2 \left[\frac{1}{\sin^2\theta} \frac{\partial^2}{\partial\phi^2} + \frac{1}{\sin\theta} \frac{\partial}{\partial\phi} \left(\sin\theta \frac{\partial}{\partial\phi} \right) \right] . \tag{3.1.3}$$

We will also use the z component of angular momentum, which is associated with the operator

$$\hat{L}_z = \frac{\hbar}{\mathrm{i}} \frac{\partial}{\partial\phi} . \tag{3.1.4}$$

If we keep the z-axis as the beam direction as in Eq. (2.4.8), and illustrated in Fig. 3.1, the coordinates can be much simplified for present case of spherical potentials. There is now no dependence on ϕ of the initial beam $\mathrm{e}^{\mathrm{i}kz}$, which implies that it is an eigensolution of $\hat{L}_z$ with eigenvalue $m = 0$. Furthermore spherical potentials $V(R)$ are independent of both θ and ϕ, which is equivalent to the Hamiltonian $\hat{T}+V$ commuting with angular momentum operator $\hat{\mathbf{L}}$, which we write as $[\hat{T}+V, \hat{\mathbf{L}}] = 0$.

These angular independences means that, since the initial wave function is cylindrically symmetric and no potential breaks that symmetry, the final state must have a wave function that is cylindrically symmetric too, as well as its external scattering amplitude. Thus we need only consider wave functions $\psi(R,\theta)$ and amplitudes $f(\theta,\phi) = f(\theta)$ that are independent of ϕ. In quantum mechanical terms, the potential commutes with $\hat{L}_z$, so the $\hat{L}_z$ eigenvalue is conserved during the reaction. Its conserved value of m=0 implies that the wave function and scattering amplitudes cannot vary with ϕ.

Our problem is therefore to solve

$$[\hat{T} + V - E]\psi(R,\theta) = 0 . \tag{3.1.5}$$

The scattering wave functions that are solutions of this equation must, from Eq. (2.4.12), match smoothly at large distances onto the asymptotic form

$$\psi^{\mathrm{asym}}(R,\theta) = \mathrm{e}^{\mathrm{i}kz} + f(\theta)\frac{\mathrm{e}^{\mathrm{i}kR}}{R} . \tag{3.1.6}$$

We will thus find a scattering amplitude $f(\theta)$ and hence the differential cross section $\sigma(\theta)$ for elastic scattering from a spherical potential.

Partial wave expansions

The wave function $\psi(R,\theta)$ is now expanded using Legendre polynomials $P_L(\cos\theta)$, in what is called a *partial wave expansion*. We choose these polynomials as they are eigenfunctions of both $\hat{L}^2$ and $\hat{L}_z$, with eigenvalues $L(L+1)$ and $m = 0$ respectively. We saw above that in the present case

we only need solutions with $m = 0$, as these solutions are independent of ϕ. Furthermore, since the potential commutes with $\hat{L}$, we can find solutions with particular values of angular momentum L. These solutions for individual L are called *partial waves*.

Let us first write a single partial wave as the product of a Legendre polynomial $P_L(\cos\theta)$ for any L=0, 1, $\cdots$, and a part that depends on radius, which we write as $\chi_L(R)/R$ for some function $\chi_L(R)$ that we have yet to determine. When operating on this partial wave product, the ∇_R^2 in the kinetic energy operator gives

$$\nabla_R^2 \; P_L(\cos\theta) \; \frac{\chi_L(R)}{R} = \frac{1}{R}\left(\frac{\mathrm{d}^2}{\mathrm{d}R^2} - \frac{L(L+1)}{R^2}\right) \chi_L(R) \; P_L(\cos\theta) \; . \quad (3.1.7)$$

The $1/R$ factor of $\chi_L(R)$ was chosen so that the second derivative $\mathrm{d}^2/\mathrm{d}R^2$ appears in a simple form on the right side of this equation.

Moreover, the $P_L(\cos\theta)$ together form an orthogonal and complete set over angles $0 \leq \theta \leq \pi$, satisfying the orthogonality and normalisation condition

$$\int_0^\pi P_L(\cos\theta) P_{L'}(\cos\theta) \sin\theta \mathrm{d}\theta = \frac{2}{2L+1}\delta_{LL'}. \quad (3.1.8)$$

This means that any function of angle can be expanded as $\sum_L b_L P_L(\cos\theta)$ for some coefficients b_L. Thus any function of angle and radius can be expanded as $\sum_L b_L(R) P_L(\cos\theta)$ for the $b_L(R)$ now functions of R.

We can therefore expand the full wave function as

$$\psi(R,\theta) = \sum_{L=0}^{\infty} (2L+1)\mathrm{i}^L P_L(\cos\theta) \frac{1}{kR} \chi_L(R) \quad (3.1.9)$$

for functions $\chi_L(R)$ to be found. The explicit factors $(2L+1)\mathrm{i}^L$ are built in for convenience, so that, as we will see, the $\chi_L(R)$ have simple forms in the limit of zero potential. The finiteness of $\psi(R,\theta)$ everywhere implies at least that $\chi_L(0) = 0$ always†.

We now substitute the partial wave sum of Eq. (3.1.9) in the Schrödinger equation Eq. (3.1.1) to find the conditions satisfied by the radial wave functions $\chi_L(R)$. For the kinetic energy applied to Eq. (3.1.9), we use the differential properties (3.1.7) of the Legendre polynomials. For the potential energy term, we use the fact that $V(R)$ is independent of θ. After multiplying on the left by $P_{L'}(\cos\theta)$, integrating over all angles, and using the orthogonality properties of Eq. (3.1.8), we conclude that for each L value

† It implies more precisely that $\chi_L(R) = O(R)$ as $R \to 0$.

there is a separate *partial wave equation*

$$\left[-\frac{\hbar^2}{2\mu}\left(\frac{\mathrm{d}^2}{\mathrm{d}R^2}-\frac{L(L+1)}{R^2}\right)+V(R)-E\right]\chi_L(R)=0\ . \tag{3.1.10}$$

The spherical nature of the potential is crucial in allowing us to solve for each partial wave function separately: this corresponds to angular momentum being conserved when potentials are spherical.

Eq. (3.1.10) is a second order equation, and so needs two boundary conditions specified in order to fix a solution. One boundary condition already known is that $\chi_L(0)=0$. The other is fixed by the large R behaviour, so that it reproduces the external form of Eq. (3.1.6). Since $f(\theta)$ is not yet known, the role of Eq. (3.1.6) is to fix the overall normalisation of the $\chi_L(R)$. We show below how to accomplish these things.

As usual in quantum mechanical matching, both the functions and their derivatives must agree continuously. We therefore match interior and exterior functions and their derivatives at some *matching radius* $R=a$ chosen outside the finite range R_n of the nuclear potential.

Radial solutions for zero potential

For $R\geq a$ we have $V(R)=0$, so at and outside the matching radius the radial wave functions must attain their external forms which we name $\chi_L^{\mathrm{ext}}(R)$. The free-field partial wave equation may be simplified from Eq. (3.1.10), and rewritten using a change of variable from R to the dimensionless radius

$$\rho\equiv kR, \tag{3.1.21}$$

so the $\chi_L^{\mathrm{ext}}(R)$ satisfy

$$\left[\frac{\mathrm{d}^2}{\mathrm{d}\rho^2}-\frac{L(L+1)}{\rho^2}+1\right]\chi_L^{\mathrm{ext}}(\rho/k)=0\ . \tag{3.1.22}$$

This equation for the external form χ_L^{ext} is a special case for $\eta=0$ of the more general *Coulomb wave equation*

$$\left[\frac{\mathrm{d}^2}{\mathrm{d}\rho^2}-\frac{L(L+1)}{\rho^2}-\frac{2\eta}{\rho}+1\right]X_L(\eta,\rho)=0\ , \tag{3.1.23}$$

which has solutions defined in Abramowitz and Stegun [1, ch. 14] and described in more detail in Box 3.1†. This second-order equation has two well-known solutions that are linearly independent: the regular function $F_L(\eta,\rho)$ and the irregular function $G_L(\eta,\rho)$. A regular function is so named

† In this section we need just the special case of $\eta=0$, but we have begun here with a definition of the complete Coulomb functions, as the $2\eta/\rho$ term will reappear in the next section when Coulomb potentials are introduced.

Coulomb functions

That $F_L(\eta,\rho)$ is regular means $F_L(\eta,\rho{=}0) = 0$, and irregularity means $G_L(\eta,\rho{=}0) \neq 0$. They are related by the Wronskian

$$\begin{aligned} G_L(\eta,\rho)\frac{\mathrm{d}F_L(\eta,\rho)}{\mathrm{d}\rho} - F_L(\eta,\rho)\frac{\mathrm{d}G_L(\eta,\rho)}{\mathrm{d}\rho} &= 1 \\ \text{or}\quad W(G,F) \equiv G\,F' - G'\,F &= k\ . \end{aligned} \tag{3.1.11}$$

Note that mathematics texts such as [1] usually define G' as $dG/d\rho$, but we denote this by $\dot{G}$. Since ρ is the dimensionless radius $\rho = kR$, we will use the prime for derivatives with respect to R, so $G' = k\dot{G}$, etc. The Wronskian is equivalently $G\dot{F} - \dot{G}F = 1$.
The Coulomb Hankel functions are combinations of F and G,

$$H_L^{\pm}(\eta,\rho) = G_L(\eta,\rho) \pm \mathrm{i}F_L(\eta,\rho)\ . \tag{3.1.12}$$

Coulomb functions for $\eta = 0$

The $\eta = 0$ functions are more directly known in terms of Bessel functions:

$$\begin{aligned} F_L(0,\rho) &= \rho\, j_L(\rho) &&= (\pi\rho/2)^{1/2} J_{L+1/2}(\rho) \\ G_L(0,\rho) &= -\rho\, y_L(\rho) &&= -(\pi\rho/2)^{1/2} Y_{L+1/2}(\rho)\ , \end{aligned} \tag{3.1.13}$$

where the irregular spherical Bessel function $y_L(\rho)$ is sometimes written as $n_L(\rho)$ (the Neumann function). The J_ν and Y_ν are the cylindrical Bessel functions. The $\eta = 0$ Coulomb functions for the first few L values are

$$F_0(0,\rho) = \sin\rho,$$
$$G_0(0,\rho) = \cos\rho; \tag{3.1.14}$$
$$F_1(0,\rho) = (\sin\rho - \rho\cos\rho)/\rho,$$
$$G_1(0,\rho) = (\cos\rho + \rho\sin\rho)/\rho; \tag{3.1.15}$$
$$F_2(0,\rho) = ((3{-}\rho^2)\sin\rho - 3\rho\cos\rho)/\rho^2,$$
$$G_2(0,\rho) = ((3{-}\rho^2)\cos\rho + 3\rho\sin\rho)/\rho^2\ . \tag{3.1.16}$$

Their behaviour near the origin, for $\rho \ll L$, is

$$F_L(0,\rho) \sim \frac{1}{(2L{+}1)(2L{-}1)\cdots 3.1}\rho^{L+1} \tag{3.1.17}$$
$$G_L(0,\rho) \sim (2L{-}1)\cdots 3.1\ \rho^{-L}\ , \tag{3.1.18}$$

and their asymptotic behaviour when $\rho \gg L$ is

$$F_L(0,\rho) \sim \sin(\rho - L\pi/2)$$
$$G_L(0,\rho) \sim \cos(\rho - L\pi/2) \tag{3.1.19}$$
$$H_L^{\pm}(0,\rho) \sim \mathrm{e}^{\pm\mathrm{i}(\rho - L\pi/2)} = \mathrm{i}^{\mp L}\mathrm{e}^{\pm\mathrm{i}\rho}\ . \tag{3.1.20}$$

So H_L^+ describes an outgoing wave $\mathrm{e}^{\mathrm{i}\rho}$, and H_L^- an incoming wave $\mathrm{e}^{-\mathrm{i}\rho}$.

Coulomb functions for $\eta \neq 0$ are described on page 55.

Box 3.1: Coulomb Functions

because it is zero at $\rho = 0$, and an irregular function because it is non-zero at $\rho = 0$. Any solution X_L can be written as $X_L = bF_L + cG_L$ for some constants b and c chosen according to the boundary conditions.

We may construct $H_L^{\pm} = G_L \pm \mathrm{i}F_L$, which are also two linearly independent solutions of Eq. (3.1.23). By Eq. (3.1.20), these functions are asymptotically proportional to $\mathrm{e}^{\pm \mathrm{i}kR}$. Since the radial momentum operator is $\hat{p} = \frac{\hbar}{\mathrm{i}}\frac{\partial}{\partial R}$, the linear combinations $H_L^{\pm}$ asymptotically have momentum eigenvalues $\pm\hbar k$, and this means that H_L^+ describes a radially *outgoing wave* and H_L^- an *incoming* wave.

The partial wave expansion of Eq. (3.1.9) can be found for any function $\psi(R, \theta)$. In particular, it can be proved [2] that the partial wave expansion for the incident plane wave is

$$\mathrm{e}^{\mathrm{i}kz} = \sum_{L=0}^{\infty} (2L{+}1)\mathrm{i}^L P_L(\cos\theta) \frac{1}{kR} F_L(0, kR) \ , \tag{3.1.24}$$

using just the regular Coulomb functions $F_L(0, kR)$. Their appearance in this equation is the reason that $(2L{+}1)\mathrm{i}^L$ were defined in Eq. (3.1.9), as we now have $\chi_L = F_L$ in the plane wave limit when the potential is zero.

In terms of the $H_L^{\pm} = G_L \pm \mathrm{i}F_L$, the plane wave expansion is equivalently

$$\mathrm{e}^{\mathrm{i}kz} = \sum_{L=0}^{\infty} (2L{+}1)\mathrm{i}^L P_L(\cos\theta) \frac{1}{kR} \frac{\mathrm{i}}{2} [H_L^-(0, kR) - H_L^+(0, kR)] \ . \tag{3.1.25}$$

From this equation we see that the incident beam has equal and opposite amplitudes of the radially ingoing wave H_L^- and the radially outgoing wave H_L^+.

Radial solutions with a potential

Outside the potential we know the external form of Eq. (3.1.6), though not the scattering amplitudes $f(\theta)$. At the origin we know that $\chi_L(0) = 0$, but not the derivatives $\chi_L'(0)$. Because the boundary conditions are thus distributed at different radii, we have to use trial solutions integrated from one radial limit, and determine any unknown parameters by using the boundary condition at the other limit.

We may therefore integrate a trial solution $u_L(R)$ of Eq. (3.1.10) outwards, starting with $u_L(0) = 0$ and some finite $u_L'(0) \neq 0$ chosen arbitrarily, using

$$u_L{}''(R) = \left[\frac{L(L{+}1)}{R^2} + \frac{2\mu}{\hbar^2}(V(R) - E) \right] u_L(R) \tag{3.1.26}$$

and some numerical integration scheme for second-order ordinary differential equations. The true solution will be some multiple of this: $\chi_L(R) = Bu_L(R)$.

In the external region outside the potential, $u_L(R)$ will be found to be a linear combination of two linearly independent solutions of Eq. (3.1.22), such as $H_L^+(0,kR)$ and $H_L^-(0,kR)$:

$$Bu_L(R) = \chi_L(R) \overset{R>R_n}{\to} \chi_L^{\rm ext}(R) = A_L \left[H_L^-(0,kR) - \mathbf{S}_L H_L^+(0,kR)\right] \quad (3.1.27)$$

for some complex constants B, A_L and $\mathbf{S}_L$. The $\mathbf{S}_L$ is called the *partial wave S matrix element*. (It will be unity for zero potential $V(R)$, as the solution must then be proportional to $F_L(0,kR)$ only, by Eq. (3.1.24).) The $\mathbf{S}_L$ is determined in general from $u_L(R)$ by matching the first and last terms of Eq. (3.1.27), and their derivatives, at the radius $R = a$ which is outside the nuclear range R_n. This is most conveniently done by constructing the inverse logarithmic derivative, which is called the R matrix element

$$\mathbf{R}_L = \frac{1}{a}\frac{\chi_L(a)}{\chi_L'(a)} = \frac{1}{a}\frac{u_L(a)}{u_L'(a)} \ , \quad (3.1.28)$$

where the a^{-1} factor is traditionally used to keep the R matrix dimensionless. Given a trial solution $u_L(R)$ in the interior region, although its absolute normalisation B is not yet known, its logarithmic derivative is the same as that of $\chi_L(R)$, and thus unambiguously determines $\mathbf{R}_L$. The $\mathbf{R}_L$ then determines the S matrix element uniquely by matching with the inverse logarithmic derivative of $\chi_L^{\rm ext}(R)$:

$$\mathbf{R}_L = \frac{1}{a}\frac{H_L^- - \mathbf{S}_L H_L^+}{H_L'^- - \mathbf{S}_L H_L'^+} \ , \quad (3.1.29)$$

implying

$$\mathbf{S}_L = \frac{H_L^- - a\mathbf{R}_L H_L'^-}{H_L^+ - a\mathbf{R}_L H_L'^+} \ . \quad (3.1.30)$$

The matrix elements $\mathbf{S}_L$ are thereby uniquely determined by the potential, and next we use them to find the scattering amplitude $f(\theta)$.

Equation (3.1.27) implies that the full scattering wave function has the external form of the partial wave sum

$$\psi(R,\theta) \overset{R>R_n}{\to} \frac{1}{kR}\sum_{L=0}^{\infty}(2L+1)\mathrm{i}^L P_L(\cos\theta) A_L\left[H_L^-(0,kR) - \mathbf{S}_L H_L^+(0,kR)\right] \quad (3.1.31)$$

which we now have to match with Eq. (3.1.6) in order to determine $f(\theta)$ in terms of the $\mathbf{S}_L$.

Substituting Eq. (3.1.25) in Eq. (3.1.6), equating to the right hand side of

Eq. (3.1.31), multiplying by kR and using the asymptotic forms of Eq. (3.1.20) for the $H_L^{\pm}$ functions, we have

$$\sum_{L=0}^{\infty}(2L{+}1)\mathrm{i}^L P_L(\cos\theta)A_L\left[\mathrm{i}^L\mathrm{e}^{-\mathrm{i}kR}-\mathbf{S}_L\mathrm{i}^{-L}\mathrm{e}^{\mathrm{i}kR}\right]$$
$$=\sum_{L=0}^{\infty}(2L{+}1)\mathrm{i}^L P_L(\cos\theta)\frac{\mathrm{i}}{2}(\mathrm{i}^L\mathrm{e}^{-\mathrm{i}kR}-\mathrm{i}^{-L}\mathrm{e}^{\mathrm{i}kR})+kf(\theta)\mathrm{e}^{\mathrm{i}kR} \quad (3.1.32)$$

when both $R > R_n$ and $kR \gg L$. Collecting together the separate terms with $\mathrm{e}^{\mathrm{i}kR}$ and $\mathrm{e}^{-\mathrm{i}kR}$ factors, we find

$$\mathrm{e}^{\mathrm{i}kR}\left[\sum_{L=0}^{\infty}(2L{+}1)\mathrm{i}^L P_L(\cos\theta)\left\{A_L\mathbf{S}_L\mathrm{i}^{-L}-\frac{\mathrm{i}}{2}\mathrm{i}^{-L}\right\}+kf(\theta)\right]$$
$$=\mathrm{e}^{-\mathrm{i}kR}\left[\sum_{L=0}^{\infty}(2L{+}1)\mathrm{i}^L P_L(\cos\theta)\left\{A_L\mathrm{i}^L-\frac{\mathrm{i}}{2}\mathrm{i}^L\right\}\right] \ . \quad (3.1.33)$$

Since the $\mathrm{e}^{\pm\mathrm{i}kR}$ are linearly independent, and the two [..] expressions in this equation are independent of R, they must each be identically zero. Furthermore, using the orthogonality (3.1.8) of the Legendre polynomials, the second {..} expression must also be zero, which implies $A_L = \mathrm{i}/2$. Substituting this result into the first zero [..] expression, we derive

$$f(\theta) \ = \ \frac{1}{2\mathrm{i}k}\sum_{L=0}^{\infty}(2L{+}1)P_L(\cos\theta)(\mathbf{S}_L-1) \ . \quad (3.1.34)$$

This important equation (3.1.34) constructs the scattering amplitude in terms of the S matrix elements. The elastic differential cross section is thus

$$\sigma(\theta)\equiv\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega}=\left|\frac{1}{2\mathrm{i}k}\sum_{L=0}^{\infty}(2L{+}1)P_L(\cos\theta)(\mathbf{S}_L-1)\right|^2 \ . \quad (3.1.35)$$

The resulting full scattering wave function is

$$\psi(R,\theta) \ = \ \sum_{L=0}^{\infty}(2L{+}1)\mathrm{i}^L P_L(\cos\theta)\frac{1}{kR}\chi_L(R) \ , \quad (3.1.36)$$

where the radial functions have external form for $R > R_n$ in detail as

$$\chi_L^{\mathrm{ext}}(R) \ = \ \frac{\mathrm{i}}{2}\left[H_L^-(0,kR)-\mathbf{S}_L H_L^+(0,kR)\right] \ . \quad (3.1.37)$$

Phase shifts

Each matrix element $\mathbf{S}_L$ is equivalently described by a *phase shift* δ_L for each partial wave by

$$\mathbf{S}_L = \mathrm{e}^{2\mathrm{i}\delta_L} \tag{3.1.38}$$

by taking complex logarithms as $\delta_L = \frac{1}{2\mathrm{i}} \ln \mathbf{S}_L$. Phase shifts are thus defined up to additive multiples of π. We often add suitable integer multiples $n(E)$ of π,

$$\delta_L(E) = \frac{1}{2\mathrm{i}} \ln \mathbf{S}_L + n(E)\pi \tag{3.1.39}$$

to make $\delta_L(E)$ continuous functions of energy E for each separate partial wave L, but no cross section should depend on this addition as $\mathrm{e}^{2\mathrm{i}\pi n} \equiv 1$.

In terms of the phase shift δ_L, the scattering amplitude can be written as

$$f(\theta) = \frac{1}{k} \sum_{L=0}^{\infty} (2L+1) P_L(\cos\theta) \mathrm{e}^{\mathrm{i}\delta_L} \sin\delta_L \ , \tag{3.1.40}$$

and the external form of Eq. (3.1.37) of the wave function is equivalently

$$\chi_L^{\mathrm{ext}}(R) = \mathrm{e}^{\mathrm{i}\delta_L} \left[\cos\delta_L F_L(0,kR) + \sin\delta_L G_L(0,kR)\right] \ . \tag{3.1.41}$$

In this form we can see the reason for the name 'phase shift'. In the asymptotic region where both $R > R_n$ and $kR \gg L$, we may use Eq. (3.1.19) to write Eq. (3.1.41) as

$$\begin{aligned} \chi_L^{\mathrm{ext}}(R) &\rightarrow \mathrm{e}^{\mathrm{i}\delta_L} [\cos\delta_L \sin(kR - L\pi/2) + \sin\delta_L \cos(kR - L\pi/2)] \\ &= \mathrm{e}^{\mathrm{i}\delta_L} \sin(kR + \delta_L - L\pi/2) \ . \end{aligned} \tag{3.1.42}$$

The oscillations are therefore shifted to smaller R when δ_L is positive, which occurs for attractive potentials at least when they are weak. The oscillatory patterns shift to larger R when $\delta_L < 0$ for repulsive potentials. Physically, attractive potentials pull the oscillations into its range, and repulsive potentials tend to expel the scattering oscillations.

The external solution can be also be written as

$$\chi_L^{\mathrm{ext}}(R) = F_L(0,kR) + \mathbf{T}_L H_L^+(0,kR) \ , \tag{3.1.43}$$

where

$$\mathbf{T}_L = \mathrm{e}^{\mathrm{i}\delta_L} \sin\delta_L \tag{3.1.44}$$

is called the *partial wave T matrix element*. By Eq. (3.1.43), it is the coefficient of $H_L^+(0,kR)$, an outgoing wave, and is related to the S matrix element

by

$$\mathbf{S}_L = 1 + 2\mathrm{i}\mathbf{T}_L \ . \tag{3.1.45}$$

The scattering amplitude in terms of the $\mathbf{T}_L$ is

$$f(\theta) = \frac{1}{k}\sum_{L=0}^{\infty}(2L{+}1)P_L(\cos\theta)\mathbf{T}_L \ . \tag{3.1.46}$$

For zero potential, $\delta_L = \mathbf{T}_L = 0$, and $\chi_L^{\mathrm{ext}}(R) = F_L(0,kR)$ only, the regular partial wave component of the incident plane wave.

A third form of the external wave function is

$$\chi_L^{\mathrm{ext}}(R) = \mathrm{e}^{\mathrm{i}\delta_L}\cos\delta_L\left[F_L(0,kR) + \mathbf{K}_L G_L(0,kR)\right] \ , \tag{3.1.47}$$

with $\mathbf{K}_L = \tan\delta_L$ called the *partial wave K matrix element*. The S matrix element in terms of this is

$$\mathbf{S}_L = \frac{1+\mathrm{i}\mathbf{K}_L}{1-\mathrm{i}\mathbf{K}_L} \ . \tag{3.1.48}$$

For zero potential, $\mathbf{K}_L = 0$. The K matrix element may be directly found from the R matrix element $\mathbf{R}_L$ of the interior solution at the matching radius a as

$$\mathbf{K}_L = -\frac{F_L - a\mathbf{R}_L F_L'}{G_L - a\mathbf{R}_L G_L'} \ , \tag{3.1.49}$$

where the arguments of the F_L and G_L are omitted for clarity. All of the above scattering phase shifts δ_L and partial wave elements $\mathbf{T}_L$, $\mathbf{S}_L$ and $\mathbf{K}_L$ are independent of a, provided that it is larger than the range R_n of the potential.

From Eq. (3.1.49) the consequences of $V(R)$ being real are clear. In this case, the trial function $u(R)$ will be real, and hence also $\mathbf{R}_L$ by Eq. (3.1.28), $\mathbf{K}_L$ by Eq. (3.1.49), and hence δ_L will be real since $\tan\delta_L = \mathbf{K}_L$. It is for these reasons that scattering from a real potential is most often described by a (real) phase shift. This corresponds to the matrix element $\mathbf{S}_L = \mathrm{e}^{2\mathrm{i}\delta_L}$ having unit modulus, $|\mathbf{S}_L| = 1$. The relations between the phase shifts and the $\mathbf{K}$, $\mathbf{T}$ and S matrix elements are summarised in Table 3.1.

Table 3.1. *Relations between the wave functions and the phase shifts,* $\mathbf{K}$*,* $\mathbf{T}$ *and* $\mathbf{S}$ *matrix elements, for an arbitrary partial wave. Partial wave indices and the arguments of the Coulomb functions are omitted for clarity. The last two lines list the consequences of zero and real potentials.*

Using:	δ	$\mathbf{K}$	$\mathbf{T}$	$\mathbf{S}$
$\chi(R) =$	$\mathrm{e}^{\mathrm{i}\delta}[F\cos\delta + G\sin\delta]$	$\dfrac{1}{1-\mathrm{i}\mathbf{K}}\,[F+\mathbf{K}G]$	$F+\mathbf{T}H^+$	$\frac{\mathrm{i}}{2}[H^- - \mathbf{S}H^+]$
$\delta =$	δ	$\arctan\mathbf{K}$	$\arctan\dfrac{\mathbf{T}}{1+\mathrm{i}\mathbf{T}}$	$\dfrac{1}{2\mathrm{i}}\ln\mathbf{S}$
$\mathbf{K} =$	$\tan\delta$	$\mathbf{K}$	$\dfrac{\mathbf{T}}{1+\mathrm{i}\mathbf{T}}$	$\mathrm{i}\dfrac{1-\mathbf{S}}{1+\mathbf{S}}$
$\mathbf{T} =$	$\mathrm{e}^{\mathrm{i}\delta}\sin\delta$	$\dfrac{\mathbf{K}}{1-\mathrm{i}\mathbf{K}}$	$\mathbf{T}$	$\dfrac{\mathrm{i}}{2}(1-\mathbf{S})$
$\mathbf{S} =$	$\mathrm{e}^{2\mathrm{i}\delta}$	$\dfrac{1+\mathrm{i}\mathbf{K}}{1-\mathrm{i}\mathbf{K}}$	$1+2\mathrm{i}\mathbf{T}$	$\mathbf{S}$
$V=0$ V real	$\delta=0$ δ real	$\mathbf{K}=0$ $\mathbf{K}$ real	$\mathbf{T}=0$ $\lvert 1+2\mathrm{i}\mathbf{T}\rvert = 1$	$\mathbf{S}=1$ $\lvert\mathbf{S}\rvert = 1$

Angle-integrated cross sections

From the cross section $\sigma(\theta) = |f(\theta)|^2$ given by Eq. (3.1.35), we may integrate over the entire sphere to find the angle-integrated cross section

$$\begin{aligned}
\sigma_{\mathrm{el}} &= \int_0^{2\pi} d\phi \int_0^{\pi} \mathrm{d}\theta \sin\theta\ \sigma(\theta) \\
&= 2\pi \int_0^{\pi} \mathrm{d}\theta \sin\theta |f(\theta)|^2 \\
&= \frac{\pi}{k^2}\sum_{L=0}^{\infty}(2L+1)|1-\mathbf{S}_L|^2 \\
&= \frac{4\pi}{k^2}\sum_{L=0}^{\infty}(2L+1)\sin^2\delta_L\ , \qquad (3.1.50)
\end{aligned}$$

using the orthogonality and normalisation Eq. (3.1.8) of the Legendre polynomials. Note that this integrated cross section is sometimes called the *total* cross section because it is the total after integration over all angles. However, we reserve the term 'total' to include all non-elastic final states too, as will be used in section 3.2.1.

