

$$V_{\text{eff}}(r) = \infty, \quad \text{for } r < 0, \quad \text{so } u = 0 \text{ for } r \leq 0.$$

Find the WKB approximation for the energy, E_n , as a function of m, k, \hbar . The boundary condition at $r = 0$ leads to a WKB solution near $r = 0$ of the form

$$u_{\text{WKB}}(r) = \frac{A}{\sqrt{P(r)}} \sin \left[\frac{1}{\hbar} \int_0^r dr' P(r') \right],$$

with $P(r) = \sqrt{2m(E - V_{\text{eff}}(r))}$. (Note: $P(r)$ is finite at $r = 0$.)

53. Show that the WKB connection formulae can be converted to the form

$$u_I = \frac{A}{\sqrt{P(x)}} e^{\pm \frac{i}{\hbar} \int_x^{x_2} d\xi P(\xi)} \quad \longleftrightarrow \quad u_{II}$$

$$u_{II} = \frac{A}{\sqrt{|P(x)|}} \left(\frac{1}{2} e^{\pm i \frac{x}{4}} e^{-\frac{1}{\hbar} \int_{x_2}^x d\xi |P(\xi)|} + e^{\mp i \frac{x}{4}} e^{+\frac{1}{\hbar} \int_{x_2}^x d\xi |P(\xi)|} \right)$$

$$\text{for the right/left running wave solutions} \quad \frac{A}{\sqrt{P(x)}} e^{\pm \frac{i}{\hbar} \int_x^{x_2} d\xi P(\xi)},$$

in region I, with a similar relation at the boundary $x = x_1$ (see Fig. P53).

Use these connection formulae to calculate the transmission and reflection coefficients for a wave incident on a potential barrier of arbitrary but smooth shape, with incident energy, $E < V_{\text{max}}$. In particular, show that the transmission coefficient, T , is given by

$$T = \frac{\text{Transm. Flux}}{\text{Inc. Flux}} = \left(\frac{4D}{D^2 + 4} \right)^2, \quad \text{with } D = e^{-\frac{1}{\hbar} \int_{x_2}^{x_1} dx \sqrt{2m(V(x)-E)}}.$$

54. For the one-dimensionalized potential of the shape shown in Fig. P54, demonstrate for arbitrary energies in the continuum, $E > 0$, but $E < V_{\text{max}}$, the solutions in general will satisfy $|u_{IV}|^2 \gg |u_{II}|^2$. Show also that for the special values of $E = E_n$, for which

$$\frac{1}{\pi} \int_{x_1}^{x_2} dx \sqrt{2\mu(E_n - V(x))} \approx \hbar(n + \frac{1}{2}),$$

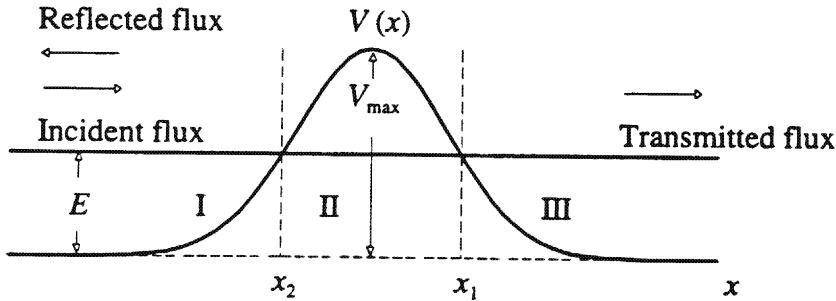


FIGURE P53.

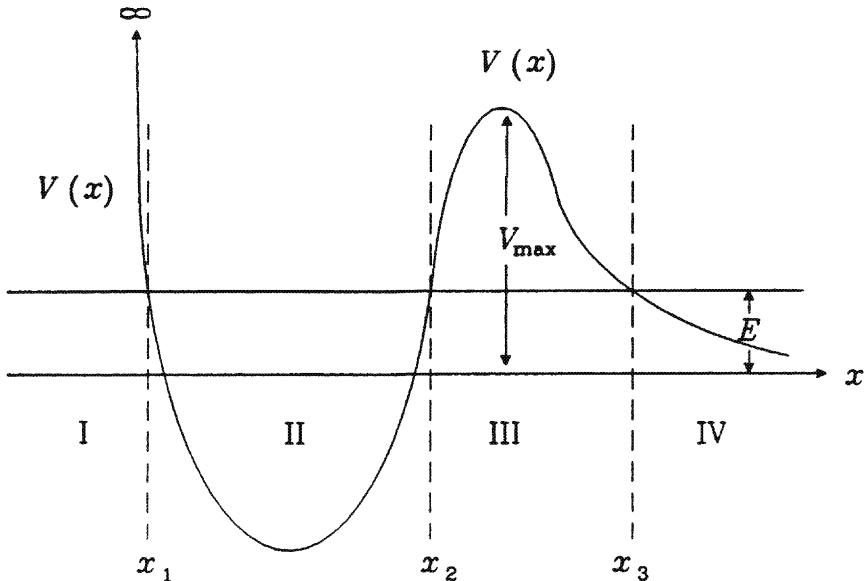


FIGURE P54.