There exists an Optical Theorem which relates the angle-integrated cross

section $\sigma_{\rm el}$ to the zero-angle scattering amplitude. Using $P_L(1) = 1$, we have

$$f(0) = \frac{1}{2\mathrm{i}k}\sum_{L=0}^{\infty}(2L{+}1)(\mathrm{e}^{2\mathrm{i}\delta_L} - 1) \ , \tag{3.1.51}$$

so

$$\begin{aligned} \mathrm{Im}f(0) &= \frac{1}{k}\sum_{L=0}^{\infty}(2L{+}1)\sin^2\delta_L \\ &= \frac{k}{4\pi}\sigma_{\rm el} \ . \end{aligned} \tag{3.1.52}$$

This relation exists because the incident and scattered waves at zero scattering angle have a fixed relative phase, and interfere in a manner that portrays the total loss of flux from the incident wave to the scattered waves.

Scattering using rotated coordinate systems

To find the scattering from an incident beam in direction $\mathbf{k}$ to direction $\mathbf{k}'$, the Legendre polynomial $P_L(\cos\theta) = P_L(\hat{\mathbf{k}}\cdot\hat{\mathbf{k}}')$ in Eq. (3.1.34) may be simply replaced using the addition theorem for spherical harmonics [2],

$$P_L(\cos\theta) = \frac{4\pi}{2L{+}1}\sum_M Y_L^M(\hat{\mathbf{k}})Y_L^M(\hat{\mathbf{k}}')^* \ . \tag{3.1.53}$$

where $\hat{\mathbf{k}}$ is the notation for a unit vector in the $\mathbf{k}$ direction. This, from Eq. (3.1.24), gives the partial wave expansion of a plane wave in direction $\hat{\mathbf{k}}$ as

$$\mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{R}} = 4\pi\sum_{LM}\mathrm{i}^L Y_L^M(\hat{\mathbf{R}})Y_L^M(\hat{\mathbf{k}})^*\frac{1}{kR}F_L(0,kR) \ . \tag{3.1.54}$$

Thus the amplitude $f(\mathbf{k}';\mathbf{k})$ for scattering from direction $\mathbf{k}$ to $\mathbf{k}'$ is

$$f(\mathbf{k}';\mathbf{k}) = \frac{2\pi}{\mathrm{i}k}\sum_{LM}Y_L^M(\hat{\mathbf{k}}')Y_L^M(\hat{\mathbf{k}})^*\ (\mathrm{e}^{2\mathrm{i}\delta_L} - 1) \tag{3.1.55}$$

$$= \frac{4\pi}{k}\sum_{LM}Y_L^M(\hat{\mathbf{k}}')Y_L^M(\hat{\mathbf{k}})^*\ \mathbf{T}_L, \tag{3.1.56}$$

and the full scattering wave function depends on the incident momentum as

$$\psi(\mathbf{R};\mathbf{k}) = 4\pi\sum_{LM}\mathrm{i}^L Y_L^M(\hat{\mathbf{R}})Y_L^M(\hat{\mathbf{k}})^*\frac{1}{kR}\chi_L(R) \ . \tag{3.1.57}$$

In both cases, the vector $\mathbf{k}$ after the semicolon indicates the incident momentum. Note that a spherical harmonic for its unit vector argument in the

$+z$ direction is $Y_L^M(\hat{\mathbf{z}}) = \delta_{M0}\sqrt{\frac{2L+1}{4\pi}}$, so another form of Eq. (3.1.24) is

$$\mathrm{e}^{\mathrm{i}kz} = \sqrt{4\pi}\sum_{L=0}^{\infty}\mathrm{i}^L\sqrt{2L+1}\;Y_L^0(\hat{\mathbf{R}})\frac{1}{kR}F_L(0,kR) \tag{3.1.58}$$

for the plane wave in the $+\hat{\mathbf{z}}$ direction.

3.1.2 Coulomb and nuclear potentials

In general, we saw in Chapter 1, nuclei have between them both a short range attractive nuclear potential and a long range Coulomb repulsion. This Coulomb component has the $1/R$ form shown in Fig. 1.3, and invalidates the theory presented above for finite range potentials. We develop below a theory for a pure $1/R$ component, and then see how to add to it the effects of an additional finite range correction to the Coulomb component. We still assume both the Coulomb and nuclear potentials to be spherical.

Pure point Coulomb scattering

If we consider *only* the point Coulomb potential between two particles with charges Z_1 and Z_2, we have

$$V_c(R) = Z_1Z_2\mathrm{e}^2/R\ . \tag{3.1.70}$$

For scattering with relative velocity v, we define a dimensionless *Sommerfeld parameter* η, as mentioned before, by

$$\eta = \frac{Z_1Z_2\mathrm{e}^2}{\hbar v} = \frac{Z_1Z_2\mathrm{e}^2\mu}{\hbar^2 k} = \frac{Z_1Z_2\mathrm{e}^2}{\hbar}\left(\frac{\mu}{2E}\right)^{\frac{1}{2}}\ . \tag{3.1.71}$$

where the energy of relative motion is $E = \hbar^2k^2/2\mu$. A beam in the direction $\mathbf{k}$ is no longer $\mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{R}}$ when $\eta \neq 0$. However, the Schrödinger equation with the Coulomb potential has been solved exactly, and the solution in terms of hypergeometric functions is

$$\psi_c(\mathbf{k},\mathbf{R}) = \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{R}}\;\mathrm{e}^{-\pi\eta/2}\;\Gamma(1{+}\mathrm{i}\eta)\;{}_1F_1(-\mathrm{i}\eta;1;\mathrm{i}(kR-\mathbf{k}\cdot\mathbf{R}))\ , \tag{3.1.72}$$

defined using the Gamma function $\Gamma(z)$ and the confluent hypergeometric function ${}_1F_1(a;b;z)$ of Eq. (3.1.61).

In partial wave form, the generalisation of the standard $+\hat{\mathbf{z}}$ plane-wave expansion Eq. (3.1.24) is

$$\psi_c(k\hat{\mathbf{z}},\mathbf{R}) = \sum_{L=0}^{\infty}(2L{+}1)\mathrm{i}^L P_L(\cos\theta)\frac{1}{kR}F_L(\eta,kR)\ . \tag{3.1.73}$$

The functions $F_L(\eta,\rho)$, $G_L(\eta,\rho)$ and $H_L^{\pm}(\eta,\rho)$ are the solutions of Eq. (3.1.23) for $\eta \neq 0$. In terms of a 'Coulomb constant'

$$C_L(\eta) = \frac{2^L \mathrm{e}^{-\pi\eta/2}|\Gamma(1+L+\mathrm{i}\eta)|}{(2L{+}1)!} \tag{3.1.59}$$

and the confluent hypergeometric function ${}_1F_1(a;b;z) \equiv M(a,b,z)$, the regular function defined in Abramowitz and Stegun [1, ch. 13] as

$$F_L(\eta,\rho) = C_L(\eta)\rho^{L+1}\mathrm{e}^{\mp\mathrm{i}\rho}\ {}_1F_1(L{+}1 \mp \mathrm{i}\eta; 2L{+}2; \pm 2\mathrm{i}\rho)\ , \tag{3.1.60}$$

where either the upper or lower signs may be taken for the same result. The ${}_1F_1(a;b;z)$ is defined by the the series expansion

$${}_1F_1(a;b;z) = 1 + \frac{a}{b}\frac{z}{1!} + \frac{a(a{+}1)}{b(b{+}1)}\frac{z^2}{2!} + \frac{a(a{+}1)(a{+}2)}{b(b{+}1)(b{+}2)}\frac{z^3}{3!} + \cdots\ . \tag{3.1.61}$$

The two irregular functions have the corresponding definitions

$$\begin{aligned} H_L^{\pm}(\eta,\rho) &= G_L(\eta,\rho) \pm \mathrm{i}F_L(\eta,\rho) && (3.1.62)\\ &= \mathrm{e}^{\pm\mathrm{i}\Theta}(\mp 2\mathrm{i}\rho)^{1+L\pm\mathrm{i}\eta}U(1{+}L \pm \mathrm{i}\eta, 2L{+}2, \mp 2\mathrm{i}\rho) && (3.1.63)\end{aligned}$$

where $U(a,b,z)$ is the corresponding irregular confluent hypergeometric function defined in [1, ch. 13]. The $\Theta \equiv \rho - L\pi/2 + \sigma_L(\eta) - \eta\ln(2\rho)$, and

$$\sigma_L(\eta) = \arg\Gamma(1+L+\mathrm{i}\eta) \tag{3.1.64}$$

is called the *Coulomb phase shift*. The functions may easily be calculated numerically [1, 3], also for complex arguments [4].

Their behaviour near the origin is thus

$$F_L(\eta,\rho) \sim C_L(\eta)\rho^{L+1}\ ,\quad G_L(\eta,\rho) \sim \left[(2L{+}1)C_L(\eta)\ \rho^L\right]^{-1}, \tag{3.1.65}$$

noting that

$$C_0(\eta) = \sqrt{\frac{2\pi\eta}{\mathrm{e}^{2\pi\eta}-1}}\ \text{ and }\ C_L(\eta) = \frac{\sqrt{L^2+\eta^2}}{L(2L{+}1)}C_{L-1}(\eta)\ . \tag{3.1.66}$$

A transition from small-ρ power law behaviour to large-ρ oscillatory behaviour occurs outside the classical turning point. This point is where $1 = 2\eta/\rho + L(L{+}1)/\rho^2$, namely

$$\rho_{tp} = \eta \pm \sqrt{\eta^2 + L(L{+}1)}\ . \tag{3.1.67}$$

In nuclear reactions η is usually positive, so with purely Coulomb and centrifugal potentials there is only one turning point. Classically the turning point is at the distance of closest approach, $R_{\rm near}$ of Eq. (3.1.77), and these quantities are related by $\rho_{tp} = kR_{\rm near}$ if the classical impact parameter b is related to the quantum mechanical partial wave L according to

$$k\ b = \sqrt{L(L{+}1)} \approx L + \tfrac{1}{2}\ . \tag{3.1.68}$$

The asymptotic behaviour of the Coulomb functions outside the turning point ($\rho \gg \rho_{tp}$) is

$$F_L(\eta,\rho) \sim \sin\Theta\ ,\quad G_L(\eta,\rho) \sim \cos\Theta\ \text{ and } H_L^{\pm}(\eta,\rho) \sim \mathrm{e}^{\pm\mathrm{i}\Theta}\ . \tag{3.1.69}$$

Box 3.2: Coulomb Functions for $\eta \neq 0$

The classical scattering orbit in a Coulomb potential is a hyperbola, in which the distance of the projectile in polar coordinates (R, α), starting at $\alpha = \pi$, is

$$\frac{1}{R(\alpha)} = \frac{1}{b}\sin\alpha - \frac{D}{2b^2}(1+\cos\alpha) \tag{3.1.75}$$

where $D = Z_1 Z_2 \mathrm{e}^2/E = 2\eta/k$ is the distance of closest approach in a head-on collision, and b is the impact parameter for a general collision: the distance between the target and a straight line continuing the initial trajectory. As $R \to \infty$ after the collision, α becomes the scattering angle θ, which from Eq. (3.1.75) is

$$\tan\frac{\theta}{2} = \frac{\eta}{bk}. \tag{3.1.76}$$

The distance of closest approach for arbitrary scattering angle θ is

$$R_{\mathrm{near}}(\theta) = \frac{\eta}{k}\left[1 + \mathrm{cosec}\frac{\theta}{2}\right] \ , \tag{3.1.77}$$

and the classical differential cross section, using Eq. (3.1.76), is

$$\sigma(\theta) \equiv \frac{b(\theta)}{\sin\theta}\frac{\mathrm{d}b}{\mathrm{d}\theta} = \frac{\eta^2}{4k^2\sin^4(\theta/2)} \ . \tag{3.1.78}$$

Box 3.3: Classical Coulomb scattering

We are now using the regular Coulomb function $F_L(\eta, kR)$ with $\eta \neq 0$. Details of F_L and G_L for general η, and their asymptotic forms for small and large ρ, are given in Box 3.2. In particular, the asymptotic form of $F_L(\eta, kR)$ is

$$F_L(\eta, kR) \sim \sin(kR - L\pi/2 + \sigma_L(\eta) - \eta\ln(2kR)) \ , \tag{3.1.74}$$

with the *Coulomb phase shift* $\sigma_L(\eta)$ is given by Eq. (3.1.64). The logarithmic term in this expression is needed to accommodate the $1/R$ coulomb potential. Thus the phase shift caused by the Coulomb potential is $\sigma_L(\eta)$, once $kR \gg \eta\ln(2kR)$.

The outgoing part in $\psi_c(k\mathbf{z}, \mathbf{R})$ is found by matching at large values of $R - z$ to

$$\psi_c(k\hat{\mathbf{z}}, \mathbf{R}) \overset{R\to\infty}{\to} \mathrm{e}^{\mathrm{i}[kz + \eta\ln k(R-z)]} + f_c(\theta)\frac{\mathrm{e}^{\mathrm{i}[kR - \eta\ln 2kR]}}{R} \ . \tag{3.1.79}$$

The $\psi_c(k\mathbf{z}, \mathbf{R})$ therefore has a scattering amplitude $f_c(\theta)$ which, following Eq. (3.1.34), is *formally* the partial wave sum

$$f_c(\theta) = \frac{1}{2\mathrm{i}k}\sum_{L=0}^{\infty}(2L+1)P_L(\cos\theta)(\mathrm{e}^{2\mathrm{i}\sigma_L(\eta)} - 1) \ , \tag{3.1.80}$$

in terms of the Coulomb phase shift. However, this series expression does not converge, because the Coulomb potential does not go to zero fast enough for large $R = L/k$, and the phase shifts $\sigma_L(\eta)$ never go to zero for large L. The series only has meaning if a screened Coulomb potential is used, and then the screening radius let tend to infinity: see Taylor [5, §14-a].

If however Eq. (3.1.72) is directly matched to Eq. (3.1.79) for large $(R-z)$ values, the asymptotic amplitude is found to be

$$f_c(\theta) = -\frac{\eta}{2k\sin^2(\theta/2)} \exp\left(-\mathrm{i}\eta\ln(\sin^2(\theta/2)) + 2\mathrm{i}\sigma_0(\eta)\right) \ , \qquad (3.1.81)$$

which is called the *point Coulomb scattering amplitude*. The point-Coulomb cross section is therefore

$$\sigma_R(\theta) = |f_c(\theta)|^2 = \frac{\eta^2}{4k^2\sin^4(\theta/2)} \ . \qquad (3.1.82)$$

and is called the *Rutherford cross section*, because it happens to be the same as in classical scattering theory (see Box 3.3).

Coulomb+nuclear scattering

With the nuclear potential included as well as the deviation at short distances of the Coulomb potential from the pure $1/R$ form, the scattering potential may be written as $V(R) = V_c(R) + V_n(R)$ for some finite range potential $V_n(R)$ in addition to the point Coulomb potential of Eq. (3.1.70). We assume that $V_n(R)$ is spherical.

The phase shift from $V(R)$ will be $\delta_L \neq \sigma_L(\eta)$, so we define an *additional nuclear phase shift* δ_L^n by

$$\delta_L = \sigma_L(\eta) + \delta_L^n \ . \qquad (3.1.83)$$

The scattering amplitude $f_{nc}(\theta)$ from the combined Coulomb and nuclear potential $V(R)$ will, using Eq. (3.1.34), have a factor

$$\mathrm{e}^{2\mathrm{i}\delta_L} - 1 = (\mathrm{e}^{2\mathrm{i}\sigma_L(\eta)} - 1) + \mathrm{e}^{2\mathrm{i}\sigma_L(\eta)}(\mathrm{e}^{2\mathrm{i}\delta_L^n} - 1) \ , \qquad (3.1.84)$$

so that the partial wave sums will be a combination of the point Coulomb amplitude of Eq. (3.1.80) and an additional 'Coulomb-distorted nuclear amplitude' $f_n(\theta)$:

$$f_{nc}(\theta) = f_c(\theta) + f_n(\theta) \ . \qquad (3.1.85)$$

To find the Coulomb-distorted nuclear phase shift δ_L^n, or equivalently the nuclear S matrix element $\mathsf{S}_L^n = \mathrm{e}^{2\mathrm{i}\delta_L^n}$, we match to a generalisation of the

asymptotic form of Eq. (3.1.37), namely to

$$\chi_L^{\rm ext}(R) = \frac{\rm i}{2}[H_L^-(\eta, kR) - \mathbf{S}_L^n H_L^+(\eta, kR)] \ . \tag{3.1.86}$$

This equation simply uses Coulomb functions with their first argument η now not zero, but given by Eq. (3.1.71). Similarly, in terms of the nuclear phase shift δ_L^n, we generalise Eq. (3.1.41) to obtain

$$\chi_L^{\rm ext}(R) = {\rm e}^{{\rm i}\delta_L^n}\left[\cos\delta_L^n\ F_L(\eta, kR) + \sin\delta_L^n\ G_L(\eta, kR)\right] \ . \tag{3.1.87}$$

The new scattering amplitude for the nuclear potential in addition to the point Coulomb scattering is found by using the second term in Eq. (3.1.84):

$$f_n(\theta) = \frac{1}{2{\rm i}k}\sum_{L=0}^{\infty}(2L{+}1)P_L(\cos\theta){\rm e}^{2{\rm i}\sigma_L(\eta)}(\mathbf{S}_L^n - 1) \ . \tag{3.1.88}$$

This is therefore *not* just the amplitude due to the short range forces alone.

Note that we can optionally multiply both f_c of Eq. (3.1.81) and f_n of Eq. (3.1.88) by a phase factor such as $\exp(-2{\rm i}\sigma_0(\eta))$, as only relative phase makes any difference to the *Coulomb+nuclear cross section*

$$\sigma_{nc}(\theta) = |f_c(\theta) + f_n(\theta)|^2 \equiv |f_{nc}(\theta)|^2 \ . \tag{3.1.89}$$

Since this cross section diverges to infinity at small angles because of Eq. (3.1.82), very often elastic scattering cross sections are presented numerically in terms of their ratio to Rutherford, written as†

$$\sigma/\sigma_R \equiv \sigma_{nc}(\theta)/\sigma_R(\theta) \ , \tag{3.1.90}$$

which becomes unity at small angles.

3.1.3 Resonances and virtual states

When cross sections are plotted as functions of energy, $\sigma(E)$ either angle-integrated or for a specific angle, these plots are called excitation functions. They often show a range of narrower and wider peaks. Many of these peaks are caused by resonances, when the interacting particles are trapped together inside a potential barrier for some period of time τ. This gives rise to variations in the excitation function with widths $\Gamma \sim \hbar/\tau$. We will see that resonance variations can be peaks, but also sometimes interference dips, or a peak next to a dip: all these patterns may result from a single resonance interfering with other scattering mechanisms.

A resonance is described by its total spin $J_{\rm tot}$ and parity $\pi = \pm 1$ (which

† Written this way for simplicity, although strictly σ is an angle-integrated cross section.

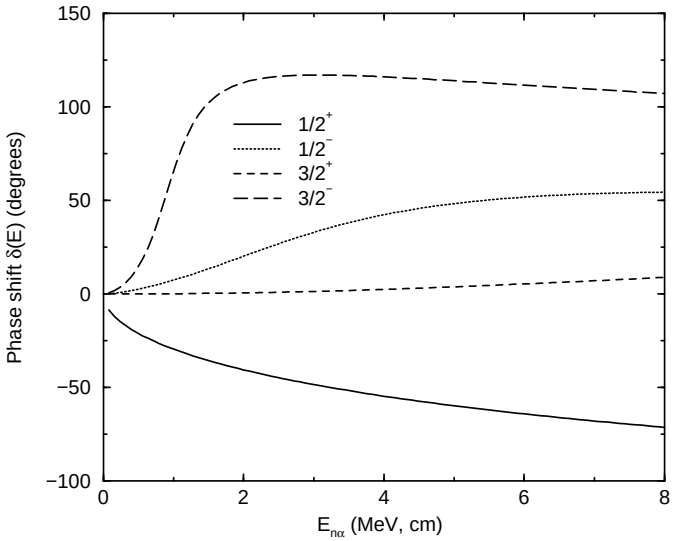

Fig. 3.2. Examples of resonant phase shifts for the $J^\pi = 3/2^-$ channel in low energy n-α scattering, with a pole at $E = 0.96 - \mathrm{i}0.92/2$ MeV. There is only a hint of a resonance in the phase shifts for the $J^\pi = 1/2^-$ channel, but it does have a wide resonant pole at $1.9 - \mathrm{i}6.1/2$ MeV.

we combine in the notation $J^\pi_{\rm tot}$)‡, along with its energy $E_{\rm r}$ and width Γ in units of energy. A resonance will show characteristically as a rapid rise of the scattering phase shift $\delta(E)$ as seen in Fig. 3.2, and this corresponds to a time delay for the scattering of a wave packet is of the order $\Delta t \sim \hbar {\rm d}\delta(E)/{\rm d}E$ [6] §.

The form of the increase is often found to be like

$$\delta(E) = \delta_{\rm bg}(E) + \delta_{\rm res}(E) \tag{3.1.91}$$

where

$$\delta_{\rm res}(E) = \arctan\left(\frac{\Gamma/2}{E_{\rm r} - E}\right) + n(E)\pi \ ,$$

for $\Gamma > 0$, and for some *background phase shift* $\delta_{\rm bg}(E)$ that varies only slowly around the resonance energy. The $n(E)$ is the integer depending on energy that may be optionally added to make $\delta_{\rm res}(E)$ a continuous function of energy. If the background phase shift $\delta_{\rm bg}(E) \approx 0$, then by Eq. (3.1.50)

‡ With the one-channel scattering considered so far, $J_{\rm tot} = L$ and $\pi = (-1)^L$.

§ This paper explains why phase shifts which *decrease* are not candidates for resonances because this corresponds to a time *advance*, which is limited by causality to the size of target divided by velocity of incident relative motion.

the resonance produces a contribution to the angle-integrated cross section of

$$\begin{aligned}\sigma_{\rm el}^{\rm res}(E) &\simeq \frac{4\pi}{k^2}(2L{+}1)\sin^2\delta_{\rm res}(E) \\ &= \frac{4\pi}{k^2}(2L{+}1)\frac{\Gamma^2/4}{(E-E_{\rm r})^2+\Gamma^2/4}\ , \end{aligned} \tag{3.1.92}$$

which shows a clear peak at $E \sim E_{\rm r}$ with a full width at half maximum (fwhm) of Γ.

A resonance with the form of Eq. (3.1.92) with $\delta_{\rm bg}(E) = 0$ called a *pure Breit-Wigner resonance*. If $\delta_{\rm bg}(E) \neq 0$ then Fig. 3.3 shows some of other Breit-Wigner patterns that may be produced. If moreover $\delta_{\rm bg}(E)$ varies with energy, a resonance may still exist even though the phase shift $\delta(E)$ does not pass $\pi/2$, such as with the $1/2^-$ scattering in Fig. 3.2.

The interference and cancellation effects shown in Fig. 3.3 for the angle-integrated elastic cross sections occur when there is a background phase shift in the *same* partial wave as the resonance. If there are contributing amplitudes from *different* (non-resonant) partial waves, then there can be no cancellation effects for the angle-integrated cross sections of Eq. (3.1.50) since these are *incoherent* in the partial wave sum. A resonance can only give coherent interference with another partial wave if the *angular* cross sections are measured, since Eq. (3.1.34) is coherent in its partial wave sum.

Because the propagation of a wave packet in the presence of a resonance experiences a time delay of $\tau \sim \hbar\ {\rm d}\delta_{\rm res}(E)/{\rm d}E$, the form of Eq. (3.1.91) implies that $\tau \sim \hbar/\Gamma$ as earlier expected.

If the S matrix is calculated for a Breit-Wigner resonance using the parametrisation of Eq. (3.1.91), then, using $\tan\delta_{\rm res}(E) = \frac{1}{2}\Gamma/(E_{\rm r}-E)$ and Eq. (3.1.48),

$$\mathbf{S}(E) = {\rm e}^{2{\rm i}\delta_{\rm bg}(E)}\frac{E-E_{\rm r}-{\rm i}\Gamma/2}{E-E_{\rm r}+{\rm i}\Gamma/2}\ . \tag{3.1.93}$$

This expression shows that if the function $\mathbf{S}(E)$ were continued to complex energies E, it would have a pole, where the denominator is zero, at $E_p = E_{\rm r} - {\rm i}\Gamma/2$. These are poles in the fourth quadrant of the complex energy plane, near but below the real energy axis. The existence of such a complex pole leads most theorists to *define* resonance by its pole position†, by the parameters $J^\pi_{\rm tot}$ and complex E_p‡. In the example of low energy n-α

† We should note, however, that there yet exist cross section peaks that are not associated with poles, as noted for example in [5].

‡ In the more general multichannel theory to be presented in section 3.2.1, we will see more how many partial wave channels may couple to the total $J^\pi_{\rm tot}$. The resonance peaks will then

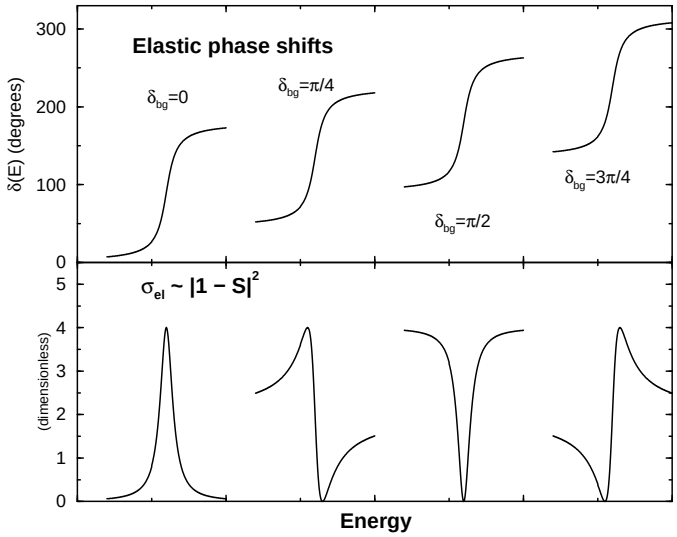

Fig. 3.3. Possible Breit-Wigner resonances. The upper panel shows resonant phase shifts with several background phase shifts $\delta_{\rm bg} = 0$, $\pi/4$, $\pi/2$ and $3\pi/4$ in the same partial wave. The lower panel gives the corresponding contributions to the total elastic scattering cross section from that partial wave.

scattering in Fig. 3.2, calculations of scattering at complex energies show that there is indeed a pole at $E = 0.96 - {\rm i}0.92/2$ MeV in the $3/2^-$ channel. There is only a hint of a resonance in the phase shifts for the $J^\pi = 1/2^-$ channel, but we find it does have a resonant pole at $1.9 - {\rm i}6.1/2$ MeV. A wide resonance (one with large Γ) such as this one has a broad effect on scattering over a large energy range.

Mathematically, therefore, a resonance is a pole of the S matrix in the fourth complex energy quadrant, with ${\rm Re}E_p > 0$ and ${\rm Im}E_p < 0$. Resonances may also be characterised as *unbound states*: states that would be bound if the nuclear potential were stronger. In the complex plane, bound states are also poles, on the negative real energy axis and the positive imaginary k axis as shown by the circles in Fig. 3.4. If the potential for a bound state becomes weaker, it moves towards zero energy according to the arrows, and then becomes a resonance (the squares in Fig. 3.4) if there is a potential barrier between large distances and the interior nuclear attraction. This trapping barrier could be a repulsive Coulomb barrier for proton–nucleus scattering such as seen in Fig. 1.3, or a centrifugal barrier for either neutrons or protons in angular momentum $L > 0$ states. The width of the resonance

occur in all the partial waves, and the definition in terms of an S matrix pole is applicable to multichannel as well as one-channel scattering.

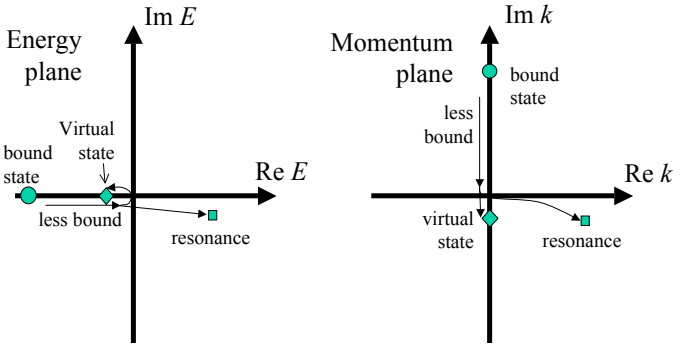

Fig. 3.4. The correspondences between the energy (left) and momentum (right) complex planes. The arrows show the trajectory of a bound state caused by a progressively weaker potential: it becomes a resonance for $L > 0$ or when there is a Coulomb barrier, otherwise it becomes a virtual state. Because $E \propto k^2$, bound states on the positive imaginary k axis and virtual states on the negative imaginary axis both map onto the negative energy axis.

is extremely sensitive to the height of these barriers. Very wide resonances, or poles a long way from the real axis, will not have a pronounced effect on scattering at real energies, especially if there are several of them. They may thus be considered less important physically.

The case of neutral scattering in $L = 0$ partial waves deserves special attention, since here there is no repulsive barrier to trap e.g. a s-wave neutron. There is no Breit-Wigner form now, and mathematically the S matrix pole S_p is found to be on the negative imaginary k axis: the diamonds in Fig. 3.4. This corresponds to a negative real pole energy, but this is *not* a bound state, for which the poles are always on the positive imaginary k axis. The neutral unbound poles are called *virtual states*, to be distinguished from both bound states and resonances. The dependence on the sign of $k_p = \pm\sqrt{2\mu E_p/\hbar^2}$ means we should write the S matrix as a function of k not E. A pure virtual state has pole at $k_p = \mathrm{i}/a$ on the negative imaginary axis, described by a negative value of a called the *scattering length*. This corresponds to the analytic form

$$S(k) = -\frac{k + \mathrm{i}/a}{k - \mathrm{i}/a} \ , \tag{3.1.94}$$

giving $\delta(k) = -\arctan ak$, or $k \cot \delta(k) = -1/a$. These formulae describe the phase shift behaviour close to the pole, in this case for low momenta where k not too much larger than $1/|a|$. For more discussion see for example Taylor [5, §13-b].

3.1.4 Nuclear currents or flux

When a charged particle is scattered from another particle, its acceleration during the reaction will in general lead to an exchange of energy with the electromagnetic field according to Maxwell's equations. The electromagnetic field depends more specifically on the *nuclear current* or *flux* of the charged particles, and therefore we need to find this current in terms of the scattering wave functions.

One definition of the nuclear probability current or flux was that given in Eq. (2.4.1), namely $\mathbf{j} = \mathbf{v}|\psi|^2$, but this definition is only preliminary as it uses for $\mathbf{v}$ the average beam velocity, and not a local property of the wave functions in the presence of potentials. A proper definition of the nuclear current $\mathbf{j}(\mathbf{r}, t)$ should at every position $\mathbf{r}$ satisfy the *continuity equation*

$$\nabla \cdot \mathbf{j}(\mathbf{r}, t) + \frac{\partial \rho(\mathbf{r}, t)}{\partial t} = 0 \tag{3.1.95}$$

with probability density $\rho(\mathbf{r}, t) = |\psi(\mathbf{r}, t)|^2$. A current satisfying this continuity equation is called a *conserved current*.

Using first the *free field* Schrödinger equation $\hat{T}\psi = i\hbar\frac{\partial\psi}{\partial t}$ with the kinetic energy operator $\hat{T} = -\frac{\hbar^2}{2\mu}\nabla^2$, we may evaluate the rate of density change for a free particle as

$$\begin{aligned} \frac{\partial \psi^*\psi}{\partial t} &= \frac{\partial \psi^*}{\partial t}\psi + \psi^*\frac{\partial \psi}{\partial t} \\ &= \frac{\hbar}{2\mathrm{i}\mu}\left[\left(\nabla^2\psi\right)^*\psi \ - \psi^*\nabla^2\psi\right] \\ &= \frac{\hbar}{2\mathrm{i}\mu}\nabla\cdot\left[(\nabla\psi)^*\psi \ - \psi^*\nabla\psi\right] \ . \end{aligned} \tag{3.1.96}$$

This yields a local conserved current or flux for the free-field case of

$$\mathbf{j}_{\text{free}} = \frac{\hbar}{2\mathrm{i}\mu}(\psi^*\nabla\psi - \psi\nabla\psi^*) \ , \tag{3.1.97}$$

and leads us to define the *free current operator* either as

$$\hat{\mathbf{j}}_{\text{free}} = \frac{\hbar}{2\mathrm{i}\mu}(\overrightarrow{\nabla} - \overleftarrow{\nabla}) \ , \tag{3.1.98}$$

where the arrows indicate the target of the differentiation, or better as a position-dependent operator

$$\hat{\mathbf{j}}_{\text{free}}(\mathbf{r}) = \frac{\hbar}{2\mathrm{i}\mu}\left\{\delta(\mathbf{r}-\mathbf{r}_i)\ \nabla_i - \nabla_i\ \delta(\mathbf{r}-\mathbf{r}_i)\right\} \ , \tag{3.1.99}$$

where the $\mathbf{r}_i$ are the variables in terms of which the wave function is written

as $\psi(\mathbf{r}_i)$, and the gradients ∇_i are with respect to the $\mathbf{r}_i$. The current operator of Eq. (3.1.99) can be used in normal matrix elements such as $\langle\phi|\hat{\mathbf{j}}_{\rm free}(\mathbf{r})|\psi\rangle$ which integrate over the internal $\mathbf{r}_i$ coordinates, and yield the current as a function of $\mathbf{r}$.

We define the *electric* current j_q by means of the *electric current operator* $\hat{\mathbf{j}}_q$ that is proportional to the charge times the nuclear current of that charged particle. That is,

$$\hat{\mathbf{j}}_q = q\hat{\mathbf{j}} \tag{3.1.100}$$

for the particle charge of q, to be used for example in section 3.5.2 for photonuclear reactions.

In the case of *interacting* particles because of a potential between them, ψ satisfies $[\hat{T}+\hat{V}]\psi = i\hbar\frac{\partial\psi}{\partial t}$, where we now allow the potential $\hat{V}$ to be a general operator that operates on functions of the $\mathbf{r}_i$. It may have derivatives (from a spin-orbit force) or may be parity- or partial-wave-dependent. These are all particular kinds of non-localities, where a non-local potential kernel such as $V(\mathbf{r}'_i, \mathbf{r}_i)$ removes flux at one position $\mathbf{r}_i$ and has it reappear at another place $\mathbf{r}'_i \neq \mathbf{r}_i$. In this case it should not be surprising that we have to adjust our definitions of the nuclear current, which is supposed to follow continuity.

Evaluating the rate of density change gives

$$\begin{aligned} \frac{\partial\psi^*\psi}{\partial t} &= (\frac{1}{i\hbar}[\hat{T}+\hat{V}]\psi)^*\psi + \psi^*\frac{1}{i\hbar}[\hat{T}+\hat{V}]\psi \\ &= \frac{\hbar}{2\mathrm{i}\mu}\nabla\cdot[(\nabla\psi)^*\,\psi\ -\psi^*\nabla\psi] + \frac{1}{i\hbar}[\psi^*\hat{V}\psi - (\hat{V}\psi)^*\psi]\ . \\ \text{Thus } \frac{\partial\rho(\mathbf{r},t)}{\partial t} &= -\nabla\cdot\mathbf{j}_{\rm free} - \frac{\mathrm{i}}{\hbar}\langle\psi|\left[\delta(\mathbf{r}-\mathbf{r}_i)\hat{V} - \hat{V}^\dagger\delta(\mathbf{r}-\mathbf{r}_i)\right]|\psi\rangle \end{aligned} \tag{3.1.101}$$

If the potential $\hat{V}$ were a local real function of position $\mathbf{r}_i$ only, then this last term disappears, and the free current operator of Eq. (3.1.98) gives a conserved current. In general, however, this is not the case, and it is a task to find a second contribution $\hat{\mathbf{j}}_2$ to the current operator so that the sum

$$\hat{\mathbf{j}} = \hat{\mathbf{j}}_{\rm free} + \ \hat{\mathbf{j}}_2 \tag{3.1.102}$$

is a conserved current when the interaction potentials are present. If this additional term comes from the two-body interaction terms, it is called the *two-body current contribution*. It must satisfy

$$\nabla\cdot\hat{\mathbf{j}}_2 = \frac{\mathrm{i}}{\hbar}[\delta(\mathbf{r}-\mathbf{r}_i)\ \hat{V} - \hat{V}^\dagger\ \delta(\mathbf{r}-\mathbf{r}_i)]\ , \tag{3.1.103}$$

so that the full current operator satisfies

$$\nabla \cdot \hat{\mathbf{j}} = \frac{\mathrm{i}}{\hbar}[\delta(\mathbf{r}-\mathbf{r}_i)\ H - H^\dagger\ \delta(\mathbf{r}-\mathbf{r}_i)]\ , \tag{3.1.104}$$

which is equivalent to the original continuity equation (3.1.95)†.

Later, in section 4.7, we will see that Eq. (3.1.104) is by itself sufficient to solve our problems for one particular important application. For electric transitions at long distances and low momentum, we will see that Siegert's theorem allows us to include two-body currents, because in that case their only relevant property is the one given by Eq. (3.1.103), that is, by the continuity equation itself. However, we cannot from a purely nucleonic model calculate the effect of two-body currents $\hat{\mathbf{j}}_2$ in *magnetic* transitions, and in electric transitions with higher momentum transfers, so in their calculations we will have in this book to omit the terms depending on $\hat{\mathbf{j}}_2$.

3.1.5 Complex potentials

Often, the effective interactions between two nuclei give the best fit to experimental cross sections if they are allowed to have *negative imaginary* as well as real components, even though the microscopic interaction potentials between individual nucleons may be entirely real valued. The effective imaginary components arise from a variety of reasons, but principally because in nature there are more reactions occurring than can be described by the spherical potentials dealt with so far. These further reactions remove flux from elastic scattering, and we will see that this removal can be equivalently described by complex potentials.

In the next section 3.2 we will see how to define multiple channels for the model wave functions, and later (section 11.5.3) it will be shown how eliminating such channels from our model induces imaginary potentials in the remaining components. Imaginary potentials are also present in a potential that reproduces amplitudes that have been averaged over a range of scattering energies (section 11.5), especially if we average over many compound-

† The continuity equation is not sufficient by itself to define the complete current, because only defines the 'longitudinal' component of $\hat{\mathbf{j}}_2$, not its 'transverse' component, because adding $\nabla \times \mathbf{X}(\mathbf{r})$ to $\hat{\mathbf{j}}_2$ does not change $\nabla \cdot \hat{\mathbf{j}}_2$ whatever vector field $\mathbf{X}(\mathbf{r})$ might be chosen.

That is, only if we have a microscopic explanation of the potential non-localities in terms of a local theory (for example of meson exchanges) do we have a unique specification of local nuclear currents. This is the case where we can start from a fully gauge-invariant Lagrangian. In other cases, it may still be possible to construct a current which is conserved. For example, Sachs [7] finds a current for isospin exchange forces, Riska [8] finds a current for spin-orbit potentials, and recently Marcucci et al [9] find conserved currents for modern fully-fitted two- and three-nucleon potentials, but these derivations, however, do not give unique results for the conserved current: that can only be obtained in definite meson exchange models. The effect of these ambiguities is that we do not really know the details of the current at short distances.

The interaction potential between a nucleon and a nucleus is usually well described by an attractive nuclear well of the form

$$V(R) = -\frac{V_r}{1 + \exp\left(\frac{R-R_r}{a_r}\right)} \tag{3.1.105}$$

which is called a 'Woods-Saxon' (or 'Saxon-Woods' or 'Fermi') shape. The central depth V_r is typically between 40 and 50 MeV, and the diffuseness a_r about 0.6 fm. The radius R_r is proportional to the size of the nucleus, and is commonly around $R_r = r_r A^{1/3}$ for a nucleus of A nucleons, with $r_r \approx 1.2$ fm. Similar potentials can be used for the interaction between two nuclei with mass numbers A_1 and A_2, if the radii are scaled instead as $R_r = r_r(A_1^{1/3} + A_2^{1/3})$, since this is proportional to the sum of the individual radii.

This potential is usually combined with an imaginary and a spin-orbit part. The imaginary part, which is present at higher scattering energies as discussed in §3.1.5, is also often given by a Woods-Saxon form

$$W(R) = -\frac{V_i}{1 + \exp\left(\frac{R-R_i}{a_i}\right)} \tag{3.1.106}$$

for a similar geometry $R_i \approx R_r$ and $a_i \approx a_r$, and a depth V_i fitted to experiments giving $V_i \sim 10 - 20$ MeV depending on energy. Sometimes a surface-peaked imaginary contribution is also included, with a shape like the derivative of Eq. (3.1.106).

The spin-orbit potentials will be described in §4.3.2.

Box 3.4: Typical nuclear scattering potentials

nucleus resonances (section 11.5.2). The potentials that fit elastic scattering are therefore generally complex, of the kind outlined in Box 3.4 and again in section 4.1.

If the potential is $V(R) + \mathrm{i}W(R)$, then it is no longer Hermitian, and the S matrix is no longer unitary. If the imaginary part $W < 0$, then we have *absorptive potentials*, and a loss of flux. This can be made to approximate the flux leaving in the exit channels that are not explicitly in our model. Potentials with both real and imaginary parts are called *optical potentials*, since they describe both the refraction and absorption in the same way as a light wave passing through a cloudy refractive medium.

If the Schrödinger equation $[\hat{T} + V + \mathrm{i}W]\psi = i\hbar\partial\psi/\partial t$ now has an imaginary potential, then we can calculate the rate of loss of flux as

$$\frac{\partial\psi^*\psi}{\partial t} = -\nabla\cdot\mathbf{j} + \frac{2}{\hbar}\, W\psi^*\psi\ . \tag{3.1.107}$$

As $W < 0$ the imaginary potential acts as a *sink* of particles. The imaginary

potential causes particles to be removed from the incident beam with an additional rate of

$$\left.\frac{\partial\rho}{\partial t}\right|_W \;=\; \frac{2}{\hbar}\,W\rho \tag{3.1.108}$$

so, if the transport from the kinetic terms could be neglected, the probability density would decay as

$$\rho(t) \;\propto\; \mathrm{e}^{2Wt/\hbar} = \mathrm{e}^{-2|W|t/\hbar}\;. \tag{3.1.109}$$

When complex potentials are introduced into scattering theory, all the previous scattering theory remains valid, but now the phase shifts δ_L become complex, and the moduli $|\mathsf{S}_L| \neq 1$. For absorptive potentials we have $|\mathsf{S}_L| < 1$.

There is now an *absorptive cross section* σ_A of flux disappearing from the elastic channel, which can be calculated as an integral of $W(R)$ multiplied by the probability density

$$\sigma_A \;=\; \frac{2}{\hbar v}\int[-W(R)]\;|\psi(\mathbf{R})|^2\;\mathrm{d}^3\mathbf{R}\;, \tag{3.1.110}$$

where v is the velocity of the incident beam so $2/\hbar v = k/E$. In terms of the partial wave radial functions $\chi_L(R)$, the absorption cross section is

$$\sigma_A \;=\; \frac{2}{\hbar v}\frac{4\pi}{k^2}\sum_L(2L+1)\int_0^\infty[-W(R)]\;|\chi_L(R)|^2\;\mathrm{d}R\;. \tag{3.1.111}$$

Since, in the L'th partial wave, the difference between the square moduli of the coefficents of the incoming and outgoing waves in Eq. (3.1.37) is $1-|\mathsf{S}_L|^2$, we define a *reaction cross section* as a sum over all partial waves,

$$\sigma_R \;=\; \frac{\pi}{k^2}\sum_L(2L{+}1)(1-|\mathsf{S}_L|^2)\;. \tag{3.1.112}$$

We can use the Schrödinger equations for χ_L and its complex conjugate for χ_L^* to integrate twice by parts and prove that

$$-\int_0^a \chi_L(R)^*\;W(R)\;\chi_L(R)\;\mathrm{d}R = \frac{\hbar^2k}{8\mu}(1-|\mathsf{S}_L|^2)\;, \tag{3.1.113}$$

and hence, in this spherical potential case, that $\sigma_A = \sigma_R$. The next section will discuss more general Hamiltonians, and as these couple also to non-elastic exit channels, we will see that, in general, σ_R will be larger than σ_A by precisely the total cross sections to these non-elastic reactions.

3.2 Multi-channel scattering

3.2.1 Multiple channels

In the reaction between two nuclei such as ^{12}C + d, a variety of mass rearrangements may be possible, such as ^{13}C + p, ^{14}N + γ, etc. Define each of these as a different *mass partition*, and label them according to variable x. We deal in this chapter only with two-body partitions, leaving three-body breakup (for example to ^{12}C + n + p) until Chapter 8, but in all cases the sum of the particle masses in each partition $\sum_i m_{xi}$ is almost the same for each x. The total is only *almost* the same because of relativistic effects, and hence the different Q-values describing the energy differences between a pair of partitions according to Eq. (1.2.2).

Each partition x will therefore consist of two bodies, one we call like the projectile, and the other we call like a target. Let the vector $\mathbf{R}_x$, extending from the target-like nucleus to the projectile-like one, describe their relative position. Let p and t label the state (the energy level) of the projectile- and target-like nuclei respectively, to distinguish their ground state from any excited states. Each state will have a definite spin and parity, so we label their spins by J_p and J_t. We denote their internal coordinates by ξ_p and ξ_t, which would be the spin states for nucleons, and sets of spin and radial coordinates for clusters of nucleons. We will use $\phi^{xp}_{J_p\mu_p}(\xi_p)$ and $\phi^{xt}_{J_t\mu_t}(\xi_t)$ to refer to the whole quantum states of the projectile and the target, respectively.

Let $\mathbf{L}$ be their relative angular momentum, as in the previous section. Now, however, we have to couple together $\mathbf{L}$, $\mathbf{J}_p$, and $\mathbf{J}_t$ to make some *total* angular momentum $\mathbf{J}_{\rm tot}$. This can be done in two ways, either by coupling $\mathbf{J}_p$ to $\mathbf{J}_t$ first, or $\mathbf{L}$ to $\mathbf{J}_p$. Thereby we introduce two intermediate angular momenta, $\mathbf{S}$ or $\mathbf{J}_a$† respectively, so these two schemes are named as 'S basis' or 'J basis'‡:

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

These are two complete and orthonormal basis schemes. The S basis has the advantage that compound nucleus resonances typically have little mixing of channel spin quantum number, whereas the J basis has the advantage that projectile spin-orbit forces are diagonal in this basis. Most often we

† The 'a' label on the summed angular momentum $\mathbf{L} + \mathbf{J}_p = \mathbf{J}_a$ is chosen arbitrarily.
‡ Sometimes they are called 'LS' and 'jj' respectively, but those names are more appropriate for coupling *four* rather than three angular momenta.

will use the J basis for both bound and scattering states. Later we give the conversion formulae between the two basis schemes.

The set of all quantum numbers for a given total $J_{\rm tot}$, in the J basis $\{xpt,\ LJ_pJ_aJ_t\}$, will be abbreviated by α. Each x denotes a mass partition, each $\{p,t\}$ denotes an *excited state pair*, and each α denotes a *partial wave channel*. The unqualified noun 'channel' will refer to one of these according to context.

The relative coordinate $\mathbf{R}_x$ depends on the partition, so the radial wave function of relative motion will be written as $\psi_\alpha(R_x)$, in place of $\chi_L(R)$ for the one-channel case. The total system wave function is now written as $\mathbf{\Psi}(\mathbf{R}_x,\xi_p,\xi_t)$, in place of $\psi(R,\theta)$ in the one channel case, and will contain a sum over the partitions, where each partition is represented by a product of the internal states $\phi^{xp}_{J_p\mu_p}(\xi_p)$ and $\phi^{xt}_{J_t\mu_t}(\xi_t)$ as well as a wave function for their relative orbital motion. We assume for now that the projectile and target nuclei are distinguishable as far as the Pauli Principle is concerned: the antisymmetrisation of the wave function for identical particles will be discussed in section 3.4.

In each partition x, we define first the state of two nuclei in relative motion with total angular momentum $J_{\rm tot}$ and projection $M_{\rm tot}$. When we include the Clebsch-Gordon coefficients for coupling the angular momenta together, in the J basis the basis set of wave functions for a given partition x is

$$\begin{aligned}
&\Psi^{M_{\rm tot}}_{xJ_{\rm tot}}(\mathbf{R}_x,\xi_p,\xi_t) \\
&\quad= \sum_{LJ_pJ_aJ_tM\mu_pM_a\mu_t} \phi^{xp}_{J_p\mu_p}(\xi_p)\phi^{xt}_{J_t\mu_t}(\xi_t)\mathrm{i}^L Y^M_L(\hat{\mathbf{R}}_x)\frac{1}{R_x}\psi_\alpha(R_x) \\
&\qquad\qquad \langle LM,J_p\mu_p|J_aM_a\rangle\langle J_aM_a,J_t\mu_t|J_{\rm tot}M_{\rm tot}\rangle \\
&\quad\equiv \sum_\alpha \left[\left[\mathrm{i}^L Y_L(\hat{\mathbf{R}}_x)\otimes\phi^{xp}_{J_p}(\xi_p)\right]_{J_a}\otimes\phi^{xt}_{J_t}(\xi_t)\right]_{J_{\rm tot}M_{\rm tot}}\frac{1}{R_x}\psi_\alpha(R_x) \\
&\quad\equiv \sum_\alpha |xpt:(LJ_p)J_a,J_t;J_{\rm tot}M_{\rm tot}\rangle\ \psi_\alpha(R_x)/R_x \\
&\quad\equiv \sum_\alpha |\alpha;J_{\rm tot}M_{\rm tot}\rangle\ \psi_\alpha(R_x)/R_x\ , \qquad (3.2.1)
\end{aligned}$$

where x on the left side selects those α on the right of the same partition. The symbol $\langle L_1M_1,L_2M_2|LM\rangle$ is the Clebsch-Gordon coefficient for coupling two angular momentum states L_1M_1 and L_2M_2 to a total of LM. The i^L coefficients are included for the same reason that they are in Eq. (3.1.9): to make the wave functions $\psi_\alpha(R_x)$ revert to the standard Coulomb functions $F_L(\eta,k_\alpha R_x)$ in the absence of a nuclear potential.

In the S (channel spin) basis, that wave functions for given $J_{\rm tot}M_{\rm tot}$ are

analogously

$$\begin{aligned}\Psi^{M_{\rm tot}}_{xJ_{\rm tot}}(\mathbf{R}_x,\xi_p,\xi_t) &= \sum_{LJ_pSJ_t}\left[{\rm i}^L Y_L(\hat{\mathbf{R}}_x)\otimes\left[\phi^{xp}_{J_p}(\xi_p)\otimes\phi^{xt}_{J_t}(\xi_t)\right]_S\right]_{J_{\rm tot}M_{\rm tot}} \\ &\qquad\qquad \times\ \psi_\beta(R_x)/R_x \\ &\equiv \sum_\beta |xpt: L(J_p,J_t)S; J_{\rm tot}M_{\rm tot}\rangle\ \psi_\beta(R_x)/R_x \\ &\equiv \sum_\beta |\beta; J_{\rm tot}M_{\rm tot}\rangle\ \psi_\beta(R_x)/R_x\ , \end{aligned} \tag{3.2.2}$$

where β is the set of quantum numbers $\{xpt,\ LJ_pJ_tS\}$, and the sum over β on the right side is restricted to those with the same x value as on the left. Partial waves in the channel spin basis are often labelled by ${}^{2S+1}L_{J_{\rm tot}}$, for example ${}^3P_2$ for S=1, L=1 and $J_{\rm tot}$=2.

There is a unitary transformation between the radial wave functions in the S and J bases for a given partition x:

$$\psi_\beta(R_x)=\sum_\alpha\langle\beta|\alpha\rangle\ \psi_\alpha(R_x) \text{ and } \psi_\alpha(R_x)=\sum_\beta\langle\alpha|\beta\rangle\ \psi_\beta(R_x) \tag{3.2.3}$$

where the transformation matrix element, the same for all R_x, is

$$\langle\alpha|\beta\rangle=\sqrt{(2S{+}1)(2J_a{+}1)}\ W(LJ_pJ_{\rm tot}J_t;J_aS)\ . \tag{3.2.4}$$

The symbol $W(abcd;ef)$ is the Racah coefficient of angular momentum recoupling theory.

The system wave function for a given $J_{\rm tot}M_{\rm tot}$ is a superposition of all partitions, as

$$\overline{\Psi}^{M_{\rm tot}}_{J_{\rm tot}}=\sum_x\Psi^{M_{\rm tot}}_{xJ_{\rm tot}}=\sum_\alpha|\alpha;J_{\rm tot}M_{\rm tot}\rangle\ \psi_\alpha(R_x)/R_x\ , \tag{3.2.5}$$

where now the α sum is unrestricted. This wave function $\overline{\Psi}^{M_{\rm tot}}_{J_{\rm tot}}$ can be written as a function of the coordinates $(\mathbf{R}_x,\xi_p,\xi_t)$ of any single partition, because the coordinates of each individual partition enable a complete set of basis states to be defined. Note that by writing Eq. (3.2.5) we are *not* assuming the coordinate sets of separate partitions are orthogonal. In the subsequent development, we will be careful to keep any terms arising from channel non-orthogonalities.

Limiting case of pure Coulomb monopole potentials

Since the one-channel wave function $\psi(R,\theta)$ reduces to a plane wave if the nuclear potentials are zero (as then $\chi_L=F_L$), so should the total wave function $\mathbf{\Psi}$ when summed over all total spins and projections $J_{\rm tot}M_{\rm tot}$. In the

multichannel case, the plane wave as an initial state must be supplemented by the m-quantum numbers of the approaching nuclei. A total system wave function must in the free-field limit reduce to

$$\mathbf{\Psi}^{\mu_p\mu_t}_{xpt}(\mathbf{R}_x,\xi_p,\xi_t;\mathbf{k}_i) \stackrel{V=0}{\to} \mathrm{e}^{\mathrm{i}\mathbf{k}_i\cdot\mathbf{R}_x}\phi^{xp}_{J_p\mu_p}(\xi_p)\phi^{xt}_{J_t\mu_t}(\xi_t) \tag{3.2.6}$$

for a projectile in state p and target in state t in partition x, m-states μ_p and μ_t respectively, and initial momenta in the c.m. frame of $\pm\mathbf{k}_i$.

Summing over $J_{\rm tot}M_{\rm tot}$, with nuclear potentials

When scattering potentials are present, the total system wavefunction $\mathbf{\Psi}^{\mu_{p_i}\mu_{t_i}}_{x_ip_it_i}$ will contain radial wavefunctions ψ_α different from the Coulomb F_L functions, and for initial m-state projections μ_{p_i} and μ_{t_i} for the incoming nuclear states $x_ip_it_i$, it will be a sum over all $J_{\rm tot}M_{\rm tot}$ that generalises Eq. (3.1.57):

$$\begin{aligned}\mathbf{\Psi}^{\mu_{p_i}\mu_{t_i}}_{x_ip_it_i}(\mathbf{R}_x,\xi_p,\xi_t;\mathbf{k}_i) = &\sum_{J_{\rm tot}M_{\rm tot}x}\Psi^{M_{\rm tot}}_{xJ_{\rm tot}}(\mathbf{R}_x,\xi_p,\xi_t)\\ &\times\frac{4\pi}{k_i}\sum_{L_iM_i}Y^{M_i}_{L_i}(\mathbf{k}_i)^*\sum_{J_{a_i}m_i}\langle L_iM_i,J_{p_i}\mu_{p_i}|J_{a_i}m_i\rangle\langle J_{a_i}m_i,J_{t_i}\mu_{t_i}|J_{\rm tot}M_{\rm tot}\rangle\end{aligned} \tag{3.2.7}$$

in the J basis, for an incoming plane wave in direction $\mathbf{k}_i$.

We now combine the indices $x_ip_it_i$ with the L_i and J_{a_i} of Eq. (3.2.7) to form a new value for the multi-index, $\alpha_i = \{x_ip_it_i,\, L_iJ_{p_i}J_{a_i}J_{t_i}\}$. This identifies the partial wave channel in which there is an incoming plane wave, so the multichannel radial functions will henceforth be labeled also with α_i, as $\psi_{\alpha\alpha_i}(R_x)$. The $\Psi^{M_{\rm tot}}_{xJ_{\rm tot}}$ therefore depends on α_i, called the *incoming channel*, so to make this dependence explicit we rewrite Eq. (3.2.7) as

$$\mathbf{\Psi}^{\mu_{p_i}\mu_{t_i}}_{x_ip_it_i}(\mathbf{R}_x,\xi_p,\xi_t;\mathbf{k}_i) = \sum_{J_{\rm tot}M_{\rm tot}}\sum_{\alpha\alpha_i}|\alpha;J_{\rm tot}M_{\rm tot}\rangle\,\frac{\psi_{\alpha\alpha_i}(R_x)}{R_x}A^{J_{\rm tot}M_{\rm tot}}_{\mu_{p_i}\mu_{t_i}}(\alpha_i;\mathbf{k}_i) \tag{3.2.8}$$

where we define the coefficient

$$A^{J_{\rm tot}M_{\rm tot}}_{\mu_{p_i}\mu_{t_i}}(\alpha_i;\mathbf{k}_i) \equiv \frac{4\pi}{k_i}\sum_{M_im_i}Y^{M_i}_{L_i}(\mathbf{k}_i)^*\langle L_iM_i,J_{p_i}\mu_{p_i}|J_{a_i}m_i\rangle\langle J_{a_i}m_i,J_{t_i}\mu_{t_i}|J_{\rm tot}M_{\rm tot}\rangle. \tag{3.2.9}$$

Here and elsewhere, the sum over α_i is not over all possible channels, but over just the partial waves that include the incoming state indices $x_ip_it_i$ defined by the properties of the beam projectile and target. Similar expressions can be derived for the S basis.

It is by means of this expansion with the incoming channel index α_i that

we determine the boundary conditions and scattering amplitudes below. In all channels $\alpha \neq \alpha_i$ there should only be outgoing flux.

Reductions to simpler cases

To confirm the meaning of the multichannel formalism, we briefly outline how it reduces to the previous one-channel theory of section 3.1 in the case of structureless spin-zero particles interacting only by spherical elastic potentials. The only non-zero $\psi_{\alpha\alpha_i}(R)$ for partial wave L will then be

$$\psi_{\alpha\alpha}(R) = \chi_L(R) \tag{3.2.10}$$

for $\alpha = \{111, L0L0\}$. The only non-zero $\Psi^{M_{\rm tot}}_{xJ_{\rm tot}}(\mathbf{R}, \xi_p, \xi_t)$ are

$$\Psi^M_{1L}(\mathbf{R}, \xi_p, \xi_t) = \mathrm{i}^L Y^M_L(\hat{\mathbf{R}})\ \chi_L(R)/R\ , \tag{3.2.11}$$

and the only non-zero $\mathbf{\Psi}^{\mu_p\mu_t}_{xpt}(\mathbf{R}_x, \xi_p, \xi_t; \mathbf{k})$ are

$$\mathbf{\Psi}^{00}_{111}(\mathbf{R}, \xi_p, \xi_t; \mathbf{k}) = \psi(\mathbf{R}; \mathbf{k}) = \frac{4\pi}{k} \sum_{LM} Y^M_L(\mathbf{k})^*\ \Psi^M_{1L}(\mathbf{R}, \xi_p, \xi_t), \tag{3.2.12}$$

where $\psi(\mathbf{R}; \mathbf{k})$ is that of Eq. (3.1.57).