the situation is reversed, and for these energies, $|u_{II}|^2 \gg |u_{IV}|^2$. Estimate the width, ΔE , of these virtual bound or quasibound states (or resonances) in terms of ω_0 , the approximate circular frequency in the well, and the penetrability factor

$$Q^2 = e^{-\frac{1}{\hbar} \int_{x_2}^{x_3} dx \sqrt{2\mu(V(x)-E_n)}}.$$

55. A symmetrical X_2Y_4 molecule, such as C_2H_4 (ethylene), has one degree of freedom, ϕ , which corresponds to a highly hindered internal rotation of one essentially rigid CH_2 unit relative to the other on the circle, as shown in Fig. 4.3 of Chapter 4. The wave equation separates approximately, so the hindered internal

rotation can be described by a one-degree-of-freedom Schrödinger equation,

$$-\frac{\hbar^2}{2I} \frac{d^2 u}{d\phi^2} + V(\phi)u(\phi) = Eu(\phi),$$

with $I = I_1 I_2 / (I_1 + I_2)$, $I_1 = I_2 = 2m_Y r_Y^2$. In Chapter 4, this problem was solved in a square well approximation. Now, we shall choose a more realistic potential that can be approximated by (see Fig. P55),

$$V(\phi) = V_0(1 - \cos 2\phi),$$

with minima at $\phi = 0$ and π and maxima at $\phi = \frac{\pi}{2}, \frac{3\pi}{2}, \dots$. The constant, V_0 , can be expected to be very large compared with the lowest allowed energy eigenvalues. In that case, the energy levels occur in closely spaced multiplets. The average position of a multiplet can be approximated by the quadratic approximation for $V(\phi)$, e. g. $V(\phi) \approx V_0 \frac{4\phi^2}{2}$ near the potential minimum at $\phi = 0$, so $E \approx E_n = \hbar\omega_0(n + \frac{1}{2})$, with $\omega_0 \approx \sqrt{(4V_0/I)}$. In particular, show how the splitting into multiplets depends on the energies, $\hbar\omega_0$, and the penetrability factors

$$Q = e^{-\frac{1}{\hbar} \int_{\frac{\pi}{2}}^{\phi} d\phi' \sqrt{2I(V(\phi')-E)}}.$$

Use the fact that solutions of the form, $(A/\sqrt{|P|}) \cosh(\dots)$ in the classically forbidden region I (see Fig. P55), must connect onto solutions of the form, $\pm(A/\sqrt{|P|}) \cosh(\dots)$ in the region $\phi \rightarrow \phi + 2\pi$, i.e., region V in Fig. P55, whereas solutions of type $(A/\sqrt{|P|}) \sinh(\dots)$ in region I must connect onto solutions of the form $\pm(A/\sqrt{|P|}) \sinh(\dots)$ in region V, in order to preserve both probability density and probability density current.

Try to generalize your result for the energy splitting for the potentials

$$V(\phi) = V_0(1 - \cos N\phi), \quad \text{with } N = 3, 4, \dots$$

For arbitrary N , show that the energy multiplets are made up of $(N+1)$ levels, with $(N-1)$ two-fold degenerate states and two nondegenerate states, now crowded into the same ΔE , viz.,

$$\Delta E = \frac{2\hbar\omega_0}{\pi} Q^2,$$

valid for $N = 2$.

For very large N , we have effectively bands of very finely spaced discrete allowed energy values, the Bloch bands of condensed matter physics.

Caution: For $N = 2$, all solutions are either symmetric or antisymmetric with respect to reflections in the plane $\phi = 3\pi/N = 3\pi/2$, in region III of Fig. P55, if they are made to have either symmetry, or antisymmetry with respect to reflections in the plane $\phi = \pi/N = \pi/2$, in region I of Fig. P55. For $N \geq 3$, symmetries in regions near $\phi = 3\pi/N, 5\pi/N, \dots$ may not be simple for the doubly degenerate states. For such doubly degenerate states, a linear combination of symmetric and antisymmetric (or even and odd) functions may also be acceptable solutions even if the solutions are made symmetric or antisymmetric with respect to reflections in the plane $\phi = \pi/N$.

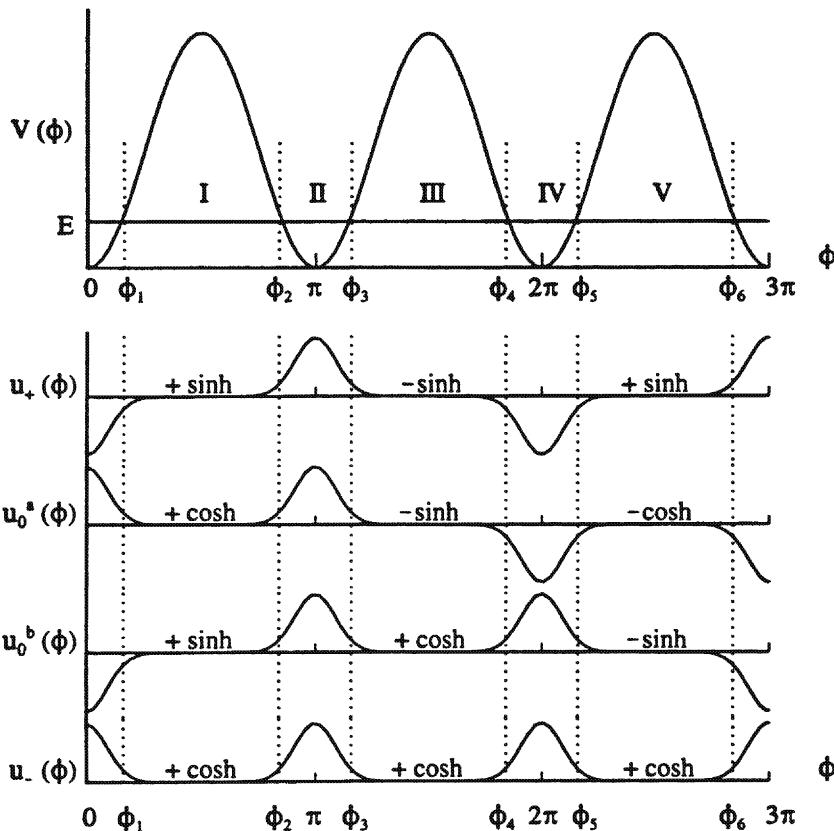


FIGURE P55. The hindering potential $V(\phi)$ for the X_2Y_4 molecule and the four eigenfunctions $u_-(\phi)$ (lowest E) $u_0^{(a)}(\phi)$, $u_0^{(b)}(\phi)$ (degenerate doublet) and $u_+(\phi)$ (highest E) for the $n = 0$ quartet.

Solution for Problem 55

The Case $N = 2$: We will start the process of finding the allowed solutions by assuming the solutions in the first classically forbidden region, near $\phi = \frac{\pi}{2}$ (region I of Fig. P55), must be either an even or an odd function of $(\phi - \frac{\pi}{2})$. Thus, in region I,

$$\begin{aligned} u_1(\phi) &= \frac{A}{\sqrt{|P(\phi)|}} \cosh \frac{1}{\hbar} \left(\int_{\frac{\pi}{2}}^{\phi} d\phi' |P(\phi')| \right) && \text{for even } u_1, \\ u_1(\phi) &= \frac{A}{\sqrt{|P(\phi)|}} \sinh \frac{1}{\hbar} \left(\int_{\frac{\pi}{2}}^{\phi} d\phi' |P(\phi')| \right) && \text{for odd } u_1. \end{aligned} \quad (1)$$

We shall continue these WKB solutions to region V, near $\phi = \frac{\pi}{2} + 2\pi$, where we will require $u_V = \pm u_1$; i.e., even functions must end up as even functions, odd functions must end up as odd functions, so the probability density and probability density current are single-valued functions in the 3-D space. Let us, however, start with exponential functions in region I:

$$\begin{aligned} u_1^{(+)} &= \frac{1}{\sqrt{|P|}} e^{+\frac{1}{\hbar} \int_{\frac{\pi}{2}}^{\phi} d\phi' |P(\phi')|} = \frac{1}{Q} \frac{1}{\sqrt{|P|}} e^{-\frac{1}{\hbar} \int_{\phi}^{\phi_2} d\phi' |P(\phi')|}, \\ u_1^{(-)} &= \frac{1}{\sqrt{|P|}} e^{-\frac{1}{\hbar} \int_{\frac{\pi}{2}}^{\phi} d\phi' |P(\phi')|} = Q \frac{1}{\sqrt{|P|}} e^{+\frac{1}{\hbar} \int_{\phi}^{\phi_2} d\phi' |P(\phi')|}, \end{aligned} \quad (2)$$

where ϕ_2 gives the right boundary of the classically forbidden region I, and where we have used

$$\int_{\frac{\pi}{2}}^{\phi} d\phi' |P(\phi')| = \int_{\frac{\pi}{2}}^{\phi_2} d\phi' |P(\phi')| - \int_{\phi}^{\phi_2} d\phi' |P(\phi')|,$$

and where Q is defined through

$$Q = e^{-\frac{1}{\hbar} \int_{\frac{\pi}{2}}^{\phi_2} d\phi' |P(\phi')|}.$$

We shall now use the WKB connection formulae to connect these solutions to the oscillatory solutions, valid in region II for $\phi_2 < \phi < \phi_3$:

$$\begin{aligned} u_1^{(+)} &\rightarrow \frac{2}{Q \sqrt{P(\phi)}} \cos\left(\frac{1}{\hbar} \int_{\phi_2}^{\phi} d\phi' P(\phi') - \frac{\pi}{4}\right), \\ u_1^{(-)} &\rightarrow \frac{Q}{\sqrt{P(\phi)}} \cos\left(\frac{1}{\hbar} \int_{\phi_2}^{\phi} d\phi' P(\phi') + \frac{\pi}{4}\right). \end{aligned} \quad (3)$$