Parity

Nuclear and Coulomb interactions do not change parity, so that each projectile and target state has a specific parity π_{xp} and π_{xt}. The parity for a partial wave L is $(-1)^L$, so the total parity of a partial wave channel is $\pi = (-1)^L \pi_{xp} \pi_{xt}$. This must be the same for all partial waves, since parities are not mixed by Coulomb or nuclear couplings.

This also means that coupled channels sets for a give $J_{\rm tot}$ can be subdivided into positive and negative parity subsets, and each subset calculated separately. We will therefore label coupled channels sets not just by $J_{\rm tot}$ but by $J^\pi_{\rm tot}$, and sums over $J_{\rm tot}$ are rewritten as over $J^\pi_{\rm tot}$. The parities will therefore be recombined in sums like that of Eq. (3.2.8), where the first summation is now over $J_{\rm tot}\pi M_{\rm tot}$.

Multichannel S matrix

The S matrix element of Section 3.1.1 is now generalised to a full *matrix* $\mathbf{S}^{J_{\rm tot}\pi}_{\alpha\alpha_i}$ for each total angular momentum and parity $J^\pi_{\rm tot}$, where α_i is the partial wave channel with the incoming plane wave, and α is an outgoing channel.

This means that Eqs. (3.1.6, 3.1.86) are generalised to depend on the

entrance channel α_i, and from Eqs. (3.2.6) and (3.2.8) we obtain for $R_x > R_n$:

$$\psi_{\alpha\alpha_i}(R_x) = \frac{\mathrm{i}}{2}\left[H^-_{L_i}(\eta_\alpha, k_\alpha R_x)\ \delta_{\alpha\alpha_i} - H^+_L(\eta_\alpha, k_\alpha R_x)\ \mathsf{S}^{J_{\rm tot}\pi}_{\alpha\alpha_i}\right]. \quad (3.2.13)$$

The S matrix $\mathsf{S}^{J_{\rm tot}\pi}_{\alpha\alpha_i}$ gives the amplitude of an outgoing wave in channel α that arises from a incoming plane wave in channel α_i, in addition to the scattering from a diagonal point Coulomb potential. For all the non-elastic channels $\alpha \neq \alpha_i$ we have

$$\psi_{\alpha\alpha_i}(R_x) \stackrel{\alpha\neq\alpha_i}{=} H^+_L(\eta_\alpha, k_\alpha R_x)\ \frac{1}{2\mathrm{i}}\mathsf{S}^{J_{\rm tot}\pi}_{\alpha\alpha_i}, \quad (3.2.14)$$

which is to be proportional to a purely outgoing wave. When $\alpha = \alpha_i$, Eq. (3.2.13) leads to a matching equation similar to Eq. (3.1.37) for the elastic channel.

The cross sections, we saw in Section 2.4.4, depend on the channel *velocity*† multiplying the square modulus of an amplitude. It is therefore convenient to combine these velocity factors with the S matrix, by defining

$$\tilde{\mathsf{S}}_{\alpha\alpha_i} = \sqrt{\frac{v_\alpha}{v_{\alpha_i}}}\mathsf{S}_{\alpha\alpha_i} \quad (3.2.15)$$

where the velocities satisfy $\mu_\alpha v_\alpha = \hbar k_\alpha$. The combination S matrix $\tilde{\mathsf{S}}_{\alpha\alpha_i}$ may now be used to find the multichannel cross sections, and its matrix elements may be more directly found from the boundary conditions of Eq. (3.2.13) expressed as

$$\psi_{\alpha\alpha_i}(R_x) = \frac{\mathrm{i}}{2}\left[H^-_{L_i}(\eta_\alpha, k_\alpha R_x)\ \delta_{\alpha\alpha_i} - H^+_L(\eta_\alpha, k_\alpha R_x)\ \sqrt{\frac{v_{\alpha_i}}{v_\alpha}}\tilde{\mathsf{S}}^{J_{\rm tot}\pi}_{\alpha\alpha_i}\right] \quad (3.2.16)$$

Both $\mathsf{S}_{\alpha\alpha_i}$ and $\tilde{\mathsf{S}}_{\alpha\alpha_i}$ can be regarded as complex numbers in *matrices* S and $\tilde{\mathsf{S}}$. The second (column) index in these matrices refers to the incoming channel, and the first (row) index names the exit channel.

We can also define a partial wave T matrix by $\mathsf{S} = \mathsf{I} + 2\mathrm{i}\mathsf{T}$ where I is the identity matrix‡, or

$$\mathsf{S}_{\alpha\alpha_i} = \delta_{\alpha\alpha_i} + 2\mathrm{i}\mathsf{T}_{\alpha\alpha_i} \quad (3.2.17)$$

$$\tilde{\mathsf{S}}_{\alpha\alpha_i} = \delta_{\alpha\alpha_i} + 2\mathrm{i}\tilde{\mathsf{T}}_{\alpha\alpha_i}\ , \quad (3.2.18)$$

noting that the velocity ratios in Eq. (3.2.15) are unity for the diagonal matrix elements, so the diagonal terms $\delta_{\alpha\alpha_i}$ are not affected.

† Strictly a *speed*, but this is the most common terminology.
‡ We will often write $\mathsf{S} = 1 + 2\mathrm{i}\mathsf{T}$ for simplicity.

In terms of these T matrix elements, the scattering boundary conditions of Eq. (3.2.13) are simply

$$\psi_{\alpha\alpha_i}(R_x) = F_{L_i}(\eta_\alpha, k_\alpha R_x)\ \delta_{\alpha\alpha_i} + H^+_L(\eta_\alpha, k_\alpha R_x)\ \mathbf{T}^{J_{\rm tot}\pi}_{\alpha\alpha_i}\ . \qquad (3.2.19)$$

Multichannel cross section

The scattering amplitude from an incoming elastic channel $(x_i p_i t_i)$ to (xpt) depends on the m-substates of the initial nuclei μ_{p_i}, μ_{t_i} and the final nuclei μ_p, μ_t, as well as on the scattering angle θ, as $\tilde{f}^{xpt}_{\mu_p\mu_t,\mu_{p_i}\mu_{t_i}}(\theta)$. We use the scattering amplitude $\tilde{f}$ calculated from the $\tilde{\mathbf{S}}$ matrix elements, so that, in contrast to Eq. (2.4.14), there are no further velocity factors for the flux ratio. The cross section for an unpolarised beam, where all $\mu_{p_i}\mu_{t_i}$ values are equally likely, is thus found by using Eq. (2.4.16), then summing over final m-states and averaging over the initial states:

$$\sigma_{xpt}(\theta) = \frac{1}{(2J_{p_i}{+}1)(2J_{t_i}{+}1)} \sum_{\mu_p\mu_t,\mu_{p_i}\mu_{t_i}} \left|\tilde{f}^{xpt}_{\mu_p\mu_t,\mu_{p_i}\mu_{t_i}}(\theta)\right|^2\ . \qquad (3.2.20)$$

By Eq. (3.2.19), in addition to the incoming wave in channel α_i, the $\psi_{\alpha\alpha_i}(R_x)$ have outgoing waves, which in the external region become

$$\psi_{\alpha\alpha_i}(R_x) \overset{R>R_n}{=} H^+_{L_\alpha}(\eta_\alpha, k_\alpha R_x)\mathbf{T}^{J_{\rm tot}\pi}_{\alpha\alpha_i} \to \mathrm{i}^{-L_\alpha}\mathrm{e}^{\mathrm{i}k_\alpha R_x}\mathbf{T}^{J_{\rm tot}\pi}_{\alpha\alpha_i}\ , \qquad (3.2.21)$$

and the $\mathbf{\Psi}(\mathbf{R}_x, \xi_p, \xi_t; \mathbf{k}_i)$ have outgoing waves proportional to the scattering amplitude as

$$\langle \phi^{xp}_{J_p\mu_p}(\xi_p)\phi^{xt}_{J_t\mu_t}(\xi_t)|\mathbf{\Psi}^{\mu_{p_i}\mu_{t_i}}_{x_i p_i t_i}(\mathbf{R}_x, \xi_p, \xi_t; \mathbf{k}_i)\rangle \overset{R_x\geq R_n}{=} f^{xpt}_{\mu_p\mu_t,\mu_{p_i}\mu_{t_i}}(\theta)\mathrm{e}^{\mathrm{i}k_\alpha R_x}/R_x\ . \qquad (3.2.22)$$

Using Eq. (3.2.8), we may determine the scattering amplitudes $f(\theta)$ in terms of the $\mathbf{T}^{J_{\rm tot}\pi}_{\alpha\alpha_i}$, for scattering from a beam in the $\mathbf{k}_i$ direction to the asymptotic $\hat{\mathbf{k}} = \hat{\mathbf{R}}$ direction differing by an angle θ:

$$f^{xpt}_{\mu_p\mu_t,\mu_{p_i}\mu_{t_i}}(\theta) = \sum_{J_{\rm tot}\pi M_{\rm tot}} \sum_{\alpha\alpha_i} \mathrm{i}^{-L_\alpha}\langle \phi^{xp}_{J_p\mu_p}\phi^{xt}_{J_t\mu_t}|\alpha; J_{\rm tot}M_{\rm tot}\rangle \times A^{J_{\rm tot}M_{\rm tot}}_{\mu_{p_i}\mu_{t_i}}(\alpha_i; \mathbf{k}_i)\ \mathbf{T}^{J_{\rm tot}\pi}_{\alpha\alpha_i}, \qquad (3.2.23)$$

where the α sum is over partial waves consistent with the outgoing xpt, and the α_i must be consistent with the incoming beam specification $x_i p_i t_i$.

We include the flux factor of Eq. (2.4.14) by using $\tilde{\mathbf{T}}$ instead of $\mathbf{T}$, to now give $\tilde{f}$, and expand the $|\alpha\rangle$ state and the $A(\alpha_i; \mathbf{k}_i)$ coefficients, cancelling the i^L factor. After also inserting appropriate Coulomb phases as in Eq. (3.1.88)

and adding the diagonal pure Coulomb amplitude $f_c(\theta)$, we have a general scattering amplitude for Coulomb + nuclear reactions

$$\begin{aligned}\tilde{f}^{xpt}_{\mu_p\mu_t,\mu_{p_i}\mu_{t_i}}(\theta) &= \delta_{\mu_p\mu_{p_i}}\delta_{\mu_t\mu_{t_i}} f_c(\theta) + \frac{4\pi}{k_i} \sum_{L_i L J_{a_i} J_a m_i m M_i J_{\rm tot}} \langle L_i M_i, J_{p_i}\mu_{p_i}|J_{a_i} m_i\rangle \\ &\quad \langle J_{a_i} m_i, J_{t_i}\mu_{t_i}|J_{\rm tot}M_{\rm tot}\rangle \langle LM, J_p\mu_p|J_a m\rangle \langle J_a m, J_t\mu_t|J_{\rm tot}M_{\rm tot}\rangle \\ &\quad Y^M_L(\mathbf{k}) Y^{M_i}_{L_i}(\mathbf{k}_i)^* \ \tilde{\mathbf{T}}^{J_{\rm tot}\pi}_{\alpha\alpha_i} \ {\rm e}^{2{\rm i}(\sigma_L(\eta_\alpha)+\sigma_{L_i}(\eta_{\alpha_i}))}, \end{aligned} \tag{3.2.24}$$

and in the S (channel spin) basis

$$\begin{aligned}\tilde{f}^{xpt}_{\mu_p\mu_t,\mu_{p_i}\mu_{t_i}}(\theta) &= \delta_{\mu_p\mu_{p_i}}\delta_{\mu_t\mu_{t_i}} f_c(\theta) + \frac{4\pi}{k_i} \sum_{L_i L S_i S s s_i M_i J_{\rm tot}} \langle J_{p_i}\mu_{p_i}, J_{t_i}\mu_{t_i}|S_i s_i\rangle \\ &\quad \langle L_i M_i, S_i s_i|J_{\rm tot}M_{\rm tot}\rangle \langle J_p\mu_p, J_t\mu_t|Ss\rangle \langle LM, Ss|J_{\rm tot}M_{\rm tot}\rangle \\ &\quad Y^M_L(\mathbf{k}) Y^{M_i}_{L_i}(\mathbf{k}_i)^* \ \tilde{\mathbf{T}}^{J_{\rm tot}\pi}_{\beta\beta_i} \ {\rm e}^{2{\rm i}(\sigma_L(\eta_\beta)+\sigma_{L_i}(\eta_{\beta_i}))}. \end{aligned} \tag{3.2.25}$$

Note that $\tilde{\mathbf{T}}^{J_{\rm tot}\pi}_{\alpha\alpha_i} = \frac{\rm i}{2}[\delta_{\alpha\alpha_i} - \tilde{\mathbf{S}}^{J_{\rm tot}\pi}_{\alpha\alpha_i}]$, and similarly for the S basis.

Polarised beams

In general, cross sections depend on the polarisation of the beam, namely on any non-uniform distribution over initial m-states μ_{p_i} for the projectile of spin J_p. The properties of any beam are defined by its density operator ρ, whereby the expectation value of any operator $\hat{O}$ is given by the trace

$$\langle\hat{O}\rangle_\rho = \sum_{\mu_{p_i}\mu'_{p_i}=-J_p}^{J_p} \langle J_p\mu_{p_i}|\rho|J_p\mu'_{p_i}\rangle\langle J_p\mu'_{p_i}|\hat{O}|J_p\mu_{p_i}\rangle \tag{3.2.26}$$

$$\equiv Tr(\rho\hat{O}) \ . \tag{3.2.27}$$

The polarisation properties of this operator are usually represented by complex numbers t_{Qq} for $Q = 1, 2, ..., 2J_p$ and $0 \le q \le Q$, according to the construction

$$\rho = \frac{1}{2J_p+1} \sum_{Qq} t^*_{Qq}\tau_{Qq} \tag{3.2.28}$$

where the spherical tensor τ_{Qq} is the operator with matrix elements

$$(\tau_{Qq})_{\mu\mu'} = \sqrt{2Q+1} \ \langle J_p\mu, Qq|J_p\mu'\rangle \ . \tag{3.2.29}$$

The degree to which the beam polarisation is reflected in the observed cross section $\sigma^{\rm pol}_{xpt}(\theta)$ for any reaction channel xpt is given by the *tensor*

analysing powers T^{xpt}_{Qq} for this reaction, according to

$$\sigma^{\rm pol}_{xpt}(\theta) = \sigma_{xpt}(\theta) \sum_{Qq} t^*_{Qq} T^{xpt}_{Qq} \tag{3.2.30}$$

where $\sigma_{xpt}(\theta)$ is the cross section of Eq. (3.2.20) for an unpolarised beam.

These tensor analysing powers can be calculated from the scattering amplitudes $f^{xpt}_{\mu_p\mu_t:\mu_{p_i}\mu_{t_i}}(\theta)$ as the ratio of traces

$$\begin{aligned} T^{xpt}_{Qq}(\theta) &= \frac{Tr(\mathbf{f}\tau_{Qq}\mathbf{f}^+)}{Tr(\mathbf{f}\mathbf{f}^+)} \qquad (3.2.31)\\ &= \sqrt{2Q+1}\frac{\sum_{\mu_p\mu_t\mu_{p_i}\mu_{t_i}} f^{xpt\ *}_{\mu_p\mu_t:\mu_{p_i}\mu_{t_i}}(\theta)\langle J_p\mu_{p_i}, Qq|J_p\mu'_{p_i}\rangle f^{xpt}_{\mu_p\mu_t,\mu'_{p_i}\mu_{t_i}}(\theta)}{\sum_{\mu_p\mu_t\mu_{p_i}\mu_{t_i}} |f^{xpt}_{\mu_p\mu_t:\mu_{p_i}\mu_{t_i}}(\theta)|^2} \end{aligned}$$

For a more complete description of polarisation, see Gómez-Camacho and Johnson [10].

Integrated cross sections

The angle-integrated outgoing cross section to a non-elastic excited state pair xpt is

$$\begin{aligned} \sigma_{xpt} &= 2\pi \int_0^\pi {\rm d}\theta \sin\theta\ \sigma_{xpt}(\theta)\\ &= \frac{\pi}{k_i^2}\frac{1}{(2J_{p_i}+1)(2J_{t_i}+1)} \sum_{J_{\rm tot}\pi LJ\alpha_i} (2J_{\rm tot}+1)|\tilde{\mathbf{S}}^{J_{\rm tot}\pi}_{\alpha\alpha_i}|^2 \qquad (3.2.32)\\ &= \frac{\pi}{k_i^2} \sum_{J_{\rm tot}\pi LJ\alpha_i} g_{J_{\rm tot}} |\tilde{\mathbf{S}}^{J_{\rm tot}\pi}_{\alpha\alpha_i}|^2\ , \qquad (3.2.33) \end{aligned}$$

where we have abbreviated a *spin weighting factor* to

$$g_{J_{\rm tot}} \equiv \frac{2J_{\rm tot}+1}{(2J_{p_i}+1)(2J_{t_i}+1)}\ . \tag{3.2.34}$$

The *reaction cross section* σ_R is defined as the flux leaving the elastic channel, and depends only on the elastic S matrix element $\mathbf{S}_{\alpha_i\alpha_i}$ as

$$\begin{aligned} \sigma_R &= \frac{\pi}{k_i^2}\frac{1}{(2J_{p_i}+1)(2J_{t_i}+1)} \sum_{J_{\rm tot}\pi\alpha_i} (2J_{\rm tot}+1)(1-|\mathbf{S}^{J_{\rm tot}\pi}_{\alpha_i\alpha_i}|^2) \qquad (3.2.35)\\ &= \frac{\pi}{k_i^2} \sum_{J_{\rm tot}\pi\alpha_i} g_{J_{\rm tot}}(1-|\mathbf{S}^{J_{\rm tot}\pi}_{\alpha_i\alpha_i}|^2) \quad \text{similarly.} \end{aligned}$$

Remember that the sum over α_i is over just the partial waves that include the incoming state indices $x_ip_it_i$, and that for elastic channels $\mathbf{S}_{\alpha_i\alpha_i} = \tilde{\mathbf{S}}_{\alpha_i\alpha_i}$.

The integrated *elastic cross section* is defined only for neutral scattering ($\eta = 0$), and is a generalisation of Eq. (3.1.50):

$$\sigma_{\rm el} = \frac{\pi}{k_i^2}\frac{1}{(2J_{p_i}{+}1)(2J_{t_i}{+}1)}\sum_{J_{\rm tot}\pi\alpha_i}(2J_{\rm tot}{+}1)|1-\mathbf{S}^{J_{\rm tot}\pi}_{\alpha_i\alpha_i}|^2\ . \qquad (3.2.36)$$

It measures all the flux being elastically scattered by any non-zero angle. The *total cross section* is the sum of the reaction and elastic cross sections

$$\begin{aligned}\sigma_{\rm tot} &= \sigma_R + \sigma_{\rm el} \\ &= \frac{2\pi}{k_i^2}\frac{1}{(2J_{p_i}{+}1)(2J_{t_i}{+}1)}\sum_{J_{\rm tot}\pi\alpha_i}(2J_{\rm tot}{+}1)[1-{\rm Re}\mathbf{S}^{J_{\rm tot}\pi}_{\alpha_i\alpha_i}], \qquad (3.2.37)\end{aligned}$$

and is the sum the fluxes leaving the incident direction for any reason: elastic scattering to another angle, or a reaction leading to any non-elastic channel.

The *absorption cross section* is the loss of flux caused by any imaginary potentials in the Hamiltonian. In multi-channel theory, we calculate it as the reaction cross section minus all the non-elastic outgoing cross sections:

$$\sigma_A = \sigma_R - \sum_{xpt\neq x_ip_it_i}\sigma_{xpt}\ . \qquad (3.2.38)$$

This reduces the result of section 3.1.5 (namely $\sigma_A = \sigma_R$) when there no non-elastic channels. With multiple channels, if the coupled equations are solved precisely in the presence of absorptive complex potentials, then σ_A will be positive, and will as before be an integral of $W(R) < 0$, now

$$\sigma_A = \frac{2}{\hbar v_i}\frac{4\pi}{k_i^2}\sum_{\alpha_i\alpha}\int_0^\infty[-W_\alpha(R_x)]\ |\psi_{\alpha\alpha_i}(R_x)|^2\ {\rm d}R_x\ . \qquad (3.2.39)$$

3.2.2 Coupled equations

The multichannel wave functions of Eqs. (3.2.1) and (3.2.2) contain the channel wave functions $\psi_\alpha(R_x)$ or $\psi_\beta(R_x)$. In order to find these wave functions, we have to write down the coupled equations that they satisfy, starting from the Schrödinger equation for the whole system. Chapter 6 will show how to solve the coupled equations that we derive in this section.

For total energy E and Hamiltonian operator H, we have to solve

$$[H-E]\Psi^{M_{\rm tot}}_{J_{\rm tot}\pi} = 0\ . \qquad (3.2.40)$$

The results will be independent of $M_{\rm tot}$ when H is rotationally invariant: when H does not depend on any particular direction in space.

The total Hamiltonian H can be written equivalently for each partition

x, in terms of that partition's internal Hamiltonians, kinetic energies, and interaction potentials:

$$H = H_{xp}(\xi_p) + H_{xt}(\xi_t) + \hat{T}_x(R_x) + V_x(R_x, \xi_p, \xi_t) \ , \tag{3.2.41}$$

where $V_x(R_x, \xi_p, \xi_t) \to 0$ as $R_x \to \infty$.

The internal nuclear states $\phi^{xp}_{J_p}(\xi_p)$ and $\phi^{xt}_{J_t}(\xi_t)$ satisfy eigen-equations for their Hamiltonians

$$\begin{aligned} H_{xp}(\xi_p)\phi^{xp}_{J_p}(\xi_p) &= \epsilon_{xp}\phi^{xp}_{J_p}(\xi_p) \ , \\ H_{xt}(\xi_t)\phi^{xt}_{J_t}(\xi_t) &= \epsilon_{xt}\phi^{xt}_{J_t}(\xi_t) \ , \end{aligned} \tag{3.2.42}$$

for eigenenergies ϵ_{xp} and ϵ_{xt} respectively†. The kinetic energy operator depends on the masses m_{xp} and m_{xt} via the partition's reduced mass $\mu_x = m_{xp}m_{xt}/(m_{xp}m_{xt})$ as

$$\hat{T}_x(R_x) = -\frac{\hbar^2}{2\mu_x}\nabla^2_{R_x} \ . \tag{3.2.43}$$

The interaction potential $V_x(R_x, \xi_p, \xi_t)$ is the residual interaction between nuclei p and t. For nucleons i in the projectile and j in the target, it may be written as the sum

$$V_x(R_x, \xi_p, \xi_t) = \sum_{i\in p, j\in t} V_{ij}(\mathbf{r}_i - \mathbf{r}_j) \tag{3.2.44}$$

of individual nucleon-nucleon forces V_{ij}. When the distance between p and t becomes large asymptotically, the residual interaction goes to zero.

For convenience, we define a *joint* projectile and target Hamiltonian as $H_x \equiv H_{xp} + H_{xt}$, a joint eigenstate as $\phi^{xpt} \equiv \phi^{xp}_{J_p}\phi^{xt}_{J_t}$, and a joint eigenenergy as $\epsilon_{xpt} \equiv \epsilon_{xp} + \epsilon_{xp}$, so we have simply $H_x\phi^{xpt} = \epsilon_{xpt}\phi^{xpt}$ for the product of internal structures. The total Hamiltonian is then $H = \hat{T}_x + H_x + V_x$ for any chosen x.

The coupled equations are now found by expanding the total wave function $\Psi^{M_{\rm tot}}_{J_{\rm tot}\pi}$ in either the S or J partial wave basis. In the J basis, for example, $\Psi^{M_{\rm tot}}_{J_{\rm tot}\pi} = \sum_\alpha |\alpha; J_{\rm tot}\pi\rangle\psi_\alpha(R_x)/R_x$, so from Eq. (3.2.40) for a given $J_{\rm tot}\pi$ value, we have‡

$$\sum_\alpha [H - E]|\alpha; J_{\rm tot}\pi\rangle\psi_\alpha(R_x)/R_x = 0 \ . \tag{3.2.45}$$

† We omit the m-state quantum numbers from this equation since the energy does not depend on these

‡ The $M_{\rm tot}$ has been omitted since the results should be the same for all $M_{\rm tot}$ values, and now we will often omit also the $J_{\rm tot}\pi$ labels when discussing a given coupled channels set.

Projecting onto one of the basis states, by operating on the left by $R_{x'}\langle\alpha'|$,

$$\sum_\alpha R_{x'}\langle\alpha'|H-E|\alpha\rangle R_x^{-1}\ \psi_\alpha(R_x) = 0\ , \tag{3.2.46}$$

abbreviated as

$$\sum_\alpha (H-E)_{\alpha'\alpha}\ \psi_\alpha(R_x) = 0\ , \tag{3.2.47}$$

which gives a separate equation for each α' combination of quantum numbers. The set of all the equations for various α' is called the set of coupled channels equations.

The Hamiltonian and energy matrix element was abbreviated by $\langle\alpha'|H-E|\alpha\rangle = (H-E)_{\alpha'\alpha}$. To evaluate all these, we note that

$$\begin{aligned}
[H-E]|\alpha\rangle &= [H-E]|xpt:(LJ_p)J_a,J_t;J_{\rm tot}\pi\rangle \\
&= [\hat{T}_x + H_x + V_x - E]|xpt:(LJ_p)J_a,J_t;J_{\rm tot}\pi\rangle \\
&= [\hat{T}_x + \epsilon_{xp} + \epsilon_{xp} + V_x - E]|xpt:(LJ_p)J_a,J_t;J_{\rm tot}\pi\rangle \\
&= [\hat{T}_x + V_x - E_{xpt}]|xpt:(LJ_p)J_a,J_t;J_{\rm tot}\pi\rangle\ ,
\end{aligned} \tag{3.2.48}$$

where $E_{xpt} = E - \epsilon_{xp} - \epsilon_{xp}$ is the external kinetic energy for a given excited-state pair xpt.

This means that the matrix elements $\langle\alpha'|H-E|\alpha\rangle$ may be written in two ways, one by replacing H either by $\hat{T}_x + H_x + V_x$ for acting on the right hand side, and the other by $\hat{T}_{x'} + H_{x'} + V_{x'}$ for acting on the left side. The first option is called the *prior* form of the matrix element, and the second the *post* form. Ideally, if all terms of the coupled equations are included and the equations are solved accurately, both choices will give the same results†. The *prior* form of the matrix element is thus

$$\begin{aligned}
(H-E)_{\alpha'\alpha} &= R_{x'}\langle\alpha'|\hat{T}_x + V_x - E_{xpt}|\alpha\rangle R_x^{-1} \\
&= R_{x'}\langle\alpha'|\alpha\rangle R_x^{-1}[\hat{T}_{xL} - E_{xpt}] + R_{x'}\langle\alpha'|V_x|\alpha\rangle R_x^{-1} \\
&\equiv \hat{N}_{\alpha'\alpha}[\hat{T}_{xL}(R_x) - E_{xpt}] + \hat{V}^{\rm prior}_{\alpha'\alpha}\ ,
\end{aligned} \tag{3.2.49}$$

where the partial-wave kinetic energy operator, the same as the one-channel operator of Eq. (3.1.10), is

$$\hat{T}_{xL}(R_x) = -\frac{\hbar^2}{2\mu_x}\left[\frac{{\rm d}^2}{{\rm d}R_x^2} - \frac{L_x(L_x+1)}{R_x^2}\right]\ , \tag{3.2.50}$$

where L_x is the orbital angular momentum in channel α. The coupling interactions *between* channels are either the *prior* or *post* matrix elements

† On page 95 we will see that there is also a simpler first-order result whereby that post and prior forms necessarily give the same first-order transition amplitudes.

defined as

$$\hat{V}^{\rm prior}_{\alpha'\alpha} = R_{x'}\langle\alpha'|V_x|\alpha\rangle R_x^{-1} \tag{3.2.51}$$

$$\hat{V}^{\rm post}_{\alpha'\alpha} = R_{x'}\langle\alpha'|V_{x'}|\alpha\rangle R_x^{-1} \tag{3.2.52}$$

respectively, and the norm overlap operators between the partial wave basis states are

$$\hat{N}_{\alpha'\alpha} = R_{x'}\langle\alpha'|\alpha\rangle R_x^{-1} \ . \tag{3.2.53}$$

Within the same partition, $x' = x$, the norm overlaps are diagonal: $\hat{N}_{\alpha'\alpha} = \delta_{\alpha'\alpha}$. This suggests treating the matrix elements of $\hat{T}_{xL} - E_{xpt}$ *within* a partition separately from those *between* partitions.