In the cosine functions, we shall now use

$$\frac{1}{\hbar} \int_{\phi_2}^{\phi} d\phi' P(\phi') = \frac{1}{\hbar} \int_{\phi_2}^{\phi_3} d\phi' P(\phi') - \frac{1}{\hbar} \int_{\phi}^{\phi_3} d\phi' P(\phi'),$$

and relate the integral over the complete oscillatory region to the action variable, $J(E)$, with $E = E^{(0)} + \Delta E$, where $E^{(0)}$ is the solution for a single oscillatory well of approximately parabolic shape, with $E^{(0)} = \hbar\omega_0(n + \frac{1}{2})$, and ΔE is the shift in this energy level caused by the presence of the potential hills. With $\Delta E \ll E^{(0)}$, we then have

$$\begin{aligned} \frac{1}{\hbar} \int_{\phi_2}^{\phi_3} d\phi' P(\phi') &= \frac{\pi}{\hbar} (J(E)) \\ &= \frac{\pi}{\hbar} \left(J(E^{(0)}) + \left(\frac{\partial J}{\partial E} \right)_{E^{(0)}} \Delta E \right) = \frac{\pi}{\hbar} \left(\hbar(n + \frac{1}{2}) + \frac{1}{\omega_0} \Delta E \right). \end{aligned}$$

Substituting this equation into eq. (3), we have

$$u_1^{(+)} \rightarrow \frac{2}{Q \sqrt{P(\phi)}} \cos\left(\frac{1}{\hbar} \int_{\phi}^{\phi_3} d\phi' P(\phi') - \frac{\pi}{4} - n\pi - \frac{\pi \Delta E}{\hbar\omega_0}\right),$$

$$u_1^{(-)} \rightarrow Q \frac{1}{\sqrt{|P(\phi)|}} \cos \left(\frac{1}{\hbar} \int_{\phi}^{\phi_3} d\phi' P(\phi') + \frac{\pi}{4} - (n+1)\pi - \frac{\pi \Delta E}{\hbar \omega_0} \right). \quad (4)$$

Now, expanding in the small quantity, $(\pi \Delta E)/(\hbar \omega_0)$, we have

$$\begin{aligned} u_1^{(+)} &\rightarrow \frac{2}{Q} \frac{1}{\sqrt{|P(\phi)|}} (-1)^n \left[\cos \left(\frac{1}{\hbar} \int_{\phi}^{\phi_3} d\phi' P(\phi') - \frac{\pi}{4} \right) \right. \\ &\quad \left. - \frac{\pi \Delta E}{\hbar \omega_0} \cos \left(\frac{1}{\hbar} \int_{\phi}^{\phi_3} d\phi' P(\phi') + \frac{\pi}{4} \right) \right], \\ u_1^{(-)} &\rightarrow Q \frac{1}{\sqrt{|P(\phi)|}} (-1)^{(n+1)} \left[\cos \left(\frac{1}{\hbar} \int_{\phi}^{\phi_3} d\phi' P(\phi') + \frac{\pi}{4} \right) \right. \\ &\quad \left. + \frac{\pi \Delta E}{\hbar \omega_0} \cos \left(\frac{1}{\hbar} \int_{\phi}^{\phi_3} d\phi' P(\phi') - \frac{\pi}{4} \right) \right]. \end{aligned} \quad (5)$$

We now use the WKB connection formulae to connect the oscillatory solutions for $\phi < \phi_3$ onto the exponential solutions for $\phi > \phi_3$, valid in region III, to obtain

$$\begin{aligned} u_1^{(+)} &\rightarrow \frac{1}{Q} \frac{(-1)^n}{\sqrt{|P(\phi)|}} \left[e^{-\frac{1}{\hbar} \int_{\phi_3}^{\phi} d\phi' |P(\phi')|} - 2 \frac{\pi \Delta E}{\hbar \omega_0} e^{+\frac{1}{\hbar} \int_{\phi_3}^{\phi} d\phi' |P(\phi')|} \right], \\ u_1^{(-)} &\rightarrow -Q \frac{(-1)^n}{\sqrt{|P(\phi)|}} \left[e^{+\frac{1}{\hbar} \int_{\phi_3}^{\phi} d\phi' |P(\phi')|} + \frac{1}{2} \frac{\pi \Delta E}{\hbar \omega_0} e^{-\frac{1}{\hbar} \int_{\phi_3}^{\phi} d\phi' |P(\phi')|} \right]. \end{aligned} \quad (6)$$