With these definitions, we have from Eq. (3.2.46) one version of the coupled channels equation set:

$$[\hat{T}_{x'L}(R'_x) - E_{x'p't'}]\psi_{\alpha'}(R'_x) + \sum_{\alpha} \hat{V}^{\rm prior}_{\alpha'\alpha}\psi_{\alpha}(R_x)$$
$$+ \sum_{\alpha, x\neq x'} \hat{N}_{\alpha'\alpha}[\hat{T}_{xL} - E_{xpt}]\psi_{\alpha}(R_x) = 0 \ ,$$

which, on interchanging primes and the unprimed, gives a perhaps more natural

$$[\hat{T}_{xL}(R_x) - E_{xpt}]\psi_{\alpha}(R_x) + \sum_{\alpha'} \hat{V}^{\rm prior}_{\alpha\alpha'}\psi_{\alpha'}(R_{x'})$$
$$+ \sum_{\alpha', x'\neq x} \hat{N}_{\alpha\alpha'}[\hat{T}_{x'L'} - E_{x'p't'}]\psi_{\alpha'}(R_{x'}) = 0 \ . \tag{3.2.54}$$

The third terms in these equations are called *non-orthogonality terms* because they involve the overlap of basis functions $\langle\alpha'|\alpha\rangle$ between different mass partitions, and arise particularly in transfer reactions. We will see in Chapter 6 that they may be neglected in some circumstances, which would allow the coupled equations to be written in the more familiar form

$$[\hat{T}_{xL}(R_x) - E_{xpt}]\psi_{\alpha}(R_x) + \sum_{\alpha'} \hat{V}^{\rm prior}_{\alpha\alpha'}\psi_{\alpha'}(R_{x'}) = 0 \ . \tag{3.2.55}$$

The equations (3.2.54) used the *prior* form. This may be discerned from the fact that the interaction potential $V_{x'}$ in the coupling matrix element $\hat{V}^{\rm prior}_{\alpha\alpha'} = \langle\alpha|V_{x'}|\alpha'\rangle$ refers to the *initial* channel α' rather than the final channel α. The same solutions should also result in the converse *post* form matrix element, obtained when Eq. (3.2.49) is replaced by

$$\begin{aligned}(H-E)_{\alpha'\alpha} &= R_{x'}\langle\alpha'|\hat{T}_{x'} + V_{x'} - E_{x'p't'}|\alpha\rangle R_x^{-1} \\ &= [\hat{T}_{x'L'} - E_{x'p't'}]\hat{N}_{\alpha'\alpha} + \hat{V}^{\rm post}_{\alpha'\alpha} \ .\end{aligned} \tag{3.2.56}$$

The detailed construction of all the coupling potentials (whether post or prior) is the subject of Chapter 4.

3.2.3 Unitarity of the multi-channel S matrix

The multi-channel S matrices $\mathbf{S}_{\alpha\alpha_i}$ and $\tilde{\mathbf{S}}_{\alpha\alpha_i}$ have certain symmetry properties when the initial Hamiltonians have specific features. These concern physical properties such as Hermiticity, time invariance and what is called reciprocity.

It may be that the couplings $\hat{V}_{\alpha\alpha'}$ are Hermitian, that is $\hat{V}_{\alpha\alpha'} = \hat{V}^*_{\alpha'\alpha}$ (whether post or prior). This is true if the coupling matrix is real and symmetric, but also hold more generally for self-adjoint or Hermitian couplings. Hermitian operators should be familiar in quantum mechanics since they have real eigenvalues and their eigenvectors form an orthogonal set.

For scattering, the consequence of Hermiticity is that the matrix $\tilde{\mathbf{S}}_{\alpha\alpha_i}$ of Eq. (3.2.15) is *unitary*:

$$\tilde{\mathbf{S}}^{-1} = \tilde{\mathbf{S}}^\dagger \equiv (\tilde{\mathbf{S}}^*)^{\mathrm{T}} \tag{3.2.57}$$

so $\tilde{\mathbf{S}}^\dagger\tilde{\mathbf{S}} = 1$. For α_i, α'_i as two incoming channels,

$$\sum_\alpha \tilde{\mathbf{S}}^*_{\alpha\alpha_i}\tilde{\mathbf{S}}_{\alpha\alpha'_i} = \delta_{\alpha_i\alpha'_i} \ , \tag{3.2.58}$$

and, in particular

$$\sum_\alpha |\tilde{\mathbf{S}}_{\alpha\alpha_i}|^2 = 1 \ . \tag{3.2.59}$$

Each row of the $\tilde{\mathbf{S}}$ matrix is therefore a vector with unit norm. From $\tilde{\mathbf{S}}\tilde{\mathbf{S}}^\dagger = 1$ we can similarly prove that each column is a unit vector.

Unitarity implies that the absorption cross section of Eq. (3.2.38) is $\sigma_A = 0$, so that the reaction cross section (the flux leaving the entrance channel) is precisely equal to the sum of all the outgoing cross sections.

3.2.4 Detailed balance

The condition of *detailed balance* in a general statistical or stochastic system in classical physics is said to hold when the forward and reverse *transition probabilities* are equal for each transition. The transition probabilities in the present context are the square moduli of the S matrix elements, which properly sum up to unity in the unitarity limit of Eq. (3.2.59). We therefore

define as the *detailed balance relation* the equation

$$|\tilde{\mathbf{S}}_{\alpha\alpha_i}|^2 = |\tilde{\mathbf{S}}_{\alpha_i\alpha}|^2 \ , \tag{3.2.60}$$

which makes all the forward and reverse transition probabilities equal.

This condition holds for the solutions of coupled Schrödinger equations if the forward and reverse couplings are identical, with the same magnitude and phase, namely that coupling matrix $\hat{V}_{\alpha\alpha'} = \hat{V}_{\alpha'\alpha}$ is symmetric. In this case, we have somewhat stronger *reciprocity* condition where the $\tilde{\mathbf{S}}$ matrix itself is also *symmetric*:

$$\tilde{\mathbf{S}} = \tilde{\mathbf{S}}^{\mathrm{T}} \ . \tag{3.2.61}$$

This will be proved not here, but in section 10.3.2, where we give an explicit construction for $\tilde{\mathbf{S}}$. (Note that it is $\tilde{\mathbf{S}}$ of Eq. (3.2.15), *with* the velocity factors, which is symmetric, not the original $\mathbf{S}$ matrix.) This symmetry is sufficient for the detailed balance relation to hold.

We often use the coupling matrices defined using the multi-channel wave functions of section 3.2.1 which are *not* symmetric, because of the i^L factors in Eq. (3.2.1). If these factors are used, the coupling matrices will satisfy rather $\hat{V}_{\alpha\alpha'} = (-1)^{L-L'}\hat{V}_{\alpha'\alpha}$, as also do the $\tilde{\mathbf{S}}$ matrices, but this is still sufficient for detailed balance, Eq. (3.2.60), to hold.

The symmetry condition (3.2.61) is distinct from unitarity, but real symmetric coupling matrices lead to both unitarity and symmetry of the $\tilde{\mathbf{S}}$ matrix. Hamiltonians as commonly used with complex potentials cannot be unitary, but can almost always be made to have symmetric matrix elements. For more discussion about unitarity, time reversal and reciprocity, see Taylor [5, §6-e, §17-e] and Satchler [11, §4.4, §9.5-6].

The above reciprocity results can also be proved for potentials that are *time-reversal invariant*. However complex potentials never satisfy this condition, but still lead to reciprocity, which is hence true more generally than just for invariance under time reversal.

From the detailed balance of the $\tilde{\mathbf{S}}$ matrix of Eq. (3.2.60), we may derive a direct connection between the *total cross sections* for the forward and reverse reactions. From Eq. (3.2.32), the cross section from entrance channel $x_i p_i t_i$ to a distinct exit channel xpt is

$$\sigma_{xpt:x_ip_it_i} \quad = \quad \frac{\pi}{k_i^2}\frac{1}{(2J_{p_i}+1)(2J_{t_i}+1)}\sum_{J_{\mathrm{tot}}\pi\alpha\alpha_i}(2J_{\mathrm{tot}}+1)|\tilde{\mathbf{S}}^{J_{\mathrm{tot}}\pi}_{\alpha\alpha_i}|^2. \tag{3.2.62}$$

The detailed balance $|\tilde{\mathbf{S}}_{\alpha\alpha_i}|^2 = |\tilde{\mathbf{S}}_{\alpha_i\alpha}|^2$ implies that the equivalent expression for the reverse reaction $\sigma_{x_ip_it_i:xpt}$, from entrance channel xpt to exit channel

$x_i p_i t_i$, satisfies

$$k_i^2(2J_{p_i}+1)(2J_{t_i}+1)\sigma_{xpt:x_ip_it_i} = k^2(2J_p+1)(2J_t+1)\sigma_{x_ip_it_i:xpt} \ , \quad (3.2.63)$$

so

$$\sigma_{x_ip_it_i:xpt} = \frac{k_i^2(2J_{p_i}+1)(2J_{t_i}+1)}{k^2(2J_p+1)(2J_t+1)}\sigma_{xpt:x_ip_it_i} \ . \quad (3.2.64)$$

This equation is therefore called the *principle of detailed balance*. The Hermiticity of the Hamiltonian leads to unitarity S matrices, but that by itself is only sufficient for detailed balance between the cross sections if the couplings are also real or can be made real by a unitary transformation.

A slightly different expression holds for photon channels. Although we will see in section 3.5.1 that they can be considered as spin 1 objects, the gauge condition implies that there are only two independent polarisation projections, and hence $(2s_\gamma+1)$ should be replaced by the value of 2.

Another slightly different expression holds for identical particles. If the reacting nuclei in either the entrance or exit channels are identical, then requirements of the Pauli principle dictate either symmetry or antisymmetry of the overall system wave function. Compared with Eq. (3.2.62), this induces an additional factor in way the cross section depends on the S matrix elements. This factor may be different in the forward and reverse channels, and affect the detailed balance equation (3.2.64). These factors will be determined in section 3.4, after isospin and (anti-)symmetries have been defined.

3.3 Integral forms

Instead of defining cross sections in terms of S or T matrix elements contained in the boundary conditions for differential equations, it is also possible to give expressions for these matrix elements that are integrals over the wave functions with some part of the Hamiltonian. These integral forms for the S or T matrix elements should in principle yield identical results, but are useful since they may suggest a new range of approximations that may still be sufficiently accurate in the relevant physical respects.

3.3.1 Green's function methods

Up to now we have solved only homogeneous Schrödinger equations like $[E - H]\Psi = 0$. Sometimes we may need to solve inhomogeneous equations like $[E - H]\Psi = \Omega$ with outgoing boundary conditions, for some radial

functions $\Omega(R)$ called *source terms*, as such equations arise as part of a coupled channels set. The inhomogenous equation may be solved by differential methods as discussed in Chapter 6, but often it is useful to give an integral expression for its solution, and it is especially useful that there exist simple integrals giving directly the asymptotic outgoing amplitude of the solution, namely its T matrix element. This section shows how to use Green's function methods to solve the inhomogeneous differential equation.

Integral solutions of inhomogeneous equations

Consider the general problem of solving the coupled equations similar to those of Eq. (3.2.55):

$$[T_{xL}(R) + U_{cx}(R) - E_{xpt}]\psi_\alpha(R) + \sum_{\alpha'}\langle\alpha|V|\alpha'\rangle\psi_{\alpha'}(R') = 0 \ . \qquad (3.3.1)$$

for some given incoming channel α_i that we assume fixed, and not always written amoung the subscripts. Here we have separated out the point Coulomb potential $U_{cx}(R) = Z_{xp}Z_{xt}e^2/R$ (if present), and put all the other couplings, local or non-local, into the matrix elements of V.

The solutions must satisfy the standard outgoing boundary conditions of Eq. (3.2.16) for the given α_i. Suppose that all the $\psi_{\alpha'}(R')$ are known for which $\langle\alpha|V|\alpha'\rangle \neq 0$, in which case we may solve the inhomogeneous equation (3.3.1) for the wave function $\psi_\alpha(R)$ using the known source term

$$\Omega_\alpha(R) = \sum_{\alpha'}\langle\alpha|V|\alpha'\rangle\psi_{\alpha'}(R') \ . \qquad (3.3.2)$$

This is to solve the inhomogeneous equation

$$[E_{xpt} - T_{xL}(R) - U_{cx}(R)]\psi_\alpha(R) = \Omega_\alpha(R) \ . \qquad (3.3.3)$$

The outgoing-wave boundary conditions from Eq. (3.2.16) may be written in the T matrix form of Eq. (3.2.19):

$$\psi_{\alpha\alpha_i}(R) = F_\alpha(R)\delta_{\alpha\alpha_i} + H^+_\alpha(R)\mathbf{T}_{\alpha\alpha_i} \ . \qquad (3.3.4)$$

where we have reinserted α_i as the given incoming elastic channel. The $\mathbf{T}_{\alpha\alpha_i}$ is the nuclear T matrix element for scattering in addition to the point Coulomb potential. We confirm that in the limit of $V = 0$, when $\Omega_\alpha(R) = 0$, only the the elastic channel wave function is non-zero with value $\psi_{\alpha_i\alpha_i}(R) = F_{\alpha_i}(R)$, and $\mathbf{T}_{\alpha\alpha_i} = 0$.

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

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

$$\left[\frac{\mathrm{d}^2}{\mathrm{d}R^2}-\breve{U}(R)+k_\alpha^2\right]\psi_\alpha(R)=\frac{2\mu_x}{\hbar^2}\Omega_\alpha(R)\ , \tag{3.3.5}$$

where $\breve{U}(R)\equiv 2\eta k_\alpha/R+L_\alpha(L_\alpha+1)/R^2$ is the sum of the Coulomb and centrifugal terms, and $k_\alpha^2=2\mu_x E_{xpt}/\hbar^2$.

Now the general source term $\Omega_\alpha(R)$ can always be formally written as a superposition of solutions for δ-function sources $\delta(R-R')$ at R', since

$$\Omega_\alpha(R)=\int\delta(R-R')\Omega_\alpha(R')\mathrm{d}R'\ . \tag{3.3.6}$$

Thus all we need is the solution, a function of R, of Eq. (3.3.5) for a δ-function source at R'. We denote this solution by $G^+(R,R')$, since it depends on both R and R', and it is precisely the Green's function $G^+(R,R')$ satisfying

$$\left[\frac{\mathrm{d}^2}{\mathrm{d}R^2}-\breve{U}(R)+k_\alpha^2\right]G^+(R,R') \quad = \quad \delta(R-R')\ . \tag{3.3.7}$$

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

$$\psi_\alpha(R)=\delta_{\alpha\alpha_i}F_\alpha(R)+\frac{2\mu_x}{\hbar^2}\int G^+(R,R')\Omega_\alpha(R')\mathrm{d}R'\ , \tag{3.3.8}$$

since the homogeneous solution $F_\alpha(R)$ is present only in the elastic channel. This equation is often written more compactly in operator notation as

$$\psi_\alpha=F_\alpha+\hat{G}^+\Omega_\alpha\ , \tag{3.3.9}$$

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

$$\hat{G}^+=[E-\hat{T}-U_c]^{-1} \tag{3.3.10}$$

with the specified outgoing boundary conditions. Eq. (3.3.9) can therefore be written as

$$\psi_\alpha=F_\alpha+[E-\hat{T}-U_c]^{-1}\Omega_\alpha\ . \tag{3.3.11}$$

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

For fixed R', when $R \neq R'$ we have from Eq. (3.3.7) that†

$$\left[\frac{\mathrm{d}^2}{\mathrm{d}R^2} - \breve{U}(R) + k^2\right] G^+(R, R') = 0 \ . \tag{3.3.12}$$

Since this is a second-order linear differential equation, any solution must be a linear combination of two fixed linearly-independent solutions. We choose for these the regular Coulomb function $F(R)$ and the irregular function $H^+(R)$ for this partial wave L. With this choice, the unknown Green's function must satisfy

$$G^+(R, R') = f(R')F(R) + h(R')H^+(R) \ , \tag{3.3.13}$$

where the coefficients f, h are as yet unknown functions of R'. We apply Eq. (3.3.12) separately for $R < R'$ and $R > R'$, in order to avoid $R = R'$.

To determine the $R < R'$ case, consider $R = 0$. Any solution of Eq. (3.3.12) must be zero at the origin in R, so $G^+(0, R') = 0$ for $R' > 0$. Since $H^+(0) \neq 0$ and $F(0) = 0$, we conclude from Eq. (3.3.13) that $h(R') = 0$ when $R < R'$.

To determine the $R > R'$ case, note that the $R \to \infty$ boundary condition of Eq. (3.3.4) implies that $G^+(R, R') \propto H_L^+(R)$. We conclude from Eq. (3.3.13) that $f(R') = 0$ when $R > R'$.

Summarising the two results,

$$G^+(R, R') = \begin{cases} f(R')F(R) \text{ for } R < R' \\ h(R')H^+(R) \text{ for } R > R' \end{cases} \ . \tag{3.3.14}$$

To fix $f(R')$, $h(R')$ we use the differential equation (3.3.7). Integrating this with respect to R over the range from just below R' to just above, we find

$$\frac{\mathrm{d}}{\mathrm{d}R}G^+(R, R')|_{R=R'_+} - \frac{\mathrm{d}}{\mathrm{d}R}G^+(R, R')|_{R=R'_-} = 1 \ , \tag{3.3.15}$$

so from Eq. (3.3.14) we have

$$h(R)H^{+\prime}(R) - f(R)F'(R) = 1 \ . \tag{3.3.16}$$

Now $G(R, R')$ is itself continuous over $R \sim R'$:

$$h(R)H^+(R) - f(R)F(R) = 0 \ . \tag{3.3.17}$$

† We are dealing with just one channel α here, so up to Eq. (3.3.21) we may omit that subscript for simplicity.

So, solving Eqs. (3.3.16, 3.3.17) simultaneously, we have

$$h(R) = \frac{F(R)}{W(F,H^+)}, \qquad f(R) = \frac{H^+(R)}{W(F,H^+)}, \tag{3.3.18}$$

where $W(f,g) = fg' - f'g$ is the Wronskian for two functions $f(R)$ and $g(R)$. For our F, H^+, the Wronskian $W(F,H^+) = W(F,G) = -k$ from Eq. (3.1.11).

The full Green's function is therefore

$$\begin{aligned} G^+(R,R') &= -\frac{1}{k}\begin{cases} H^+(R')F(R) \text{ for } R < R' \\ F(R')H^+(R) \text{ for } R > R' \end{cases} & (3.3.19) \\ &= -\frac{1}{k}F(R_<)H^+(R_>) & (3.3.20) \end{aligned}$$

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

We wanted the solution of the original inhomogeneous equation (3.3.3). Now restoring the channel indices α and incoming index α_i, that solution is

$$\psi_\alpha(R) = \delta_{\alpha\alpha_i}F_\alpha(R) - \frac{2\mu_x}{\hbar^2 k_\alpha}\int F_\alpha(R_<)H^+_\alpha(R_>)\Omega_\alpha(R')\mathrm{d}R' \ . \tag{3.3.21}$$

At large distances $R > \max(R', R_n)$, we have $\psi_\alpha(R) \to \delta_{\alpha\alpha_i}F_\alpha(R) + \mathbf{T}_{\alpha\alpha_i}H^+(R)$ from Eq. (3.3.4), so

$$\mathbf{T}_{\alpha\alpha_i}H^+_\alpha(R) = -\frac{2\mu_x}{\hbar^2 k_\alpha}H^+_\alpha(R)\int F_\alpha(R')\Omega_\alpha(R')\mathrm{d}R' \ , \tag{3.3.22}$$

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

$$\mathbf{T}_{\alpha\alpha_i} = -\frac{2\mu_x}{\hbar^2 k_\alpha}\int F_\alpha(R')\Omega_\alpha(R')\mathrm{d}R' \ . \tag{3.3.23}$$

This may be rewritten in Dirac bra-ket notation as

$$\begin{aligned} \mathbf{T}_{\alpha\alpha_i} &= -\frac{2\mu_x}{\hbar^2 k_\alpha}\langle F^*_\alpha|\Omega_\alpha\rangle & (3.3.24) \\ &= -\frac{2\mu_x}{\hbar^2 k_\alpha}\langle F^{(-)}_\alpha|\Omega_\alpha\rangle \ . & (3.3.25) \end{aligned}$$

The complex conjugation in Eq. (3.3.24) is necessary to cancel the conjugation implicit in the matrix elements. A $^{(-)}$ superscript in the Eq. (3.3.25) is used for the same purpose, for reasons to be explained on page 90.

In the operator notation, Eq. (3.3.11) may be rewritten as

$$\begin{aligned} \psi &= \phi + \hat{G}^+\Omega \\ &= \phi + \hat{G}^+V\psi \ , \end{aligned} \tag{3.3.26}$$

using ϕ to refer to the homogeneous solution present only in the elastic channel, and with the + sign indicating outgoing boundary conditions of Eqs. (3.3.4). An equation like (3.3.26) is called a partial-wave *Lippmann-Schwinger equation*, and in this notation the T-matrix (3.3.25) is the integral

$$\mathsf{T} = -\frac{2\mu}{\hbar^2 k}\langle\phi^{(-)}|V|\psi\rangle \equiv -\frac{2\mu}{\hbar^2 k}\int \phi(R)V(R)\psi(R)\mathrm{d}R\ . \tag{3.3.27}$$

In the 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.

3.3.2 Vector-form T matrix for plane waves

If the above analysis is repeated for every partial wave L in the spherical potential case, then the resulting T_L may be substituted in Eq. (3.1.56) to yield the angle-dependent scattering amplitude $f(\theta)$. If $U_c(R) = 0$, for example, the ϕ are the partial wave components $F_L(0, kR)$ of a plane wave and the ψ are the partial waves χ_L for scattering with the potential. Summing over L gives

$$f(\theta) = -\frac{8\pi\mu}{\hbar^2 k_i}\sum_{LM}\int_0^\infty Y_L^M(\hat{\mathbf{k}}')^* F_{L'}(0,k'R)\ V(R)\ Y_L^M(\hat{\mathbf{k}}_i)\chi_L(R)\ \mathrm{d}R. \tag{3.3.28}$$

Then, expanding $V(R)\delta_{LL'}\delta_{MM'} = \int_{4\pi}\mathrm{d}\hat{\mathbf{R}}\, Y_L^M(\mathbf{R})V(\mathbf{R})Y_{L'}^{M'}(\mathbf{R})$ for a spherical potential, we have

$$\begin{aligned} f(\theta) &= -\frac{\mu}{2\pi\hbar^2}\int \mathrm{d}\mathbf{R}\ \mathrm{e}^{-\mathrm{i}\mathbf{k}'\cdot\mathbf{R}}\ V(\mathbf{R})\ \mathbf{\Psi}(\mathbf{R};\mathbf{k}_i) && (3.3.29)\\ &= -\frac{\mu}{2\pi\hbar^2}\langle \mathrm{e}^{\mathrm{i}\mathbf{k}'\cdot\mathbf{R}}|V|\mathbf{\Psi}(\mathbf{R};\mathbf{k}_i)\rangle, && (3.3.30)\end{aligned}$$

where θ is the scattering angle from the initial momentum $\mathbf{k}_i$ to the final momentum $\mathbf{k}'$ (with $|\mathbf{k}'| = |\mathbf{k}_i|$), and the bra-ket is a three-dimensional integral. This integral form is also called a 'T matrix', but is one that depends on initial and final $\mathbf{k}$ values, not on partial waves L or α. We call this *vector form* of the $\mathbf{T}$ matrix (as distinct from the partial wave form T), with the notation $\mathbf{T}(\mathbf{k}', \mathbf{k})$.

The vector form $\mathbf{T}$ matrix is defined in relation to the two-body scattering amplitude as

$$f(\mathbf{k}';\mathbf{k}) = -\frac{\mu}{2\pi\hbar^2}\mathbf{T}(\mathbf{k}',\mathbf{k}), \tag{3.3.31}$$

so we have just shown that for a plane wave final state,

$$\mathbf{T}(\mathbf{k}',\mathbf{k}) = \langle \mathrm{e}^{\mathrm{i}\mathbf{k}'\cdot\mathbf{R}}|V|\mathbf{\Psi}(\mathbf{R};\mathbf{k})\rangle. \tag{3.3.32}$$

3.3.3 Two potential formula

If a channel potential can be composed of two parts $V(R) = U_1(R) + U_2(R)$, then it is possible to treat U_1 as the distorting potential and U_2 as the remaing interaction. Then, using the T matrix integral expression for the scattering from their combined potential V, we can derive an exact *two-potential formula* involving the T matrix *difference* between U_1 scattering and V scattering. This difference will be proportional to U_2.

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. (3.3.26) to write down the corresponding Lippmann-Schwinger equations:

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

From Eq. (3.3.27), the $\mathbf{T}$-matrix integral $\mathbf{T}^{(1)} = -\frac{2\mu}{\hbar^2 k}\langle \phi^{(-)}|U_1|\chi\rangle$ describes the scattering from U_1 only. Similarly the T matrix $\mathbf{T}^{(1+2)}$ for the combined potentials $U_1 + U_2$ satisfies

$$\begin{aligned} -\frac{\hbar^2 k}{2\mu}\mathbf{T}^{(1+2)} &= \int \phi(U_1+U_2)\psi \, \mathrm{d}R \\ &= \int (\chi - \hat{G}_0^+ U_1\chi)(U_1+U_2)\psi \, \mathrm{d}R \\ &= \int \Big[\chi(U_1+U_2)\psi - (\hat{G}_0^+ U_1\chi)(U_1+U_2)\psi\Big] \, \mathrm{d}R \,. \end{aligned} \tag{3.3.33}$$

Because the kernel function of Eq. (3.3.19) for the operator $\hat{G}_0^+$ is symmetric under $R \leftrightarrow R'$ interchange,

$$\begin{aligned} -\frac{\hbar^2 k}{2\mu}\mathbf{T}^{(1+2)} &= \int [\chi(U_1+U_2)\psi - \chi U_1 \hat{G}_0^+ (U_1+U_2)\psi] \, \mathrm{d}R \\ &= \int [\chi(U_1+U_2)\psi - \chi U_1(\psi - \phi)] \, \mathrm{d}R \\ &= \int \phi[U_1\chi + \chi U_2\psi] \, \mathrm{d}R \qquad (3.3.34) \\ &= \langle \phi^{(-)}|U_1|\chi\rangle + \langle \chi^{(-)}|U_2|\psi\rangle \, . \qquad (3.3.35) \end{aligned}$$

Note that in Eq. (3.3.34) the two terms in the integrand are products of three complex functions, and the product order is unimportant. In Eq. (3.3.35), by contrast, the functions are no longer interchangeable.

Thus $\mathbf{T}^{(1+2)} = \mathbf{T}^{(1)} + \mathbf{T}^{2(1)}$, defining an additional term

$$\mathbf{T}^{2(1)} = -\frac{2\mu}{\hbar^2 k} \int \chi U_2 \psi \, \mathrm{d}R \tag{3.3.36}$$

as the scattering T matrix contribution from coupling U_2, with U_1 appearing as a distorting potential in χ. The previous equation (3.3.35) is called the *two potential formula*, and is an exact equation for both real and complex potentials U_1, U_2.

We use the $^{(-)}$ superscript to indicate complex conjugation for the left-hand wave function, as in Eq. (3.3.25). The reason for this notation can now be explained. The χ^* satisfies a boundary condition with an *incoming* boundary conditions for all the asymptotic parts in addition to the plane wave. Since externally

$$\chi = F + \mathbf{T}^{(1)} H^+ \to \sin(kR) + \mathbf{T}^{(1)} \, \mathrm{e}^{\mathrm{i}kR} \, , \tag{3.3.37}$$

$$\text{we have} \quad \chi^* = F^* + \mathbf{T}^{(1)*} H^{+*} \to \sin(kR) + \mathbf{T}^{(1)*} \mathrm{e}^{-\mathrm{i}kR} \, , \tag{3.3.38}$$

where $\mathbf{T}^{(1)}$ is the scattering from the potential $U_1(R)$ that defines the homogeneous functions $\chi(R)$. Thus χ^* is asymptotically a plane wave plus some coefficient multiplying an *incoming* spherical wave $\mathrm{e}^{-\mathrm{i}kR}$, and hence is frequently written as $\chi^{(-)}$.

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

$$\psi = \chi + \hat{G}_1^+ U_2 \psi \, , \tag{3.3.39}$$

using $\hat{G}_1^+ = [E - T - U_1]^{-1}$ with outgoing wave boundary conditions. The first term χ represents the contribution present if $U_2 = 0$. By methods analogous to that of section 3.3.1, the $\hat{G}_1^+$ operator has the integral kernel

$$\hat{G}_1^+(R, R') = -\frac{1}{k} \chi(R_<) \chi^+(R_>), \tag{3.3.40}$$

where $\chi^+(R)$ is the new irregular solution of $[E - T - U_1]\chi^+(R) = 0$ that equals $H^+(R)$ everywhere outside the range of $U_1(R)$.

3.3.4 Vector-form T matrix for distorted waves

When the distorting potential $U_1(R) \neq 0$ is spherical, let $\mathbf{X}(\mathbf{R}; \mathbf{k}')$ be the system wave function like Eq. (3.2.1) obtained by solving the Schrödinger equation with that potential. The two-potential formula of Eq. (3.3.35) will now give the vector-form T matrix for the additional scattering by potential U_2, namely

$$\mathbf{T}(\mathbf{k}', \mathbf{k}) = \langle \mathbf{X}^{(-)}(\mathbf{R}; \mathbf{k}') | U_2 | \mathbf{\Psi}(\mathbf{R}; \mathbf{k}) \rangle, \tag{3.3.41}$$

where the superscript $\mathbf{X}^{(-)}$ again indicates incoming waves everywhere in addition to the elastic plane wave in the boundary conditions. The scattering amplitude f is related again to $\mathbf{T}$ by Eq. (3.3.31).