Now using

$$e^{-\frac{1}{\hbar} \int_{\phi_3}^{\phi} d\phi' |P(\phi')|} = e^{-\frac{1}{\hbar} \int_{\phi_3}^{\frac{3\pi}{2}} d\phi' |P(\phi')|} e^{-\frac{1}{\hbar} \int_{\frac{3\pi}{2}}^{\phi} d\phi' |P(\phi')|} = Q e^{-\frac{1}{\hbar} \int_{\frac{3\pi}{2}}^{\phi} d\phi' |P(\phi')|},$$

we get

$$\begin{aligned} u_1^{(+)} &\rightarrow \frac{(-1)^n}{\sqrt{|P(\phi)|}} \left[e^{-\frac{1}{\hbar} \int_{\frac{3\pi}{2}}^{\phi} d\phi' |P(\phi')|} - \frac{2}{Q^2} \frac{\pi \Delta E}{\hbar \omega_0} e^{+\frac{1}{\hbar} \int_{\frac{3\pi}{2}}^{\phi} d\phi' |P(\phi')|} \right], \\ u_1^{(-)} &\rightarrow \frac{(-1)^n}{\sqrt{|P(\phi)|}} \left[-e^{+\frac{1}{\hbar} \int_{\frac{3\pi}{2}}^{\phi} d\phi' |P(\phi')|} - \frac{Q^2}{2} \frac{\pi \Delta E}{\hbar \omega_0} e^{-\frac{1}{\hbar} \int_{\frac{3\pi}{2}}^{\phi} d\phi' |P(\phi')|} \right]. \end{aligned} \quad (7)$$

For levels far below the potential barriers, we expect the penetration factor, Q^2 , to be such that $Q^2 \ll 1$. Also, the energy shift caused by barrier penetration should be proportional to Q^2 . The quantity $\frac{\Delta E}{\hbar \omega_0} Q^2$ can thus be expected to be completely negligible, so the negative exponential in the last expression can be neglected. If we now name

$$\frac{1}{\sqrt{|P(\phi)|}} e^{\pm \int_{\frac{3\pi}{2}}^{\phi} d\phi' |P(\phi')|} = u_{\text{III}}^{(\pm)},$$

and introduce the shorthand notation

$$\beta \equiv \frac{\pi \Delta E}{\hbar \omega_0 Q^2},$$

the above equations give us the connection formulae

$$\begin{aligned} u_I^{(+)} &\rightarrow (-1)^n \left[u_{III}^{(-)} - 2\beta u_{III}^{(+)} \right], \\ u_I^{(-)} &\rightarrow (-1)^n \left[-u_{III}^{(+)} \right]. \end{aligned} \quad (8)$$

We can now iterate this procedure to connect the $u_{III}^{(\pm)}$ onto the corresponding $u_V^{(\pm)}$ in region V, where the original ϕ has been incremented by 2π . This equation yields

$$\begin{aligned} u_I^{(+)} &\rightarrow (-1)^{2n} \left[-u_V^{(+)} - 2\beta(u_V^{(-)} - 2\beta u_V^{(+)}) \right] = [(4\beta^2 - 1)u_V^{(+)} - 2\beta u_V^{(-)}], \\ u_I^{(-)} &\rightarrow (-1)^{2n} \left[-u_V^{(-)} + 2\beta u_V^{(+)} \right] = [2\beta u_V^{(+)} - u_V^{(-)}]. \end{aligned} \quad (9)$$

Combining these formulae to make even or odd functions of ϕ in region I, these even or odd functions in region I would connect to a linear combination of even and odd functions in region V, where ϕ has been incremented by 2π :

$$\begin{aligned} \frac{1}{\sqrt{|P(\phi)|}} \cosh \left(\frac{1}{\hbar} \int_{\frac{\pi}{2}}^{\phi} d\phi' |P(\phi')| \right) &= \frac{1}{2} (u_I^{(+)} + u_I^{(-)}) \\ &\rightarrow \frac{1}{2} \left[(2\beta^2 - 1)(u_V^{(+)} + u_V^{(-)}) + 2\beta(1 + \beta)(u_V^{(+)} - u_V^{(-)}) \right] \\ &= \frac{1}{\sqrt{|P(\phi)|}} \left[(2\beta^2 - 1) \cosh \left(\frac{1}{\hbar} \int_{\frac{5\pi}{2}}^{\phi} d\phi' |P(\phi')| \right) \right. \\ &\quad \left. + 2\beta(1 + \beta) \sinh \left(\frac{1}{\hbar} \int_{\frac{5\pi}{2}}^{\phi} d\phi' |P(\phi')| \right) \right], \end{aligned} \quad (10)$$

and

$$\begin{aligned} \frac{1}{\sqrt{|P(\phi)|}} \sinh \left(\frac{1}{\hbar} \int_{\frac{\pi}{2}}^{\phi} d\phi' |P(\phi')| \right) &= \frac{1}{2} (u_I^{(+)} - u_I^{(-)}) \\ &\rightarrow \frac{1}{2} \left[2\beta(\beta - 1)(u_V^{(+)} + u_V^{(-)}) + (2\beta^2 - 1)(u_V^{(+)} - u_V^{(-)}) \right] \\ &= \frac{1}{\sqrt{|P(\phi)|}} \left[2\beta(\beta - 1) \cosh \left(\frac{1}{\hbar} \int_{\frac{5\pi}{2}}^{\phi} d\phi' |P(\phi')| \right) \right. \\ &\quad \left. + (2\beta^2 - 1) \sinh \left(\frac{1}{\hbar} \int_{\frac{5\pi}{2}}^{\phi} d\phi' |P(\phi')| \right) \right]. \end{aligned} \quad (11)$$

Thus, we see from eq. (10) $u_{\text{even}}(\phi) \rightarrow \pm u_{\text{even}}(\phi + 2\pi)$ only if $\beta = -1$, or if $\beta = 0$. From eq. (11), $u_{\text{odd}}(\phi) \rightarrow \pm u_{\text{odd}}(\phi + 2\pi)$ only if $\beta = +1$, or if $\beta = 0$. The potential $V_0(1 - \cos 2\phi)$ thus splits the zeroth-order energies $E^{(0)} = \hbar\omega_0(n + \frac{1}{2})$ into three closely spaced levels, one of them with $\Delta E = 0$, being doubly degenerate. The four values of ΔE are

$$\begin{aligned} \Delta E &= -Q^2 \frac{\hbar\omega_0}{\pi} && \text{with } u_{\text{even}}(\phi) \rightarrow +u_{\text{even}}(\phi + 2\pi), \\ \Delta E &= 0 && \text{with } u_{\text{even}}(\phi) \rightarrow -u_{\text{even}}(\phi + 2\pi), \\ \Delta E &= 0 && \text{with } u_{\text{odd}}(\phi) \rightarrow -u_{\text{odd}}(\phi + 2\pi), \end{aligned}$$

$$\Delta E = +Q^2 \frac{\hbar\omega_0}{\pi} \quad \text{with} \quad u_{\text{odd}}(\phi) \rightarrow +u_{\text{odd}}(\phi + 2\pi). \quad (12)$$

The four eigenfunctions for the case $n = 0$ are shown qualitatively in Fig. P55. The four eigenfunctions are also either even or odd functions of $(\phi - \frac{3\pi}{2})$; i.e., they are even or odd with respect to reflections in the plane $\phi = \frac{3\pi}{2}$, where the potential again has a maximum. In particular, the eigenfunction u_- of the nondegenerate level, with $\Delta E = -Q^2 \hbar\omega_0/\pi$, is even with respect to reflections in planes through any potential maximum, and the eigenfunction u_+ of the nondegenerate level, with $\Delta E = +Q^2 \hbar\omega_0/\pi$, is odd with respect to reflections in planes through any potential maximum. Conversely, the eigenfunctions u_0 for the doubly degenerate level, with $\Delta E = 0$, are alternately even and odd functions when reflected in planes through successive potential maxima. Because any linear combination of the two eigenfunctions u_0 is again an eigenfunction with the same eigenvalue, we would, however, have to exercise care in using the symmetry with respect to reflections in successive planes of symmetry of the potential.

The case for $V(\phi) = V_0(1 - \cos N\phi)$, arbitrary N :

In this case, the maxima of the potentials will be centered about the angles

$$\begin{aligned} \frac{\pi}{N}, \left(\frac{\pi}{N} + \frac{2\pi}{N}\right), \left(\frac{\pi}{N} + 2\frac{2\pi}{N}\right), \dots, \left(\frac{\pi}{N} + k\frac{2\pi}{N}\right), \dots, \left(\frac{\pi}{N} + N\frac{2\pi}{N}\right) \\ = \left(\frac{\pi}{N} + 2\pi\right) \end{aligned}$$

Let us rename these regions with the index k , starting with $k = 0$ for the starting hill and ending with $k = N$, for which we have incremented ϕ by 2π . Eqs. (8) and (9) can now be put in the form

$$\begin{aligned} u_{0,\text{even}} &\rightarrow (-1)^n \left[-\beta u_{1,\text{even}} - (1 + \beta) u_{1,\text{odd}} \right], \\ u_{0,\text{odd}} &\rightarrow (-1)^n \left[-\beta u_{1,\text{odd}} + (1 - \beta) u_{1,\text{even}} \right]. \end{aligned} \quad (13)$$

$$\begin{aligned} u_{0,\text{even}} &\rightarrow (-1)^{2n} \left[(2\beta^2 - 1) u_{2,\text{even}} + 2\beta(1 + \beta) u_{2,\text{odd}} \right], \\ u_{0,\text{odd}} &\rightarrow (-1)^{2n} \left[(2\beta^2 - 1) u_{2,\text{odd}} - 2\beta(1 - \beta) u_{2,\text{even}} \right]. \end{aligned} \quad (14)$$