In the multi-channel case, we sum over all coupled channels sets $J^\pi_{\rm tot}$, and following Eq. (3.2.7) construct the wave functions $\mathbf{\Psi}^{\mu_{p_i}\mu_{t_i}}_{x_ip_it_i}(\mathbf{R}_x;\mathbf{k}_i)$ for the potential U_1+U_2 with coupled radial functions $\psi_{\alpha\alpha_i}(R_x)$, and $\mathbf{X}^{\mu_{p'}\mu_{t'}}_{x'p't'}(\mathbf{R}_{x'};\mathbf{k}')$ with uncoupled radial functions $\chi_{\alpha'}(R_{x'})$ for the spherical potential U_1 only. Both depend on the m-state projections of the nuclei in the relevant partition. The vector-form T matrix is now

$$\begin{aligned}
&\mathbf{T}^{\mu_{p'}\mu_{t'}:\mu_{p_i}\mu_{t_i}}_{x'p't':x_ip_it_i}(\mathbf{k}',\mathbf{k}_i)\\
&\quad= \langle \mathbf{X}^{\mu_{p'}\mu_{t'}(-)}_{x'p't'}(\mathbf{R}_{x'};\mathbf{k}')|U_2|\mathbf{\Psi}^{\mu_{p_i}\mu_{t_i}}_{x_ip_it_i}(\mathbf{R}_x;\mathbf{k}_i)\rangle &(3.3.42)\\
&\quad= \sum_{J_{\rm tot}M_{\rm tot}}\sum_{\alpha'\alpha_i} A^{J_{\rm tot}M_{\rm tot}}_{\mu_{p'}\mu_{t'}}(\alpha';\mathbf{k}')^* A^{J_{\rm tot}M_{\rm tot}}_{\mu_{p_i}\mu_{t_i}}(\alpha_i;\mathbf{k}_i)\sum_\alpha\langle\chi_{\alpha'}|U_2|\psi_{\alpha\alpha_i}\rangle &(3.3.43)\\
&\quad= -\frac{\hbar^2k_{\alpha'}}{2\mu_{\alpha'}}\sum_{J_{\rm tot}M_{\rm tot}}\sum_{\alpha'\alpha_i} A^{J_{\rm tot}M_{\rm tot}}_{\mu_{p'}\mu_{t'}}(\alpha';\mathbf{k}')^* A^{J_{\rm tot}M_{\rm tot}}_{\mu_{p_i}\mu_{t_i}}(\alpha_i;\mathbf{k}_i)\ \mathbf{T}^{J_{\rm tot}M_{\rm tot}}_{\alpha'\alpha_i} &(3.3.44)
\end{aligned}$$

where the $A^{J_{\rm tot}M_{\rm tot}}_{\mu_p\mu_t}(\alpha;\mathbf{k})$ are given by Eq. (3.2.9). This last equation gives the general multichannel relationship between the *partial wave* matrix elements $\mathbf{T}_{\alpha'\alpha_i}$ and the *vector form* matrix elements $\mathbf{T}(\mathbf{k}',\mathbf{k}_i)$. Note that the wave number $k_{\alpha'}$ and reduced mass $\mu_{\alpha'}$ in the final channel are entirely determined by $x'p't'$. The final equation holds generally: also when U_1 is non-spherical and the $\chi_{\alpha''\alpha'}(R_{x''})$ are thus solutions of a set of coupled equations.

The Eq. (3.3.44) also yields another expression for the nuclear-only scattering amplitude in terms of the partial wave T matrix elements:

$$\begin{aligned}
f^{xpt}_{\mu_p\mu_t,\mu_{p_i}\mu_{t_i}}(\mathbf{k};\mathbf{k}_i) &= -\frac{\mu_\alpha}{2\pi\hbar^2}\mathbf{T}^{\mu_p\mu_t:\mu_{p_i}\mu_{t_i}}_{xpt:x_ip_it_i}(\mathbf{k},\mathbf{k}_i)\\
&= \frac{k_\alpha}{4\pi}\sum_{J_{\rm tot}M_{\rm tot}}\sum_{\alpha\alpha_i} A^{J_{\rm tot}M_{\rm tot}}_{\mu_p\mu_t}(\alpha;\mathbf{k})^* A^{J_{\rm tot}M_{\rm tot}}_{\mu_{p_i}\mu_{t_i}}(\alpha_i;\mathbf{k}_i)\mathbf{T}^{J_{\rm tot}M_{\rm tot}}_{\alpha\alpha_i}. \quad (3.3.45)
\end{aligned}$$

3.3.5 Born series and approximations

One-potential scattering

For a fixed potential $U(R)$, solving the Lippmann-Schwinger equation $\chi = \phi + \hat{G}^+_0 U\chi$ should provide an exact solution for the wave function χ with potential U. This however is an implicit equation, as χ appears on both the left and right sides. To find it explicitly, we could perhaps sum the iterated

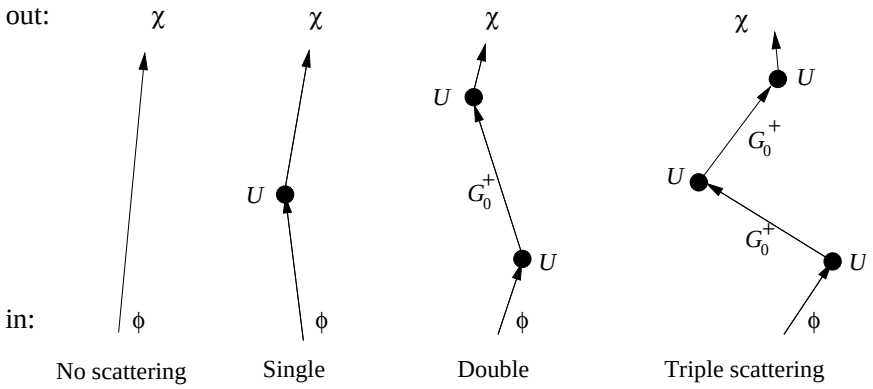

Fig. 3.5. Illustrating the Born series (3.3.46) for the wave function χ, as a sum of a homogeneous term with single, double, and higher-order rescattering contributions to the outgoing wave χ.

Born series:

$$\begin{aligned}\chi &= \phi + \hat{G}_0^+ U[\phi + \hat{G}_0^+ U[\phi + \hat{G}_0^+ U[\cdots]]] \\ &= \phi + \hat{G}_0^+ U\phi + \hat{G}_0^+ U\hat{G}_0^+ U\phi + \hat{G}_0^+ U\hat{G}_0^+ U\phi\hat{G}_0^+ U\phi + \cdots \quad ,\end{aligned} \tag{3.3.46}$$

from which the outgoing T matrix amplitude is

$$\mathsf{T} = -\frac{2\mu}{\hbar^2 k}\left[\langle\phi^{(-)}|U|\phi\rangle + \langle\phi^{(-)}|U\hat{G}_0^+ U|\phi\rangle + \cdots \quad\right] . \tag{3.3.47}$$

The equation (3.3.46) may be illustrated by the figure 3.5, 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 in Eq. (3.3.47) is called the *plane wave Born approximation* (PWBA):

$$\mathsf{T}^{\rm PWBA} = -\frac{2\mu}{\hbar^2 k}\langle\phi^{(-)}|U|\phi\rangle \ . \tag{3.3.48}$$

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

$$\mathsf{T}_L^{\rm PWBA} = -\frac{2\mu}{\hbar^2 k}\int_0^\infty F_L(0,kR)\ U(R)\ F_L(0,kR)\ {\rm d}R \ . \tag{3.3.49}$$

Substituting again these T matrix elements into Eq. (3.1.46), or by a special case of Eq. (3.3.29), the three-dimensional form for the PWBA scattering

amplitude is

$$f^{\rm PWBA}(\theta) = -\frac{\mu}{2\pi\hbar^2}\int {\rm d}\mathbf{R}\ {\rm e}^{-i\mathbf{q}\cdot\mathbf{R}}\ U(\mathbf{R})\ , \tag{3.3.50}$$

where the momentum transfer $\mathbf{q} = \mathbf{k} - \mathbf{k}_i$, 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. (3.3.35), the two-potential formula, the exact T matrix expression is again

$$\mathsf{T}^{(1+2)} = \mathsf{T}^{(1)} - \frac{2\mu}{\hbar^2 k}\langle\chi^{(-)}|U_2|\psi\rangle \tag{3.3.51}$$

where, from Eq. (3.3.39), the exact wave function is the solution of the implicit equation $\psi = \chi + \hat{G}_1 U_2\psi$. We may again by iteration, therefore, form a Born series

$$\mathsf{T}^{(1+2)} = \mathsf{T}^{(1)} - \frac{2\mu}{\hbar^2 k}\left[\langle\chi^{(-)}|U_2|\chi\rangle + \langle\chi^{(-)}|U_2\hat{G}_1U_2|\chi\rangle + \cdots\right]\ . \tag{3.3.52}$$

We might expect this series to converge if U_2 is weak in a suitable sense. We do *not* here require that U_1 is weak.

Post and prior T matrix integrals

The exact expression (3.3.51) 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. (3.3.52) as

$$\mathsf{T}^{(1+2)} = \mathsf{T}^{(1)} - \frac{2\mu}{\hbar^2 k}\left[\langle\chi^{(-)}| + \langle\chi^{(-)}|U_2\hat{G}_1 + \cdots\right]U_2|\chi\rangle\ , \tag{3.3.53}$$

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

$$\begin{aligned}\psi^{(-)} &= \chi^{(-)} + \hat{G}_1^- U_2^*\chi^{(-)} + \cdots \\ &= \chi^{(-)} + \hat{G}_1^- U_2^*\psi^{(-)}\ .\end{aligned} \tag{3.3.54}$$

The Green's function $\hat{G}_1^-$ is the complex conjugate of $\hat{G}_1^+$, and thus describes incoming boundary conditions like Eq. (3.3.38). 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 T matrix integral*

$$\mathbf{T}^{(1+2)} = \mathbf{T}^{(1)} - \frac{2\mu}{\hbar^2 k}\langle\psi^{(-)}|U_2|\chi\rangle \ . \tag{3.3.55}$$

The wave functions on the kets of Eqs. (3.3.51) and (3.3.55) are often written with a (+) to remind that they are calculated with normal *outgoing* boundary conditions:

$$\mathbf{T}^{(1+2)} = \mathbf{T}^{(1)} - \frac{2\mu}{\hbar^2 k}\langle\chi^{(-)}|U_2|\psi^{(+)}\rangle = \mathbf{T}^{(1)} - \frac{2\mu}{\hbar^2 k}\langle\psi^{(-)}|U_2|\chi^{(+)}\rangle \ . \tag{3.3.56}$$

If now in multichannel theory 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

$$\mathbf{T}^{(1+2)}_{\alpha\alpha_i} = \mathbf{T}^{(1)}_{\alpha\alpha_i} - \frac{2\mu_\alpha}{\hbar^2 k_\alpha}\langle\chi^{(-)}_\alpha|U_2|\psi^{(+)}_{\alpha_i}\rangle \quad \text{[post]}, \tag{3.3.57a}$$

$$= \mathbf{T}^{(1)}_{\alpha\alpha_i} - \frac{2\mu_\alpha}{\hbar^2 k_\alpha}\langle\psi^{(-)}_\alpha|U_2|\chi^{(+)}_{\alpha_i}\rangle \quad \text{[prior]}. \tag{3.3.57b}$$

Remember here that the $\chi^{\pm}$ are the wave functions with U_1 only, and that the $\psi^{\pm}$ are the full coupled wave functions with $V = U_1 + U_2$, so the potential in the matrix element is $U_2 = V - U_1$. The superscript (+) refers to the normal boundary conditions with outgoing waves except in the elastic channel, while the minus (−) superscript refers to the unusual *incoming* boundary condition in all waves (in addition to the plane wave component in the elastic channel).

If the second terms of Eq. (3.3.57) are inserted in Eq. (3.3.44) and summed over all partial waves, there are analogous three-dimensional integrals for the vector-form T matrices $\mathbf{T}_{xpt:x_ip_it_i}(\mathbf{k}', \mathbf{k}_i)$ from Eq. (3.3.42). If $\mathbf{X}$ is the system scattering function for potential $U(R)$ and $\mathbf{\Psi}$ with $V(R)$, then the scattering from V that is in addition to the U scattering has vector-form T matrix expressions in two versions:

$$\mathbf{T}^{2(1):\text{post}}_{xpt:x_ip_it_i}(\mathbf{k}', \mathbf{k}_i) = \langle\mathbf{X}^{(-)}_{xpt}(\mathbf{R}, \mathbf{k}')|\ V - U\ |\mathbf{\Psi}_{x_ip_it_i}(\mathbf{R}; \mathbf{k}_i)\rangle \quad \text{[post]}, \tag{3.3.58a}$$

$$\mathbf{T}^{2(1):\text{prior}}_{xpt:x_ip_it_i}(\mathbf{k}', \mathbf{k}_i) = \langle\mathbf{\Psi}^{(-)}_{xpt}(\mathbf{R}; \mathbf{k}')|\ V - U\ |\mathbf{X}_{x_ip_it_i}(\mathbf{R}, \mathbf{k}_i)\rangle \quad \text{[prior]} \tag{3.3.58b}$$

that should be equal. Both of these give scattering amplitudes $f = -\frac{\mu}{2\pi\hbar^2}\mathbf{T}$ according to Eq. (3.3.31), and then cross sections $\sigma = |f|^2$ as a function of angle. Strictly speaking, the $\mathbf{\Psi}$ and $\mathbf{X}$ both carry m-state quantum numbers: these carry over together to the $\mathbf{T}$ as in Eq. (3.3.42), and hence to the scattering amplitudes f and cross sections σ.

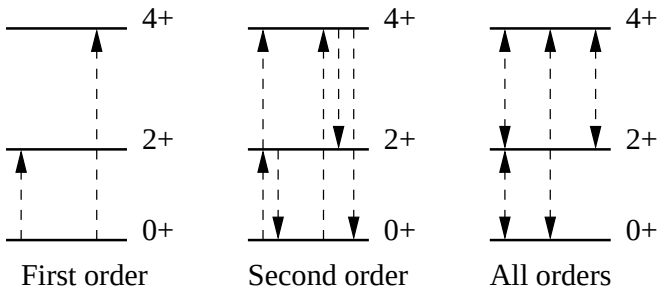

Fig. 3.6. First, second and all-order couplings within a set of 0^+, 2^+ and 4^+ nuclear levels, starting from the ground state.

Distorted wave Born approximation (DWBA)

If the series (3.3.52) is truncated after the first term, linear in U_2, then

$$\mathsf{T}^{\rm DWBA} = \mathsf{T}^{(1)} - \frac{2\mu}{\hbar^2 k}\langle\chi^{(-)}|U_2|\chi\rangle \tag{3.3.59}$$

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 $\mathsf{T}^{(1)} = 0$, and we have the convenient DWBA expression for the T matrix from incoming channel α_i to exit channel α:

$$\mathsf{T}^{\rm DWBA}_{\alpha\alpha_i} = -\frac{2\mu_\alpha}{\hbar^2 k_\alpha}\langle\chi^{(-)}_\alpha|U_2|\chi_{\alpha_i}\rangle\ . \tag{3.3.60}$$

Fig. 3.6 illustrates first and second-order couplings, in contrast to including all couplings in a full coupled channels solution.

First-order DWBA for transfer reactions

If we write the DWBA T-matrix element of Eq. (3.3.60) using the formalism for multiple mass partitions developed in section 3.2.2, then we have a DWBA expression that can be used for simple transfer reactions that couple one mass partition to another. In that formalism, we have

$$\mathsf{T}^{\rm DWBA}_{\alpha\alpha_i} = -\frac{2\mu_\alpha}{\hbar^2 k_\alpha}\left\langle\chi^{(-)}_\alpha\left|R_x\langle\alpha|H-E|\alpha_i\rangle R^{-1}_{x_i}\right|\chi_{\alpha_i}\right\rangle\ . \tag{3.3.61}$$

where the inner matrix element $\langle\alpha|H-E|\alpha_i\rangle$ integrates over the internal nuclear coordinates ξ, and yields a non-local function of R_x and R_{x_i} that is then integrated in a matrix element with $\chi^{(-)}_\alpha(R_x)$ and $\chi_{\alpha_i}(R_{x_i})$. As

discussed in section 3.2.2, the inner Hamiltonian H may be written in either *prior* or *post* forms. If we take the prior form of Eq. (3.2.49), and keep a diagonal optical potential U_α with each kinetic energy term, we have now

$$\begin{aligned}
\mathbf{T}^{\rm dw-prior}_{\alpha\alpha_i} &= -\frac{2\mu_\alpha}{\hbar^2 k_\alpha}\left\langle \chi^{(-)}_\alpha \left| \hat{N}_{\alpha\alpha_i}[T_{x_iL_i}+U_{\alpha_i}-E_{x_ip_it_i}] + \hat{V}^{x_i}_{\alpha\alpha_i}\right| \chi_{\alpha_i}\right\rangle \\
&= -\frac{2\mu_\alpha}{\hbar^2 k_\alpha}\left[\langle\chi^{(-)}_\alpha|\hat{V}^{x_i}_{\alpha\alpha_i}|\chi_{\alpha_i}\rangle + \langle\chi^{(-)}_\alpha|\hat{N}_{\alpha\alpha_i}|[T_{x_iL_i}+U_{\alpha_i}-E_{x_ip_it_i}]\chi_{\alpha_i}\rangle\right] \\
&= -\frac{2\mu_\alpha}{\hbar^2 k_\alpha}\langle\chi^{(-)}_\alpha|\hat{V}^{x_i}_{\alpha\alpha_i}|\chi_{\alpha_i}\rangle \qquad (3.3.62)
\end{aligned}$$

since the one-channel functions χ_{α_i} are found by $[T_{x_iL_i}+U_{\alpha_i}-E_{x_ip_it_i}]\chi_{\alpha_i}=0$. A similar calculation of the *post* DWBA matrix element yields

$$\begin{aligned}
\mathbf{T}^{\rm dw-post}_{\alpha\alpha_i} &= -\frac{2\mu_\alpha}{\hbar^2 k_\alpha}\left\langle \chi^{(-)}_\alpha \left| [T_{xL}+U_\alpha-E_{xpt}]\hat{N}_{\alpha\alpha_i} + \hat{V}^{x}_{\alpha\alpha_i}\right| \chi_{\alpha_i}\right\rangle \\
&= -\frac{2\mu_\alpha}{\hbar^2 k_\alpha}\langle\chi^{(-)}_\alpha|\hat{V}^{x}_{\alpha\alpha_i}|\chi_{\alpha_i}\rangle\ . \qquad (3.3.63)
\end{aligned}$$

We therefore see that in these first order DWBA expressions for for transfer reactions, the non-orthogonality terms $\hat{N}_{\alpha\alpha_i}$ disappear. Moreover, if both Eqs. (3.3.62) and (3.3.63) are derived consistently from Eq. (3.3.61), then the above derivations show that they must yield the same T matrix element. Neither of these conclusions are true for second- and higher-order DWBA calculations with transfer reactions, but the necessary post-prior agreement of first-order T (or S) matrix elements in all partial waves yields good checks on the accuracy of our calculations.

Approximate coupled channels solutions

As discussed on page 83, the result of these integral expressions may be equally obtained by solving inhomogeneous differential equations. This means that the above PWBA and DWBA approximations may be also reached by modifications to the coupled channels equations. In particular, the first-order DWBA result may be identically obtained by removing all couplings but keeping the diagonal potentials in the elastic (α_i) and final (α) channel (U_1), and keeping the couplings *from* the elastic channel *to* the final channel (U_2).

Allowing for a distinct potential U_{α_i} in the entrance channel, this modified coupled channels set is

$$\begin{aligned}
[T_{\alpha_i}+U_{\alpha_i}-E_{\alpha_i}]\psi_{\alpha_i} &= 0 \\
[T_\alpha\ +U_1\ -\ E_\alpha]\psi_\alpha\ \ &+\ \ U_2\ \psi_{\alpha_i}=0\ . \qquad (3.3.64)
\end{aligned}$$

These equations may be equivalently solved in three ways:

(i) By solving the differential equations according to the exact methods of section 6.3.2.

(ii) By solving the inhomogeneous differential equation (3.3.64) by the iterative method of section 6.3.3. The elastic channel wave function will be just the uncoupled solution $\psi_{\alpha_i} = \chi_{\alpha_i}$, and the final channel will be populated after the first iteration.

(iii) By evaluating the T-matrix for the final channel by the DWBA integral of Eq. (3.3.60).

For the restricted set of equations (3.3.64), which do not have the back couplings from the second to the first channel, these three methods will give identical results.

3.4 Identical particles

The *spin-statistics theorem* is a fundamental result in quantum field theory. This states that spin-half objects obey Fermi-Dirac statistics and have antisymmetric wave functions, whereas integer-spin objects obey Bose-Einstein statistics and have symmetric wave functions. An (anti-)symmetry of the collective wave functions means that, on interchanging the coordinates of any two particles, the wave function changes sign (antisymmetric for fermions), or remains the same (symmetric, for bosons).

Up to now we have not taken into account the Pauli Principle for identical fermions, such as for protons and for neutrons. This principle is most universally followed if the wave function for a set of identical particles is *antisymmetric* under the interchange of the coordinates of any pair of these particles.

3.4.1 Isospin

The proton and neutron are almost the same in mass ($\Delta m/m = 1.4 \times 10^{-3}$), and their different electric potentials and magnetic moments make only a small difference compared with the strong nuclear forces. This suggests treating them as identical in some sense, and including the electromagnetic effects (etc.) by perturbation theory.

The only sense that the neutron and proton need to be distinguished, then, is for the Pauli Principle, and to make antisymmetric wave functions. For this purpose (alone) we have the option of following the standard derivation of two 'states' for a *nucleon*, to be regarded as in one of two states depending on an *isobaric variable* τ_z. This distinguishes a neutron ($\tau_z = 1$) from

a proton ($\tau_z = -1$)†. Thus a full specification of a nucleon depends on position $\mathbf{r}$, spin z-component σ_z, *and* now also isospin z-component τ_z as $\psi(\mathbf{r}, \sigma_z, \tau_z)$.

If we define the neutron state vector as $|n\rangle = \begin{pmatrix}1\\0\end{pmatrix}$ and $|p\rangle = \begin{pmatrix}0\\1\end{pmatrix}$, then the $\hat{\tau}_z$ operator $\begin{pmatrix}1 & 0\\0 & -1\end{pmatrix}$ has as eigenstates the above vectors:

$$\hat{\tau}_z|n\rangle = +1\ |n\rangle \text{ and } \hat{\tau}_z|p\rangle = -1\ |p\rangle\ . \tag{3.4.1}$$

The $\hat{\tau}_z$ may be supplemented by $\hat{\tau}_x$ and $\hat{\tau}_y$ which follow the familiar algebra for components of a spin-1/2 particle, namely

$$\hat{\tau}_x = \begin{pmatrix}0 & 1\\1 & 0\end{pmatrix}; \quad \hat{\tau}_y = \begin{pmatrix}0 & -\mathrm{i}\\\mathrm{i} & 0\end{pmatrix} \tag{3.4.2}$$

satisfying the commutators $[\tau_p, \tau_q] = 2\mathrm{i}\tau_r$ for (pqr) cyclic permutations of (xyz), by analogy with the Pauli spin operators. This justifies the name of *isospin*. In terms of the original $|n\rangle$ and $|p\rangle$ states, the isospin operators may be written

$$\begin{aligned}\hat{\tau}_x &= |p\rangle\langle n| + |n\rangle\langle p|\\ \hat{\tau}_y &= \mathrm{i}[|p\rangle\langle n| - |n\rangle\langle p|]\\ \hat{\tau}_z &= |n\rangle\langle n| - |p\rangle\langle p|\ .\end{aligned} \tag{3.4.3}$$

From the $\hat{\tau}_i$ matrix operators, we obtain the *isotopic spin operators*

$$\hat{\mathbf{t}} = \frac{1}{2}\hat{\boldsymbol{\tau}} = \frac{1}{2}(\hat{\tau}_x, \hat{\tau}_y, \hat{\tau}_z)\ . \tag{3.4.4}$$

Since $\hat{t}^2 = 3/4$, the nucleon has total isospin $t = 1/2$, and z-components $m_t = t_z = +1/2$ for the neutron and $-1/2$ for the proton. The operators $\hat{t}_+ = t_x + \mathrm{i}t_y$ and $\hat{t}_- = t_x - \mathrm{i}t_y$ are the raising and lowering operators respectively, as from Eq. (3.4.3) we see that $\hat{t}_+ = \frac{1}{2}|n\rangle\langle p|$ and $\hat{t}_- = \frac{1}{2}|p\rangle\langle n|$.

Composite systems

For systems of two or more nucleons ($k = 1, 2, ..$), the isospins may be coupled to a total isospin

$$\hat{\mathbf{T}} = \sum_k \hat{\mathbf{t}}_k \tag{3.4.5}$$

with z-component $T_z = \frac{1}{2}(N - Z)$ for N neutrons and Z protons. For even numbers of nucleons, $T = 0, 1, ...$, and for odd numbers $T = \frac{1}{2}, \frac{3}{2}, ...$ Two

† This assignment is a matter of conventional choice

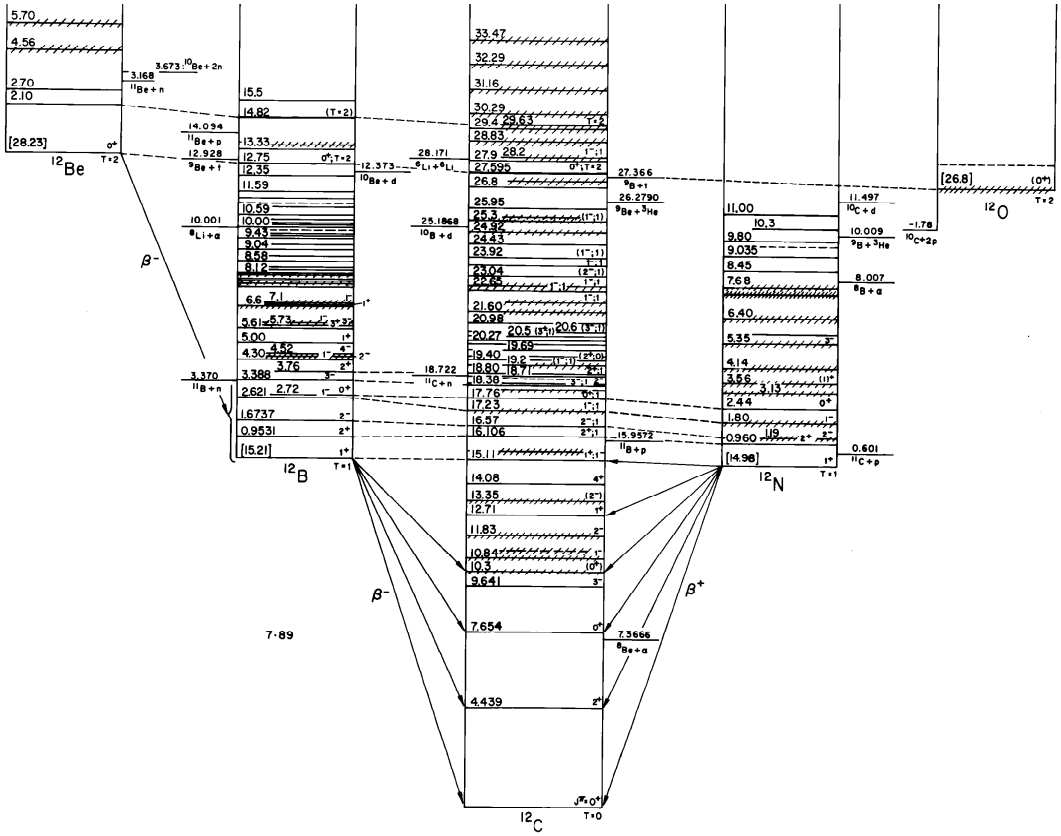

Fig. 3.7. The dashed lines indicate some of the isobaric analogue states in the $A = 12$ nuclear multiplet, from the compilation [14]. Each state is labeled by $J^\pi; T$ for total isospin T, where these are known.

neutrons have $T_z = 1$ and two protons have $T_z = -1$, and this is only possible if $T = 1$. A neutron and a proton together, by comparison, have $T_z = 0$, and hence either $T = 0$ or 1.

Antisymmetrisation can be applied to neutrons and to protons separately, but we can make for nucleons what Bohr and Mottelson [12] call a *generalised antisymmetrisation principle*, that the wave function for a set of fermions is antisymmetric with respect to the interchange of *all* coordinates (space, spin, *and* isospin) of any pair of nucleons.

Consider the case of two nucleons with coordinates $(\mathbf{r}_i, \sigma_{zi}, \tau_{zi})$, $i = 1, 2$. Antisymmetry requires $\Psi(1, 2) = -\Psi(2, 1)$. Let the spins s_1, s_2 be coupled to S, the isospins t_1, t_2 to T, the relative angular momentum be L, and

$\mathbf{L} + \mathbf{S} = \mathbf{J}$ the total spin. Then

$$\Psi_J(1,2) = [Y_L(\mathbf{R}) \otimes [s_1 \otimes s_2]_S]_J \; [t_1 \otimes t_2]_T \; , \tag{3.4.6}$$

which gives, on interchanging the particles 1 and 2,

$$\begin{aligned} \Psi_J(2,1) &= [Y_L(-\mathbf{R}) \otimes [s_2 \otimes s_1]_S]_J \; [t_2 \otimes t_1]_T \\ &= (-1)^L \; (-1)^{S-s_1-s_2} \; (-1)^{T-t_1-t_2} \Psi_J(1,2) \\ &= (-1)^{L+S+T} \Psi_J(1,2) \end{aligned} \tag{3.4.7}$$

as all $s_i = t_i = 1/2$. The factors like $(-1)^{S-s_1-s_2}$ come from the symmetry properties of the Clebsch-Gordon coefficients:

$$\langle s_1\mu_1, s_2\mu_2 | S\mu \rangle = (-1)^{S-s_1-s_2} \langle s_2\mu_2, s_1\mu_1 | S\mu \rangle. \tag{3.4.8}$$

Antisymmetrisation for two nucleons as fermions then requires that they be in a state where $L + S + T$ is *odd*.