Iterating this once more, we have the connection into the next hill

$$\begin{aligned} u_{0,\text{even}} &\rightarrow (-1)^{3n} \left[\beta(3 - 4\beta^2) u_{3,\text{even}} - (1 + \beta)(4\beta^2 - 1) u_{3,\text{odd}} \right], \\ u_{0,\text{odd}} &\rightarrow (-1)^{3n} \left[\beta(3 - 4\beta^2) u_{3,\text{odd}} + (1 - \beta)(4\beta^2 - 1) u_{3,\text{even}} \right]. \end{aligned} \quad (15)$$

Before iterating this into the k^{th} hill, it will be convenient to change the notation, and rename $\beta \equiv \cos \alpha$. With this notation, the above relations and the continued iteration process give

$$\begin{aligned} u_{0,\text{even}} &\rightarrow (-1)^n \left[-\cos \alpha u_{1,\text{even}} - (1 + \cos \alpha) u_{1,\text{odd}} \right], \\ u_{0,\text{odd}} &\rightarrow (-1)^n \left[-\cos \alpha u_{1,\text{odd}} + (1 - \cos \alpha) u_{1,\text{even}} \right], \end{aligned}$$

$$\begin{aligned}
u_{0,\text{even}} &\rightarrow (-1)^{2n} \left[\cos(2\alpha) u_{2,\text{even}} + (1 + \cos \alpha) \frac{\sin(2\alpha)}{\sin \alpha} u_{2,\text{odd}} \right], \\
u_{0,\text{odd}} &\rightarrow (-1)^{2n} \left[\cos(2\alpha) u_{2,\text{odd}} - (1 - \cos \alpha) \frac{\sin(2\alpha)}{\sin \alpha} u_{2,\text{even}} \right], \\
u_{0,\text{even}} &\rightarrow (-1)^{3n} \left[-\cos(3\alpha) u_{3,\text{even}} - (1 + \cos \alpha) \frac{\sin(3\alpha)}{\sin \alpha} u_{3,\text{odd}} \right], \\
u_{0,\text{odd}} &\rightarrow (-1)^{3n} \left[-\cos(3\alpha) u_{3,\text{odd}} + (1 - \cos \alpha) \frac{(\sin 3\alpha)}{\sin \alpha} u_{3,\text{even}} \right], \\
&\dots \\
u_{0,\text{even}} &\rightarrow (-1)^{k(n+1)} \left[\cos(k\alpha) u_{k,\text{even}} + (1 + \cos \alpha) \frac{\sin(k\alpha)}{\sin \alpha} u_{k,\text{odd}} \right], \\
u_{0,\text{odd}} &\rightarrow (-1)^{k(n+1)} \left[\cos(k\alpha) u_{k,\text{odd}} - (1 - \cos \alpha) \frac{(\sin k\alpha)}{\sin \alpha} u_{k,\text{even}} \right], \\
&\dots \\
u_{0,\text{even}} &\rightarrow (-1)^{N(n+1)} \left[\cos(N\alpha) u_{N,\text{even}} + (1 + \cos \alpha) \frac{\sin(N\alpha)}{\sin \alpha} u_{N,\text{odd}} \right], \\
u_{0,\text{odd}} &\rightarrow (-1)^{N(n+1)} \left[\cos(N\alpha) u_{N,\text{odd}} - (1 - \cos \alpha) \frac{\sin(N\alpha)}{\sin \alpha} u_{N,\text{even}} \right], \quad (16)
\end{aligned}$$

where the last iteration must give

$$u_{N,\text{even}} = u_{\text{even}}(\phi + 2\pi) = \pm u_{0,\text{even}}(\phi),$$

or

$$u_{N,\text{odd}} = u_{\text{odd}}(\phi + 2\pi) = \pm u_{0,\text{odd}}(\phi).$$

A single (nondegenerate) even solution exists if $\cos \alpha = -1$, and a single (nondegenerate) odd solution if $\cos \alpha = +1$. In addition, both an even and an odd solution exists if

$$\sin N\alpha = 0, \quad \cos N\alpha = \pm 1, \quad \text{or}$$

$$\alpha = \frac{\ell\pi}{N}, \quad \ell = 1, 2, \dots, (N-1).$$

Recalling $\cos \alpha = (\pi \Delta E)/Q^2 \hbar \omega_0$, the final spectrum of allowed energies is

$$\Delta E = -Q^2 \frac{\hbar \omega_0}{\pi}, \quad \text{with nondegenerate even eigenfunction,}$$

$$\Delta E = +Q^2 \frac{\hbar \omega_0}{\pi}, \quad \text{with nondegenerate odd eigenfunction,}$$

$$\Delta E = Q^2 \frac{\hbar \omega_0}{\pi} \cos \frac{\ell\pi}{N}, \quad \text{with } \ell = 1, 2, \dots, (N-1), \text{ all doubly degenerate.}$$