For more complex nuclei composed of antisymmetric pairs of nucleons, T is still a good quantum number even though there are greater effects of Coulomb forces, which depend on the projections t_z. We find that isobaric sets of nuclei (those with constant A) have many sets of energy levels that are similar in absolute energy when $T > 0$ is a constant, and varying slightly only because of the additional Coulomb repulsion when a neutron is replaced by a proton. These sets of levels, illustrated for $T = 0$, 1 and 2 in Fig. 3.7, are called *isobaric analogue states*, and have very similar internal nuclear structure. There is little mixing between T values, only slight energy shifts that hardly change the structure.

3.4.2 Direct and exchange amplitudes in elastic scattering

The scattering analysis so far has dealt with reactions of the form $p + t \rightarrow p' + t'$ for projectile p, target t, ejectile p' and residue t' that are considered distinguishable nuclei. In the light of the previous section, however, we have to consider the cases of

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: $p' = t$ & $t' = p$, and p is distinguishable from t,

where p and t may be clusters, not just individual nucleons. This is a way of taking into account one important overall property of clusters without considering their internal structure in detail. If the nuclei were distinguishable, the wave function $\Psi^{M_{\rm tot}}_{xJ_{\rm tot}}(\mathbf{R}_x, \xi_p, \xi_t)$ for their combination in a system

would simply be the product of their separate states ϕ_{J_p} and ϕ_{J_t} with angular momentum and orbital factors as in section 3.2.1. Now, however, we cannot always use such as product wave function if we are to satisfy the Pauli Principle.

Let us define an 'exchange index' $\epsilon = +1$ for boson-boson and $\epsilon = -1$ for fermion-fermion collisions, so the a) and b) cases may be considered with one formalism. Define the operator $\hat{P}_{pt}$ which exchanges projectile and target coordinates in the wave function of the combined system. The spin-statistics theorem implies that $\epsilon = (-1)^{2J_p}$, where J_p is the overall spin of the projectile. A complete wave function Ψ_ϵ should therefore satisfy $\hat{P}_{pt}\Psi_\epsilon(\mathbf{R}) = \epsilon\Psi_\epsilon(-\mathbf{R})$, or

$$\hat{P}_{pt}\Psi^{M_{\rm tot}}_{xJ_{\rm tot}}(\mathbf{R}_x, \xi_p, \xi_t) = \epsilon\Psi^{M_{\rm tot}}_{xJ_{\rm tot}}(-\mathbf{R}_x, \xi_t, \xi_p). \tag{3.4.9}$$

Identical spinless scattering

Consider first the simple case of spinless scattering†, but keep explicit reference to ϵ. The asymptotic form for non-identical scattering on spherical potentials is given by of Eq. (2.4.12), namely

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

so a suitable wave function for identical particles is

$$\Psi^{\rm asym}_\epsilon(\mathbf{R}) = \psi^{\rm asym}(\mathbf{R}) + \epsilon\ \psi^{\rm asym}(-\mathbf{R}) . \tag{3.4.10}$$

We now calculate the initial flux j_i and final angular flux $\hat{j}_f$, in order to calculate the cross section $\sigma = \hat{j}_f/j_i$. The incident wave is

$$\Psi^{\rm inc}_\epsilon(\mathbf{R}) = A[\mathrm{e}^{\mathrm{i}kz} + \epsilon\ \mathrm{e}^{-\mathrm{i}kz}] \tag{3.4.11}$$

and the scattered outgoing radial wave is

$$\Psi^{\rm out}_\epsilon(\mathbf{R}) = A[f(\theta) + \epsilon f(\pi-\theta)]\frac{\mathrm{e}^{\mathrm{i}kR}}{R} \equiv Af_\epsilon(\theta)\frac{\mathrm{e}^{\mathrm{i}kR}}{R} . \tag{3.4.12}$$

The total flux in $\Psi^{\rm inc}_\epsilon(\mathbf{R})$ is numerically zero. Goldberger and Watson give more detailed analysis using wave packets [13, §4.3], which shows that that the incident flux is a combination of a projectile flux $\frac{\hbar k}{\mu}|A|^2$ in the $+z$ direction, and an (identical) target flux in the $-z$ direction. The projectile flux in the beam is therefore $j_i = \frac{\hbar k}{\mu}|A|^2$. The scattered flux is $\hat{j}_f = \frac{\hbar k}{\mu}|A|^2|f_\epsilon(\theta)|^2$, so the needed cross section for identical particle scattering is

$$\begin{aligned} \sigma(\theta) &= |f_\epsilon(\theta)|^2 = |f(\theta) + \epsilon f(\pi-\theta)|^2 && (3.4.13)\\ &= |f(\theta)|^2 + |f(\pi-\theta)|^2 + 2\epsilon\,\mathrm{Re}f(\theta)^* f(\pi-\theta) . && (3.4.14)\end{aligned}$$

† This section is thus strictly applicable only to boson scattering, but the exercise is useful.

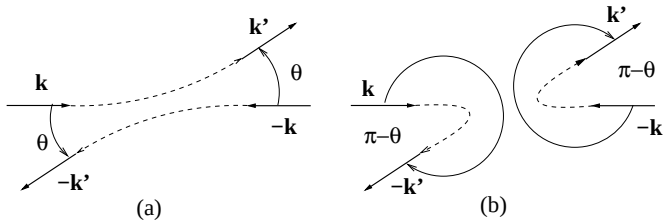

Fig. 3.8. Direct (a) and exchange (b) paths which interfere with each other, in the scattering of identical particles from c.m. momenta $\pm\mathbf{k}$ to $\pm\mathbf{k}'$ or $\mp\mathbf{k}'$, after scattering by angles θ or $\pi - \theta$.

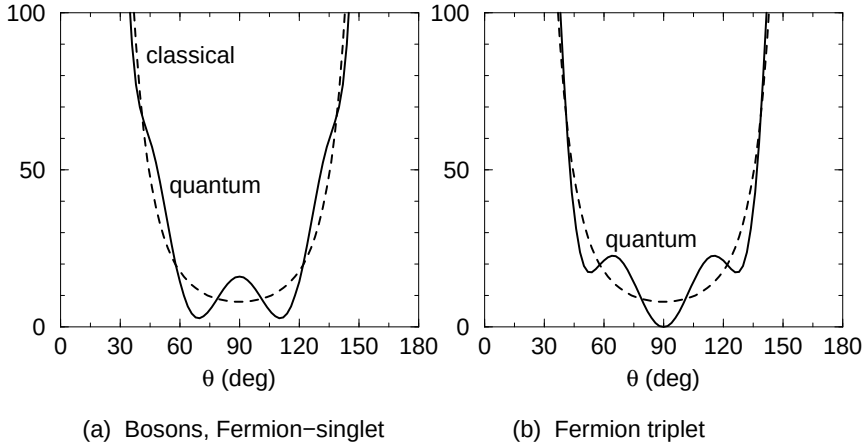

Fig. 3.9. Boson (a) and fermion triplet (b) nucleon-nucleon scattering cross sections, assuming pure Coulomb scattering with $\eta = 5$. Case (a) also applies for fermion singlet scattering. The cross section is in units of $\eta^2/4k^2$.

Fig. 3.8 shows interfering classical paths.

Since $P_L(\cos(\pi-\theta)) = (-1)^L P_L(\cos\theta)$, the new amplitude has the partial wave expansion

$$f_\epsilon(\theta) = \frac{1}{k}\sum_{L=0}^{\infty}(2L+1)P_L(\cos\theta)\mathbf{T}_L[1+\epsilon(-1)^L] \ , \tag{3.4.15}$$

where $\mathbf{T}_L$ is the scattering T matrix that would be obtained if the particles were distinguishable. This implies for the scattering of identical bosons, where $\epsilon = 1$, that odd partial waves should be removed, and that the *amplitude* for the remaining even partial waves should be doubled.

Identical particles with spin

The above analysis for $J_p = J_t = 0$ is necessarily restricted to $\epsilon = 1$ for identical bosons. For identical fermions it is essential to include spin. This is easiest in the S (channel spin) partial wave basis, where the effect of the $\hat{P}_{pt}$ exchange operator is

$$\hat{P}_{pt}|L(J_p, J_t)S; J_{\rm tot}x\rangle = (-1)^L(-1)^{S-J_p-J_t}\epsilon|L(J_t, J_p)S; J_{\rm tot}x\rangle \quad (3.4.16)$$

with the radial wave function itself, $\psi_\epsilon(R_x)$, not being affected. The $(-1)^L$ factor comes from reversing the direction of the radius vector in the spherical harmonic, and $(-1)^{S-J_p-J_t}$ comes from reordering the coupling of particle spins to make the channel spin. The expression like Eq. (3.4.15)) for the scattering amplitude is therefore different for different channel spin values S:

$$\begin{aligned} f_S(\theta) &= \frac{1}{k}\sum_{L=0}^{\infty}(2L{+}1)P_L(\cos\theta)\mathbf{T}_L[1+\epsilon(-1)^{L+S-J_p-J_t}] \\ &= \frac{1}{k}\sum_{L=0}^{\infty}(2L{+}1)P_L(\cos\theta)\mathbf{T}_L[1+(-1)^{L+S}] \end{aligned} \quad (3.4.17)$$

since $J_p = J_t$ and $\epsilon = (-1)^{2J_p}$ for two identical particles. (This formula holds for bosons if we set $S = 0$ in that case.) The partial waves that give non-zero scattering are those with $L + S$ even. We say that the partial waves with $L + S$ odd are *blocked* by the Pauli Principle. Nucleon-nucleon scattering, for example, is thus different in singlet ($S = 0$) and triplet ($S = 1$) states, and gives rise to the characteristic interference patterns shown in Fig. 3.9. The singlet scattering on the left is the same as would be obtained for the scattering of two bosons.

We can repeat the above analysis using a total isospin T for the combined projectile and target system, and we will find that the allowed partial waves are those with $L + S + T$ odd. Two colliding neutrons or protons require $T = 1$, so this the same conclusion as above.

If there are spin-dependent forces (such as the spin-orbit or tensor forces to be defined in the next chapter) then full multichannel scattering theory must be used, not the simplified theory above where the T matrix only depends on L.

3.4.3 Integrated cross sections

The definition of angle-integrated cross sections has to be specified carefully for identical particles, since for every nucleus removed from the beam, the

elastic scattering produces *two* identical nuclei to be detected. The differential cross section $\sigma(\theta) = |\tilde{f}_S(\theta)|^2$ measures the outgoing probability of detecting a specified product no matter how it was produced, but now the angular integral of this can be more than the flux leaving the initial beam! By convention, we resolve this discrepancy by *defining* the elastic $\sigma_{\rm el}$ as the cross section for removal from the *beam*. Then, using Eq. (3.4.17) in an derivation like that for Eq. (3.1.50),

$$\sigma_{\rm el} = \frac{1}{2}\int_0^{2\pi} d\phi \int_0^{\pi} {\rm d}\theta \sin\theta \ \sigma(\theta) \tag{3.4.18}$$

$$= 2\frac{\pi}{k^2} \sum_{L+S \text{ even}} (2L{+}1)|1 - \mathbf{S}_L|^2 \ . \tag{3.4.19}$$

The reaction cross section is given by a similar expression

$$\sigma_R = 2\frac{\pi}{k^2} \sum_{L+S \text{ even}} (2L{+}1)[1 - |\mathbf{S}_L|^2] \ . \tag{3.4.20}$$

The same definition is used for the non-elastic products from the reaction of two identical nuclei. The cross sections $\sigma_{xpt:x_ip_it_i}$ from incoming channel $x_ip_it_i$ to exit channel xpt are defined as the flux from the beam of *projectiles* that goes to the exit channel. If the projectile and target are identical, then, in order that individual cross sections add up to this above total, the relation between the transition S matrix elements and the angle-independent cross sections must be

$$\sigma_{xpt:x_ip_it_i} = \frac{\pi}{k_i^2}\frac{1+\delta_{p_it_i}}{(2J_{p_i}{+}1)(2J_{t_i}{+}1)} \sum_{J_{\rm tot}\pi\alpha\alpha_i} (2J_{\rm tot}{+}1)|\tilde{\mathbf{S}}^{J_{\rm tot}\pi}_{\alpha\alpha_i}|^2. \tag{3.4.21}$$

The generalised extra factor $1 + \delta_{p_it_i}$ doubles the cross section when the projectile and the target are identical *and* in the same excited state. This equation assumes that S matrix elements have been set to zero for those partial waves blocked by the Pauli Principle in either the entrance channel α_i or the exit channel α (or, suitable linear combinations set to zero, depending on the choice of partial wave basis).

We still have the detailed balance $|\tilde{\mathbf{S}}_{\alpha\alpha_i}|^2 = |\tilde{\mathbf{S}}_{\alpha_i\alpha}|^2$, so the reverse cross section should now be related not by Eq. (3.2.64) but by

$$\sigma_{x_ip_it_i:xpt} = \frac{k_i^2\ (1+\delta_{pt})\ (2J_{p_i}{+}1)(2J_{t_i}{+}1)}{k^2\ (1+\delta_{p_it_i})\ (2J_p{+}1)(2J_t{+}1)}\sigma_{xpt:x_ip_it_i} \tag{3.4.22}$$

to the forward cross section $\sigma_{xpt:x_ip_it_i}$. The new factors will appear again in Chapter 12 when we use the cross sections to find reaction rates in gases, and will in fact be cancelled in their effect.

3.4.4 Exchange transfer

This occurs in transfer reactions such as ^{6}He + ^{4}He $\rightarrow$ ^{4}He + ^{6}He, where the transfer process adds coherently to the elastic scattering amplitude, but with revised relative coordinate. In general, consider $p+t \rightarrow t'+p'$ reactions where the primes indicate the transfer channels. We construct a total wave function

$$\Psi_\epsilon = \psi_{pt} + \epsilon \hat{P}_{p't'} \psi_{t'p'} \tag{3.4.23}$$

where $\epsilon = 1$ for $p \neq t$ and $\epsilon = (-1)^{2J_p}$ for $p = t$, and where again $\hat{P}_{p't'}$ is operator which exchanges the p' and t' nuclear coordinates. In the S basis, we saw that $\hat{P}_{pt}\psi_{tp}$ generates a diagonal factor $(-1)^{L+S-J_p-J_t}$. In the J basis, it generates a linear combination of $|\alpha\rangle$ basis states. The effect of elastic transfer is generally to give a backward-angle peak in the elastic scattering distribution.

3.5 Electromagnetic channels

3.5.1 Maxwell equations and photon channels

The Maxwell equations for the magnetic **H** and electric **E** field vectors are, in Gaussian units,

$$\begin{aligned} \nabla \times \mathbf{H} &= \frac{4\pi}{c}\mathbf{j} + \frac{1}{c}\frac{\mathrm{d}\mathbf{E}}{\mathrm{d}t} \\ \nabla \times \mathbf{E} &= -\frac{1}{c}\frac{\mathrm{d}\mathbf{H}}{\mathrm{d}t} \\ \nabla \cdot \mathbf{H} &= 0 \\ \nabla \cdot \mathbf{E} &= 4\pi\rho \ , \end{aligned} \tag{3.5.1}$$

where the source terms **j** and ρ are the charge current and charge density respectively. These describe the classical electromagnetic field surrounding a nucleus. At low velocities, this is predominantly the electrostatic field arising from ρ, the charge density of the protons in the nucleus.

In addition to this electrostatic field, there can be radiative photons of higher energies produced by capture reactions, and similar photons that may lead to the breakup of nuclei. To a first approximation, these need only be considered one at a time, since (unlike a coherent laser field), radiative photons will generally react individually. In this section, therefore, we consider the coupling of *one radiative photon* with the charges in a nucleus that may lead to its excitation, and also the reverse: the production of a photon by a decaying nuclear state. The higher energy states in a nucleus may be in the continuum, in which case these reactions are photodisintegration and

photoproduction reactions, respectively. The photon by itself will have a specific energy $E = \hbar\omega$ and momentum $p_\gamma = \hbar k_\gamma = E_\gamma/c$.

Vector potential

We define, in the standard manner, the *vector potential* $\mathbf{A}(t)$ and *scalar potential* $\phi(t)$ such that

$$\mathbf{H} = \nabla \times \mathbf{A}(t) \ , \tag{3.5.2a}$$

$$\mathbf{E} = -\nabla\phi(t) - \frac{1}{c}\frac{\mathrm{d}\mathbf{A}}{\mathrm{d}t} \ . \tag{3.5.2b}$$

Substituting these into the Maxwell equations (3.5.1) we find

$$\nabla^2\mathbf{A}(t) + \frac{1}{c^2}\frac{\mathrm{d}^2\mathbf{A}}{\mathrm{d}t^2} = -\frac{4\pi}{c}\mathbf{j} + \nabla(\nabla\cdot\mathbf{A}(t)) + \frac{1}{c}\nabla\frac{\mathrm{d}\phi}{\mathrm{d}t} \tag{3.5.3}$$

$$\nabla^2\phi(t) = -4\pi\rho(t) - \frac{1}{c}\frac{\mathrm{d}}{\mathrm{d}t}(\nabla\cdot\mathbf{A}(t)) \ , \tag{3.5.4}$$

where we have used the identity $\nabla\times(\nabla\times\mathbf{A}) = \nabla(\nabla\cdot\mathbf{A}) - \nabla^2\mathbf{A}$.

The potentials $\mathbf{A}(t)$ and $\phi(t)$ are not fixed, but may be changed according to some arbitrary spatial *gauge* function $\chi(t)$ by

$$\mathbf{A}'(t) = \mathbf{A}(t) + \nabla\chi(t) \tag{3.5.5}$$

$$\phi'(t) = \phi(t) + \partial\chi(t)/\partial t \ . \tag{3.5.6}$$

This means that we are free to choose the gauge $\chi(t)$, for example so that

$$\nabla\cdot\mathbf{A}(t) = 0 \ , \tag{3.5.7}$$

which is called the *Coulomb* or *transverse gauge*. In this gauge, the scalar potential satisfies Poisson's equation

$$\nabla^2\phi(t) = -4\pi\rho(t) \tag{3.5.8}$$

and the vector potential satisfies an inhomogeneous wave equation

$$\nabla^2\mathbf{A}(t) + \frac{1}{c^2}\frac{\mathrm{d}^2\mathbf{A}}{\mathrm{d}t^2} = -\frac{4\pi}{c}\mathbf{j} + \frac{1}{c}\nabla\frac{\mathrm{d}\phi}{\mathrm{d}t} \ . \tag{3.5.9}$$

We now make our physical approximation, separating the electrostatic field caused by the charges ρ from the radiative photon that couples to the current $\mathbf{j}$. In this case, ϕ becomes time-independent like ρ, and the electromagnetic wave equation for a radiative single photon becomes

$$\nabla^2\mathbf{A}(t) + \frac{1}{c^2}\frac{\mathrm{d}^2\mathbf{A}}{\mathrm{d}t^2} = -\frac{4\pi}{c}\mathbf{j} \ . \tag{3.5.10}$$

For a fixed monochromatic photon energy $E_\gamma = \hbar\omega$, we can write the time-dependent vector potential $\mathbf{A}(t)$ in terms of a time-independent $\mathbf{A}$ and current $\mathbf{j}$ as

$$\mathbf{A}(t) = \mathbf{A}\mathrm{e}^{-i\omega t} + \mathbf{A}^*\mathrm{e}^{\mathrm{i}\omega t} \tag{3.5.11}$$

$$\mathbf{j}(t) = \mathbf{j}\mathrm{e}^{-i\omega t} + \mathbf{j}^*\mathrm{e}^{\mathrm{i}\omega t} \ . \tag{3.5.12}$$

The wave equation for the stationary state $\mathbf{A}$ vector potential is thus

$$\nabla^2\mathbf{A} + k_\gamma^2\mathbf{A} = -\frac{4\pi}{c}\mathbf{j} \ . \tag{3.5.13}$$

3.5.2 Coupling photons and particles

This classical description of the electromagnetic field will now be connected to a quantum description of the particle dynamics, by using for the source flux $\mathbf{j}$ the quantum mechanical matrix element, at each spatial position $\mathbf{r}$, of the electric form of the general current operator of Eq. (3.1.100)

$$\mathbf{j}(\mathbf{r}) = \langle\Phi|\hat{\mathbf{j}}_q(\mathbf{r})|\Psi\rangle \ . \tag{3.5.14}$$

where both $\Phi(\mathbf{r}_i)$ and $\Psi(\mathbf{r}_i)$ are wave functions depending in vector positions such as $\mathbf{r}_i$ for each charged particle i, and the bra-ket implies integration over all the $\mathbf{r}_i$. Both $\mathbf{r}$ and all the $\mathbf{r}_i$ are actual positions in the centre of mass frame, not relative coordinates.

In the free field case this matrix element is that of $\hat{\mathbf{j}}_q = q\hat{\mathbf{j}}_{\mathrm{free}}$,

$$\langle\Phi|q\hat{\mathbf{j}}_{\mathrm{free}}|\Psi\rangle = \frac{\hbar q}{2\mathrm{i}\mu}\left[\Phi^*(\nabla\Psi) - (\nabla\Phi)^*\Psi\right] \ . \tag{3.5.15}$$

The bra and ket wave functions are allowed to be different, giving off-diagonal matrix elements whereby electromagnetic effects of particle *transitions* may be described.

Photo-production

Photonuclear couplings may work in two directions. A current of charged particles may produce photons, for example in the *photo-production* reaction ^{7}Be(p,γ)^{8}B. At other times, the photons may cause the movement of charged particles and the breakup of bound states as in ^{8}B(γ,p)^{7}Be, and this is called *photo-disintegration* and described in the following subsection.

The coupling from particle current to photon production, for particle initial scattering state Ψ and final bound state Φ_b, is therefore described by

$$\nabla^2\mathbf{A} + k_\gamma^2\mathbf{A} \ = \ -\frac{4\pi}{c}\langle\Phi_b|\hat{\mathbf{j}}_{\mathrm{free}}|\Psi\rangle \ . \tag{3.5.16}$$

It is convenient to multiply this equation by $-\hbar c/k_\gamma$, so that the coefficient of $\mathbf{A}$ becomes $\hbar c/k_\gamma \times k_\gamma^2 = \hbar c k_\gamma = E_\gamma$, and has the same units of energy as in a Schrödinger equation:

$$\left[-\frac{\hbar c}{k_\gamma}\nabla^2 - E_\gamma\right]\mathbf{A}(\mathbf{r}) = \frac{4\pi\hbar}{k_\gamma}\langle\Phi_b|\hat{\mathbf{j}}_{\rm free}(\mathbf{r})|\Psi\rangle \ . \tag{3.5.17}$$

This equation has the form of a particle-to-photon coupled equation, linking the initial particle state Ψ to an outgoing photon field $\mathbf{A}$ with an 'interaction Hamiltonian' $H_{\gamma p} = \frac{4\pi\hbar}{k_\gamma}\langle\Phi_b|\hat{\mathbf{j}}_{\rm free}|$.

Photo-disintegration

The standard *minimal gauge coupling* describing the influence of an electromagnetic field on particle motion is found by transforming the Schrödinger equation $[\hat{\mathbf{p}}^2/2m + V - E]\Psi = 0$ by the 'minimal' replacement

$$\hat{\mathbf{p}} \to \hat{\mathbf{p}} - \frac{q}{c}\mathbf{A} \ , \tag{3.5.18}$$

where $\mathbf{A}$ is the vector potential for the electromagnetic field. Expanding the square we have

$$\left[\frac{1}{2\mu}\left(\hat{\mathbf{p}}^2 - \frac{q}{c}\{\mathbf{A}\cdot\hat{\mathbf{p}} + \hat{\mathbf{p}}\cdot\mathbf{A}\} + \frac{q^2}{c^2}|\mathbf{A}|^2\right) + V - E\right]\Psi = 0 \ . \tag{3.5.19}$$

Neglecting the $|\mathbf{A}|^2$ term according to our one-photon approximation, using $\hat{\mathbf{p}} = \hbar/\mathrm{i}\,\overrightarrow{\nabla}$ this particle equation becomes

$$\begin{aligned}
[\hat{T} + V - E]\Psi &= \frac{1}{2\mu}\frac{q}{c}\frac{\hbar}{\mathrm{i}}\{\mathbf{A}\cdot\overrightarrow{\nabla} + \overrightarrow{\nabla}\cdot\mathbf{A}\}\Psi \\
&= \frac{1}{2\mu}\frac{q}{c}\frac{\hbar}{\mathrm{i}}\{\mathbf{A}\cdot\overrightarrow{\nabla} - \overleftarrow{\nabla}\cdot\mathbf{A}\}\Psi \\
&= \frac{1}{c}\int \mathrm{d}\mathbf{r}\mathbf{A}(\mathbf{r})\cdot\hat{\mathbf{j}}^q_{\rm free}(\mathbf{r})\ \Psi
\end{aligned} \tag{3.5.20}$$

where in the second step we use integration by parts, assuming that in any matrix element the product of both the initial and final wave functions goes to zero asymptotically, which is true for transitions to or from bound states. In the final step we used the electric current operator $\hat{\mathbf{j}}^q_{\rm free}(\mathbf{r})$ defined in Eq. (3.1.98), with a charge q factor.

If the potential V in the Schrödinger equation is non-local, then it will be momentum-dependent, and strictly we should perform the minimal replacement of Eq. (3.5.18) in these operators as well. Without knowing the details of the non-locality we cannot give a general derivation, so for now we will assume that the effect of these non-localities is to supplement the free

current operator in Eq. (3.5.20) by the 'two-body current' terms $\hat{\mathbf{j}}_2$ discussed in section 3.1.4. This gives the more general photo-disintegration result of

$$[\hat{T}+V-E]\Psi-\frac{1}{c}\int \mathrm{d}\mathbf{r}\mathbf{A}(\mathbf{r})\cdot\hat{\mathbf{j}}(\mathbf{r})\ \Psi=0\ . \tag{3.5.21}$$

For a photo-disintegration reaction with particle initial state Φ_b and final scattering state Ψ, this equation is often used in the form

$$[\hat{T}+V-E]\Psi-\frac{1}{c}\int \mathrm{d}\mathbf{r}\ \mathbf{A}(\mathbf{r})\cdot\hat{\mathbf{j}}(\mathbf{r})\ \Phi_b=0\ , \tag{3.5.22}$$

where we have an effective 'interaction Hamiltonian' $H_{\rm int}=-\frac{1}{c}\mathbf{A}\cdot\hat{\mathbf{j}}$ that couples between two particle states.

Equally, if Eq. (3.5.20) is written as

$$[\hat{T}+V-E]\Psi-\frac{1}{c}\int \mathrm{d}\mathbf{r}\ \hat{\mathbf{j}}(\mathbf{r})\Phi_b\cdot\mathbf{A}(\mathbf{r})=0\ , \tag{3.5.23}$$

for fixed initial particle state Φ_b, then this again appears as an equation coupling the incoming photon field $\mathbf{A}$ to the particle state Ψ in the continuum. The coupling operator is $H_{p\gamma}=-\frac{1}{c}\int \mathrm{d}\mathbf{r}\ \hat{\mathbf{j}}(\mathbf{r})\Phi_b\cdot$.

3.5.3 Photon cross sections

When the photon outgoing wave is $\mathbf{A}$ in direction $\mathbf{k}$, so $\mathbf{A}(\mathbf{r})=\mathbf{a}\mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{r}}$, the cross section depends on the *number flux* of photons. In order to determine this from the magnitude of $\mathbf{A}$, we calculate the Poynting vector, which is the energy flux, and then divide by the energy of each photon.

Given $\mathbf{A}$, the physical vector potential of Eq. (3.5.11) is

$$\begin{aligned}\mathbf{A}(t) &= 2\mathrm{Re}(\mathbf{A}\mathrm{e}^{-i\omega t})\\ &= 2\mathrm{Re}(\mathbf{a}\mathrm{e}^{\mathrm{i}(\mathbf{k}\cdot\mathbf{r}-\omega t)})\\ &= 2\mathbf{a}\cos(\mathbf{k}\cdot\mathbf{r}-\omega t)\ .\end{aligned} \tag{3.5.24}$$

The time independence of ϕ, as used to derive Eq. (3.5.10), thus uses

$$\mathbf{E}(t) = -\nabla\phi(t)-\frac{1}{c}\frac{\mathrm{d}\mathbf{A}}{\mathrm{d}t}$$

$$\text{to give}\quad \mathbf{E}(t) = 2k_\gamma\mathbf{a}\sin(\mathbf{k}\cdot\mathbf{r}-\omega t) \tag{3.5.25}$$

$$\text{and}\quad \mathbf{H}(t) = 2(\mathbf{k}\times\mathbf{a})\sin(\mathbf{k}\cdot\mathbf{r}-\omega t)\ . \tag{3.5.26}$$

The Poynting vector is

$$\mathbf{S}=\frac{c}{4\pi}\mathbf{E}\times\mathbf{H}\ . \tag{3.5.27}$$

Far from the source, where the radiative field has **E** and **H** mutually perpendicular, the magnitudes $|\mathbf{H}|$ and $|\mathbf{E}|$ become equal, so

$$|\mathbf{S}| \simeq \frac{c}{4\pi}|\mathbf{E}|^2 = \frac{c}{4\pi}|\mathbf{H}|^2 \ . \tag{3.5.28}$$

As $\langle|\sin(t)|^2\rangle = 1/2$, the time-averaged $\langle|\mathbf{E}(t)|^2\rangle = \frac{1}{2}|2k_\gamma \mathbf{a}|^2 = 2k_\gamma^2|\mathbf{a}|^2$, and the time-averaged energy flux is

$$\langle|\mathbf{S}(t)|\rangle = \frac{k_\gamma^2 c}{2\pi}|\mathbf{a}|^2 \ . \tag{3.5.29}$$

Dividing by the photon energy $E_\gamma = \hbar k_\gamma c$, we find the outgoing photon number flux

$$j_\gamma = \frac{k_\gamma}{2\pi\hbar}|\mathbf{a}|^2 \ . \tag{3.5.30}$$

Because the flux has factors additional to the usual expression of Eq. (2.4.1) in quantum mechanics, it is now convenient to define a vector *photon wave function*

$$\mathbf{Z}(\mathbf{r}) = \sqrt{\frac{k_\gamma}{2\pi\hbar c}}\ \mathbf{A}(\mathbf{r}) \tag{3.5.31}$$

so that photon number density is simply $|\boldsymbol{Z}(\mathbf{r})|^2$, and the photon number flux now appears as should be expected:

$$j_\gamma = c|\mathbf{Z}(\mathbf{r})|^2 \ . \tag{3.5.32}$$

By Eq. (2.4.1) this is appropriate for a quantum mechanical object moving at the speed of light c.

In terms of this new photon wave function, the photo-production 'coupled equation' (3.5.17) becomes

$$\begin{aligned}\left[-\frac{\hbar c}{k_\gamma}\nabla^2 - E_\gamma\right]\mathbf{Z}(\mathbf{r}) &= \sqrt{\frac{k_\gamma}{2\pi\hbar c}}\frac{4\pi\hbar}{k_\gamma}\langle\Phi_b|\hat{\mathbf{j}}(\mathbf{r})|\Psi\rangle \\ &= 2\sqrt{\frac{2\pi\hbar}{k_\gamma c}}\langle\Phi_b|\hat{\mathbf{j}}(\mathbf{r})|\Psi\rangle \\ &= 2\sqrt{h/\omega}\langle\Phi_b|\hat{\mathbf{j}}(\mathbf{r})|\Psi\rangle \ ,\end{aligned} \tag{3.5.33}$$

and the photo-disintegration equation (3.5.23) becomes

$$\begin{aligned}[\hat{T} + V - E]\Psi &= \sqrt{\frac{2\pi\hbar c}{k_\gamma}}\frac{1}{c}\int \mathrm{d}\mathbf{r}\ \hat{\mathbf{j}}(\mathbf{r})\Phi_b \cdot \mathbf{Z} \\ &= \sqrt{h/\omega}\int \mathrm{d}\mathbf{r}\ \hat{\mathbf{j}}(\mathbf{r})\Phi_b \cdot \mathbf{Z}\end{aligned} \tag{3.5.34}$$

These two equations (3.5.33, 3.5.34) have *almost* the same kind of coupling interaction, namely the operators

$$V_{\gamma p} = 2\sqrt{h/\omega}\langle\Phi_b|\hat{\mathbf{j}}(\mathbf{r}) \ , \tag{3.5.35}$$

$$V_{p\gamma} = \sqrt{h/\omega}\int \mathrm{d}\mathbf{r}\ \hat{\mathbf{j}}(\mathbf{r})\Phi_b\cdot \tag{3.5.36}$$

respectively, using the bound particle state Φ_b in each case. The factor of 2 difference in magnitude of these two couplings arises from the relativistic kinematics for photons, as explained in the chapter Appendix.

The electromagnetic coupling operators of Eq. (3.5.35) are written in their *current* form, as they use the derivative current operator of Eq. (3.1.98). This is commonly judged as too complicated for everyday use, so in section 4.7 an approximate form for the couplings will be derived. This form will be valid for long photon wavelengths (low energy photons).

3.5.4 Partial waves and vector spherical harmonics

The photon vector potential $\mathbf{A}(\mathbf{r})$ and its normalised form $\mathbf{Z}(\mathbf{r})$ are described by a three-dimensional vector at every spatial position $\mathbf{r}$. These three coordinates may be equivalently mapped onto the three m-state amplitudes $\mu = -1, 0, +1$ for the photon as a spin-1 object. Let $\boldsymbol{\xi}_\mu$ be three (complex) unit vectors in 3D space, such that the complex coefficients Z_μ in $\mathbf{Z} = \sum_\mu Z_\mu \boldsymbol{\xi}_\mu$ in this basis transform as the components of a spin-1 vector. One choice for the $\boldsymbol{\xi}_\mu$ is

$$\boldsymbol{\xi}_0 = \hat{\mathbf{z}} \quad \text{and} \quad \boldsymbol{\xi}_{\pm 1} = \mp(\hat{\mathbf{x}} \pm i\hat{\mathbf{y}})/\sqrt{2} \ . \tag{3.5.37}$$

The vector field $\mathbf{Z}(\mathbf{r})$ can therefore be expanded as the coupling of a spatial angular momentum Λ with photon spin 1 to form a total spin J_γ. In a capture or disintegration reaction, this is coupled with the spin J_b of the bound state to give $J_{\rm tot}$, the total angular momentum which must equal that from the particle scattering channel, $|\alpha\rangle = |(LJ_p)J_a, J_t; J_{\rm tot}\rangle$. In the normal manner of section 3.2.1 we use partial wave expansions to write the total wave function as a sum of photon (γ) and particle (p) channels as

$$\begin{aligned}
\Psi^{M_{\rm tot}}_{J_{\rm tot}} &= \Psi^{M_{\rm tot}}_{\gamma J_{\rm tot}} + \Psi^{M_{\rm tot}}_{pJ_{\rm tot}} \\
&= \sum_{\Lambda J_\gamma b} |(\Lambda 1)J_\gamma, J_b; J_{\rm tot}\rangle \zeta_\gamma(r)/r + \sum_{LJxpt} |(LJ_p)J_a, J_t; J_{\rm tot}\rangle \psi_\alpha(R)/R \\
&\equiv \sum_\gamma |\gamma\rangle\zeta_\gamma(r)/r + \sum_\alpha |\alpha\rangle\psi_\alpha(R)/R
\end{aligned} \tag{3.5.38}$$

where $|\gamma\rangle$ refers to the set of photon partial waves, as well as coupling to the spin J_b of the bound state $\Phi_b(\mathbf{R})$. Both the $|\gamma\rangle$ and $|\alpha\rangle$ contain just the *angular* part of the basis states, with $\zeta_\gamma(r)$ and $\psi_\alpha(R)$ being the respective radial parts. As usual, the particle channels are written using the relative separation R instead of the distance r from the centre of mass, but these are linearly proportional.

The coupled state $|(\Lambda 1)J_\gamma\rangle$ in Eq. (3.5.38) is often called a *vector spherical harmonic*, explicitly the basis component

$$\mathbf{Y}^M_{\Lambda J}(\hat{\mathbf{r}}) = |(\Lambda 1)J\rangle = \sum_{m\mu} \langle \Lambda m, 1\mu | JM\rangle \; \boldsymbol{\xi}_\mu \; Y^m_\Lambda(\hat{\mathbf{r}}) \tag{3.5.39}$$

that includes the photon vector states $\boldsymbol{\xi}_\mu$. It is defined for each $\Lambda = J_\gamma{-}1$, J_γ, $J_\gamma{+}1$, and has spatial parity $(-1)^\Lambda$. The vector spherical harmonics transform under coordinate rotations by the normal rotation matrices $D^{J_\gamma}_{MM'}(\mathcal{R})$ for a spin-J_γ object.

The electromagnetic field $\mathbf{Z}(\mathbf{r})$ can therefore be expanded in vector spherical harmonics, with a sum over a range of Λ and J_γ values. The J_γ value gives the total spin or *multipole* of the photon, and the spatial form of that multipole is determined by the Λ value in the range $|J_\gamma{-}1| \le \Lambda \le J_\gamma{+}1$.

Using Eq. (3.5.38), the coupled equations of Eqs. (3.5.33) and (3.5.34) may be rewritten in terms of radial functions for each partial wave $|\gamma\rangle$ and $|\alpha\rangle$:

$$\begin{aligned} [T_\Lambda - E_\gamma] \; \zeta_\gamma(r) &= \sum_\alpha \langle \gamma | V_{\gamma p} | \alpha \rangle \; \psi_\alpha(R) \\ [T_\alpha + V_\alpha - E_\alpha] \; \psi_\alpha(R) &= \sum_\gamma \langle \alpha | V_{p\gamma} | \gamma \rangle \; \zeta_\gamma(r) \; , \end{aligned} \tag{3.5.40}$$

and solved to get S (or T) matrices from which we have cross sections following the pattern established for particle channels. When a photon T matrix element is defined as the asymptotic amplitude $\mathbf{T}^{J_{\rm tot}\pi}_{\gamma\alpha_i}$ of the outgoing solution of Eq. (3.5.40) for an incoming particle channel α_i and for system parity π, the photo-production (capture) cross section

$$\sigma_{\gamma p} = \frac{4\pi}{k_i^2} \frac{1}{(2J_{p_i}{+}1)(2J_{t_i}{+}1)} \frac{c}{v_i} \sum_{J_{\rm tot}\pi\alpha_i} (2J_{\rm tot}{+}1) \; |\mathbf{T}^{J_{\rm tot}\pi}_{\gamma\alpha_i}|^2 \tag{3.5.41}$$

since the outgoing photon speed is that of light, c.

The T matrix elements can also be found by the equivalent integral expression

$$\mathbf{T}^{J_{\rm tot}\pi}_{\gamma\alpha_i} = -\frac{1}{k_\gamma} \frac{k_\gamma}{\hbar c} \sum_\alpha \langle \zeta^{(-)}_\gamma(r) \langle \gamma | V_{\gamma p} | \alpha \rangle \psi_{\alpha\alpha_i}(R) \rangle, \tag{3.5.42}$$

where the inner matrix element is an angular integral and the outer one a radial one. Since there is no potential in the photon wave equation, the $\zeta_\gamma^{(-)}(r)$ are simply the free-field solutions, giving

$$\mathbf{T}^{J_{\rm tot}\pi}_{\gamma\alpha_i} = -\frac{1}{\hbar c}\sum_\alpha \langle F_\Lambda(0,k_\gamma r)\langle\gamma|V_{\gamma p}|\alpha\rangle\psi_{\alpha\alpha_i}(R)\rangle, \tag{3.5.43}$$

$$= -\frac{1}{\hbar c}\sum_\alpha \int {\rm d}\mathbf{r}\ \frac{1}{rR}\ F_\Lambda(0,k_\gamma r)\ \phi^*_\gamma\ V_{\gamma p}\ \phi_\alpha\ \psi_{\alpha\alpha_i}(R)\,, \tag{3.5.44}$$

where the radial and angular integrals have been recombined into one integral over all space, and ϕ_γ, ϕ_α are the wave functions of the respective basis functions.

We can further calculate the vector-dependent T matrix amplitude $\mathbf{T}(\mathbf{k}_\gamma,\mathbf{k}_i)$ from the $\mathbf{T}^{J_{\rm tot}\pi}_{\gamma\alpha_i}$ using Eq. (3.3.44). Since the photon wave functions in Eq. (3.5.43) are components of plane waves, we have the integral

$$\mathbf{T}^{\mu\mu_b:\mu_{p_i}\mu_{t_i}}(\mathbf{k}_\gamma,\mathbf{k}_i) = \langle\xi_\mu {\rm e}^{{\rm i}\mathbf{k}_\gamma\cdot\mathbf{r}}|V_{\gamma p}|\mathbf{\Psi}^{\mu_{p_i}\mu_{t_i}}_{x_i p_i t_i}(\mathbf{R};\mathbf{k}_i)\rangle \tag{3.5.45}$$

over $\mathbf{r}$, remembering that $V_{\gamma p}$ already contains an integral with respect to the particle positions $\mathbf{r}_i$, and contains the bound state wavefunction $\Phi_b^{\mu_b}$. The scattering amplitude in the photon exit channel is then

$$f_{\mu\mu_b:\mu_{p_i}\mu_{t_i}}(\mathbf{k}_\gamma:\mathbf{k}_i) = -\frac{1}{4\pi}\frac{k_\gamma}{\hbar c}\mathbf{T}^{\mu\mu_b:\mu_{p_i}\mu_{t_i}}(\mathbf{k}_\gamma,\mathbf{k}_i)\ . \tag{3.5.46}$$

Following the usual pattern of Eq. (3.2.20), the m-states are summed over the exit μ,μ_b and averaged over the entrance μ_{p_i},μ_{t_i} to obtain the cross section for unpolarised beams.

A general photon field is therefore a linear combination of vector spherical harmonics with mixed parities and multipoles. The parity of the field is $(-1)^\Lambda$, and this parity is used to distinguish electric from magnetic multipole components of the electromagnetic field. The *electric* part of a field $\mathbf{A}$ (or $\mathbf{Z}$) is defined as that with parity $(-1)^{J_\gamma+1}$, and the *magnetic* part as that with parity $(-1)^{J_\gamma}$. That is, *the electric part has* $\Lambda = J_\gamma \pm 1$*, and the magnetic part has* $\Lambda = J_\gamma$. Both components are included on an equal footing in Eqs. (3.5.40) and (3.5.42), etc.

All the analysis of this subsection, however, has ignored the requirements of gauge invariance. The above theory assumes *three* m-states for the photon, $\mu = -1, 0, +1$, which is incorrect. We next show, therefore, what must be done to satisfy a specific Coulomb gauge condition. This procedure will remove some components from the plane wave $\xi_\mu {\rm e}^{{\rm i}\mathbf{k}_\gamma\cdot\mathbf{r}}$ in Eq. (3.5.45).

Nuclear transitions, we will see in general in Chapter 4, are classified as dipole, quadrupole, etc. Electric and magnetic transitions are classified not according their spatial part Λ but their multipolarity: the total angular momentum J_γ that is transferred to or from the nucleus by the photon.
E1 and M1 photons have $J_\gamma = 1$, whereas the E2 and M2 have $J_\gamma = 2$, etc. When the parity change from the current operator is taken into account, electric transitions change nuclear parities according to $(-1)^{J_\gamma}$, and magnetic transitions by $(-1)^{J_\gamma - 1}$. Parities are not changed by M1, E2 and M3 transitions, for example, but *are* changed by E1, and M2 multipoles.

Box 3.5: Electromagnetic multipoles

3.5.5 Electric and magnetic parts in the Coulomb gauge

If the coordinate system of Eq. (3.5.37) is not the laboratory system, but is specifically chosen so that the z axis coincides with $\hat{\mathbf{k}}_\gamma$, the *local* direction of photon propagation, the Coulomb gauge condition

$$\nabla \cdot \mathbf{A} = \nabla \cdot \mathbf{Z} = 0 \tag{3.5.47}$$

is simply $A_0 = Z_0 = 0$, as the polarisation vectors $\boldsymbol{\xi}_{\pm 1}$ cover all the allowed transverse directions. In order to satisfy this condition, we first construct a suitable plane wave, and then reuse this gauged plane wave in the T matrix integral (3.5.45) for the general photon cross section.

Consider first a general plane wave vector field travelling in the $+z$-direction, $\mathbf{A}_\mu = \boldsymbol{\xi}_\mu \mathrm{e}^{\mathrm{i}kz}$. The polarisation states allowed by the Coulomb gauge condition (3.5.47) are $\mu = \pm 1$, so we may set $\mathbf{A}_0 = 0$. Following the standard specification of Eq. (3.2.7) for coupling a spin-1 object to a plane wave in the direction of $\mathbf{k}$,

$$\boldsymbol{\xi}_{\mu_i} \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{r}} = \sum_{JM\Lambda m\mu} \mathrm{i}^L \; Y^m_\Lambda(\mathbf{r}) \; \boldsymbol{\xi}_\mu \; \langle \Lambda m, 1\mu | JM \rangle \; F_\Lambda(0, kr)/r \\ \times \frac{4\pi}{k} \sum_{\Lambda_i m_i} Y^{m_i}_{\Lambda_i}(\mathbf{k})^* \langle \Lambda_i m_i, 1\mu_i | JM \rangle \; . \tag{3.5.48}$$

We now specialise to $\mathbf{k}$ in the +z direction so $m = 0$, use the definition of the vector spherical harmonics above, note that in this free-field case there is no spin-flip so $\mu = \mu_i$, and rename Λ_i as Λ. This gives

$$\boldsymbol{\xi}_\mu \mathrm{e}^{\mathrm{i}kz} = \sqrt{4\pi} \sum_{J\Lambda} \sqrt{2\Lambda{+}1} \; \mathrm{i}^L \mathbf{Y}^\mu_{\Lambda J}(\mathbf{r}) \; \langle \Lambda 0, 1\mu | J\mu \rangle F_\Lambda(0, kr)/(kr) \; . \tag{3.5.49}$$

Now the electric parts that have $J = \Lambda \pm 1$ need to be grouped together.

We therefore reassemble the above equation as

$$\boldsymbol{\xi}_\mu \mathrm{e}^{\mathrm{i}kz} = \sqrt{2\pi}\sum_J \sqrt{2J{+}1}\ \mathrm{i}^J \times \left[\sum_\Lambda \mathbf{Y}^\mu_{\Lambda J}(\mathbf{r})\ \mathrm{i}^{\Lambda-J}\sqrt{\frac{2\Lambda{+}1}{2J{+}1}}\langle\Lambda 0, 1\mu|J\mu\rangle\ F_\Lambda(0,kr)/(kr)\right]. \quad (3.5.50)$$

Let us split the $[\cdots]$ into two terms, and using the analytical forms of the $\langle\Lambda 0, 1\mu|J\mu\rangle$, define the $\Lambda = J$ magnetic part as

$$\mathbf{A}_{JM}(\mathbf{r};\mathcal{M}) = (kr)^{-1}F_J(0,kr)\ \mathbf{Y}^M_{JJ}(\hat{\mathbf{r}})\ , \quad (3.5.51)$$

and electric part as the sum of the $\Lambda = J \pm 1$ terms

$$\begin{aligned}\mathbf{A}_{JM}(\mathbf{r};\mathcal{E}) &= \sqrt{\frac{J{+}1}{2J{+}1}}(kr)^{-1}F_{J-1}(0,kr)\ \mathbf{Y}^M_{J-1,J}(\hat{\mathbf{r}}) \\ &\quad -\sqrt{\frac{J}{2J{+}1}}(kr)^{-1}F_{J+1}(0,kr)\ \mathbf{Y}^M_{J+1,J}(\hat{\mathbf{r}})\ . \quad (3.5.52)\end{aligned}$$

Finally, we multiply the electric part by μ^2 so ensure that it is zero when $\mu = 0$, and combine the electric and magnetic parts to give the complete field $\boldsymbol{\xi}_\mu \mathrm{e}^{\mathrm{i}kz}$ satisfying the gauge condition:

$$\mathbf{A}_\mu = \boldsymbol{\xi}_\mu \mathrm{e}^{\mathrm{i}kz} = \mu\sqrt{2\pi}\sum_J \sqrt{2J{+}1}\ \mathrm{i}^J[\mathbf{A}_{J\mu}(\mathbf{r};\mathcal{M}) + \mathrm{i}\mu\mathbf{A}_{J\mu}(\mathbf{r};\mathcal{E})]\ . \quad (3.5.53)$$

Both these electric and magnetic basis components are normalised like plane waves,

$$\int \mathbf{A}_{JM}(\mathbf{r};e)\cdot\mathbf{A}_{J'M'}(\mathbf{r};e')d\mathbf{r} = \delta(k{-}k')\ \delta_{JJ'}\delta_{MM'}\delta_{ee'} \quad (3.5.54)$$

where $e, e' = \mathcal{M}$ or $\mathcal{E}$, and they are related by

$$\mathbf{A}_{JM}(\mathbf{r};\mathcal{M}) = \frac{1}{\mathrm{i}k}\nabla\times\mathbf{A}_{JM}(\mathbf{r};\mathcal{E}) \quad (3.5.55)$$

$$\mathbf{A}_{JM}(\mathbf{r};\mathcal{E}) = \frac{1}{\mathrm{i}k}\nabla\times\mathbf{A}_{JM}(\mathbf{r};\mathcal{M}), \quad (3.5.56)$$

$$\text{so}\quad \nabla\cdot\mathbf{A}_{JM}(\mathbf{r};e) = 0 \qquad \text{for } e = \mathcal{M} \text{ or } \mathcal{E}. \quad (3.5.57)$$

The Eq. (3.5.53) can be used directly for photon *entrance* channels, since then we do have a plane wave in the $+z$ direction. For *exit* channels, however, we need the expansion for a wave travelling in an arbitrary direction $\mathbf{k}$. We cannot use Eq. (3.5.48) directly, since the μ_i are components in the $+z$ direction, not in the $\mathbf{k}$, and it is the $\mu = 0$ component *in the direction of*

travel that the gauge condition requires to be zero. We therefore have to rotate Eq. (3.5.53) to obtain the μ-projections in the $\mathbf{k}$ direction as

$$\boldsymbol{\xi}_\mu \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{r}} \;=\; \mu\sqrt{2\pi}\sum_{JM}\sqrt{2J{+}1}\;\;\mathrm{i}^J[\mathbf{A}_{JM}(\mathbf{r};\mathcal{M}) \;+\; \mathrm{i}\mu\mathbf{A}_{JM}(\mathbf{r};\mathcal{E})]D^J_{M\mu}(\mathcal{R}_k), \tag{3.5.58}$$

where $\mathcal{R}_k$ is the rotation taking the z-axis to the direction of $\mathbf{k}$. Because the laboratory z axis is not now the direction of motion, all M values contribute to this superposition even in the Coulomb gauge.

These components can now be used to construct a scattering amplitude for photons in the Coulomb gauge if the Eq. (3.5.58) is inserted into Eq. (3.5.45), yielding a sum of magnetic and electric parts

$$\mathbf{T}^\mu(\mathbf{k}_\gamma,\mathbf{k}_i;\mathcal{M}) = \mu\sqrt{2\pi}\sum_{JM}\hat{J}\;\mathrm{i}^{-J}D^J_{M\mu}(\mathcal{R}_{k_\gamma})^*\langle\mathbf{A}_{JM}(\mathbf{r};\mathcal{M})|V_{\gamma p}|\boldsymbol{\Psi}(\mathbf{R};\mathbf{k}_i)\rangle \tag{3.5.59}$$

$$\mathbf{T}^\mu(\mathbf{k}_\gamma,\mathbf{k}_i;\mathcal{E}) = -\mathrm{i}\mu^2\sqrt{2\pi}\sum_{JM}\hat{J}\;\mathrm{i}^{-J}D^J_{M\mu}(\mathcal{R}_{k_\gamma})^*\langle\mathbf{A}_{JM}(\mathbf{r};\mathcal{E})|V_{\gamma p}|\boldsymbol{\Psi}(\mathbf{R};\mathbf{k}_i)\rangle, \tag{3.5.60}$$

suppressing the particle m-state labels and using $\hat{J}{=}\sqrt{2J{+}1}$. The $\langle..\rangle$ matrix elements appear in

$$\mathbf{T}^{(e)}_{JM} = \langle\sqrt{4\pi}\sqrt{2J{+}1}\;\mathrm{i}^J\;\mathbf{A}_{JM}(\mathbf{r};(e))|V_{\gamma p}|\boldsymbol{\Psi}(\mathbf{R};\mathbf{k}_i)\rangle, \tag{3.5.61}$$

and so may be calculated by normal integral or coupled-channels methods as shown in the next chapter, and the results rotated to obtain the μ-projections for the photon in its direction of travel as

$$\begin{aligned}\mathbf{T}^\mu(\mathbf{k}_\gamma,\mathbf{k}_i;\mathcal{M}) &= \frac{\mu}{\sqrt{2}}\sum_{JM}D^J_{M\mu}(\mathcal{R}_{k_i\to k_\gamma})^*\;\mathbf{T}^{(\mathcal{M})}_{JM}\\ \mathbf{T}^\mu(\mathbf{k}_\gamma,\mathbf{k}_i;\mathcal{E}) &= -\frac{\mathrm{i}\mu^2}{\sqrt{2}}\sum_{JM}D^J_{M\mu}(\mathcal{R}_{k_i\to k_\gamma})^*\;\mathbf{T}^{(\mathcal{E})}_{JM}\;.\end{aligned} \tag{3.5.62}$$

This method is therefore equivalent to calculating the photon amplitudes $\mathbf{T}_{JM}$ for quantum numbers JM from forward scattering (0°), and then rotating the amplitudes to other angles according to the various JM values.

Finally, we may define a *longitudinal* part of the field, another combination of the $\Lambda = J \pm 1$ terms, as

$$\begin{aligned}&\mathbf{A}_{JM}(\mathbf{r};\mathrm{long}) \equiv \frac{1}{k}\nabla\left(\frac{1}{kr}F_J(0,kr)Y^M_J(\hat{\mathbf{r}})\right)\\ &= \sqrt{\frac{J}{2J{+}1}}\frac{1}{kr}F_{J-1}(0,kr)\mathbf{Y}^M_{J-1,J}(\hat{\mathbf{r}}) + \sqrt{\frac{J{+}1}{2J{+}1}}\frac{1}{kr}F_{J+1}(0,kr)\mathbf{Y}^M_{J+1,J}(\hat{\mathbf{r}})\;.\end{aligned} \tag{3.5.63}$$

Though $\nabla \cdot \mathbf{A}_{J_\gamma M_\gamma}(\mathbf{r};\text{long}) \neq 0$, and hence does not satisfying the transverse gauge condition, this longitudinal component will be useful later since it differs from Eq. (3.5.52) only by the coefficients of its two terms. If the second terms in both Eqs. (3.5.52) and (3.5.63) could be neglected in some circumstances, for example when $kr \ll 1$, then

$$\begin{aligned} \mathbf{A}_{JM}(\mathbf{r};\mathcal{E}) &\approx \sqrt{\frac{J+1}{2J+1}}(kr)^{-1}F_{J-1}(0,kr)\ \mathbf{Y}^M_{J-1,J}(\hat{\mathbf{r}}) \\ &= \sqrt{\frac{J+1}{J}}\sqrt{\frac{J}{2J+1}}(kr)^{-1}F_{J-1}(0,kr)\mathbf{Y}^M_{J-1,J}(\hat{\mathbf{r}}) \\ &\approx \sqrt{\frac{J+1}{J}}\mathbf{A}_{JM}(\mathbf{r};\text{long})\ . \end{aligned} \tag{3.5.64}$$

This approximation will be used in the next chapter to simplify Eq. (3.5.60).

Appendix

S matrix symmetry with relativistic kinematics

For low-energy nuclear reactions, Newtonian non-relativistic kinematics is sufficiently accurate. Later we will discuss breakup reactions at intermediate energies, but photons themselves, with zero rest mass, are necessarily relativistic, so here we apply the relativistic kinematics of section 2.3.3 to reactions that couple photon and particle channels.

In a coupled channels scheme $[T_\alpha - E_\alpha]\psi_\alpha + \sum_\beta V_{\alpha\beta}\psi_\beta = 0$, the channel kinetic energy is $E_\alpha = E_{\rm tot} - E_0$ for total relativistic energy $E^2_{\rm tot} = (\hbar kc)^2 + E_0^2$ and rest energy $E_0 = m_0c^2$.

The kinetic energy operator is in general $T_\alpha = -t_\alpha\nabla^2$ with coefficient

$$t_\alpha = (E_{\rm tot} - E_0)/k^2 = E_0(\gamma - 1)/k^2 \tag{3.5.65}$$

for $k = m_0\gamma v/\hbar$ with $\gamma = (1 - v^2/c^2)^{-1/2}$. In the non-relativistic limit, $t_\alpha \to \hbar^2/2\mu_0$.

The T matrix integrals of Eq. (3.3.23) can be also written more generally, for elastic channel α_i, as

$$\mathbf{T}_{\alpha\alpha_i} = -\frac{1}{t_\alpha k_\alpha}\int \tilde{F}_\alpha \textstyle\sum_\beta V_{\alpha\beta}\psi_\beta \mathrm{d}R\ , \tag{3.5.66}$$

from which the symmetric S matrix form of Eq. (3.2.15) is

$$\tilde{\mathbf{S}}_{\alpha\alpha_i} = 2\mathrm{i}\sqrt{\frac{v_\alpha}{v_{\alpha_i}}}\mathbf{T}_{\alpha\alpha_i} \tag{3.5.67}$$

$$= -\frac{2\mathrm{i}}{\hbar\sqrt{v_\alpha v_{\alpha_i}}}\frac{\hbar v_\alpha}{t_\alpha k_\alpha}\int \tilde{F}_\alpha \textstyle\sum_\beta V_{\alpha\beta}\psi_\beta \mathrm{d}R\ . \tag{3.5.68}$$

Non-relativistically, the quantity $w_\alpha \equiv \hbar v_\alpha / t_\alpha k_\alpha = 2$, the same for all channels. The general relativistic expression, however, is $w_\alpha = 1 + (1 - v_\alpha^2/c^2)^{1/2}$, namely $w_\alpha = 2$ for $v_\alpha \ll c$, but $w_\alpha = 1$ for $v_\alpha = c$ with photons. This implies that for a symmetric S matrix $\tilde{\mathbf{S}}$ we must have $w_\alpha V_{\alpha\beta} = w_\beta V_{\beta\alpha}$. The photon and particle coupling interactions of Eq. (3.5.35) indeed satisfy

$$V_{\gamma p} = 2\ V_{p\gamma}\ , \tag{3.5.69}$$

in contrast to nonrelativistic particle-particle couplings which must all be symmetric.

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