For $N = 3$, which might apply to the X_2Y_6 molecule, each zeroth-order energy, $E_n^{(0)}$, is split into four levels with

$$(\Delta E)_n = +Q_n^2 \frac{\hbar \omega_0}{\pi}, \quad +\frac{1}{2} Q_n^2 \frac{\hbar \omega_0}{\pi}, \quad -\frac{1}{2} Q_n^2 \frac{\hbar \omega_0}{\pi}; \quad -Q_n^2 \frac{\hbar \omega_0}{\pi}.$$

The penetration factor, Q_n^2 , may of course be so small for the ground state, $n = 0$, the splitting may be unobservable (e.g., in C_2H_6).

The case of very large N is of relevance in solid-state physics, where periodic boundary conditions are used. If we have a crystalline lattice with N repeat units, we assume the $(N + 1)^{\text{th}}$ unit is identical with the first. If N is very large, the spacing of our multiplet of $2 + (N - 1) = (N + 1)$ sublevels can effectively be replaced by a band of continuum states of width $2Q_n^2\hbar\omega_0/\pi$. The penetration factor Q_n^2 is a sensitive function of $E_n^{(0)}$. For $n = 0$, far below the top of the potential barriers, we may have $Q_0^2 \ll 1$, leading to a narrow band. For $n > 0$, Q_n^2 may grow dramatically with n , leading to ever wider bands as the top of the potential barriers is approached.

Systems of Identical Particles

The Two-Electron Atom

The indistinguishability of identical particles in quantum mechanics plays a very important role. In macroscopic, classical physics we can tag our particles (by painting infinitesimally small labels on them!) so we can distinguish those labelled, 1, 2, etc., even though they have exactly the same mass, internal constitution, etc. The impossibility of such a tagging procedure plays a very fundamental role in quantum mechanics.

Consider one of the simplest systems with identical particles, the two-electron He atom, with Hamiltonian

$$H = \frac{\vec{p}_1^2}{2\mu} + V(r_1) + \frac{\vec{p}_2^2}{2\mu} + V(r_2) + \frac{e^2}{|\vec{r}_1 - \vec{r}_2|} + H_{\text{f.s.}}(\vec{r}_1, \vec{p}_1, \vec{\sigma}_1; \vec{r}_2, \vec{p}_2, \vec{\sigma}_2), \quad (1)$$

where only the last term is dependent on the spins of the two electrons and depends on these through their Pauli $\vec{\sigma}$ vectors. This fine structure term will include one-body spin-orbit and Thomas terms, two-body spin-magnetic moment-spin-magnetic moment interactions, and so on, and can be treated as truly small perturbations on the zeroth-order terms including the Coulomb repulsion term, e^2/r_{12} . Even with all fine structure terms, however, the Hamiltonian has a strictly valid symmetry. It is invariant under the interchange of the particle indices, 1 and 2.

$$\begin{aligned} H(\vec{r}_1, \vec{p}_1, \vec{\sigma}_1; \vec{r}_2, \vec{p}_2, \vec{\sigma}_2) &= H(\vec{r}_2, \vec{p}_2, \vec{\sigma}_2; \vec{r}_1, \vec{p}_1, \vec{\sigma}_1) \\ &= P_{12} H(\vec{r}_1, \vec{p}_1, \vec{\sigma}_1; \vec{r}_2, \vec{p}_2, \vec{\sigma}_2) P_{12}^{-1}, \end{aligned} \quad (2)$$

where the operator $P_{12} \equiv P_{12}^{-1}$ exchanges the indices 1 and 2 on all electron variables. P_{12} commutes with the Hamiltonian, H . The eigenfunctions of the operator

P_{12} are the symmetric and antisymmetric functions

$$\begin{aligned}\psi^{(s)} &= \frac{1}{\sqrt{2}} [\psi(\vec{r}_1, \vec{\sigma}_1; \vec{r}_2, \vec{\sigma}_2) + \psi(\vec{r}_2, \vec{\sigma}_2; \vec{r}_1, \vec{\sigma}_1)], \\ \psi^{(a)} &= \frac{1}{\sqrt{2}} [\psi(\vec{r}_1, \vec{\sigma}_1; \vec{r}_2, \vec{\sigma}_2) - \psi(\vec{r}_2, \vec{\sigma}_2; \vec{r}_1, \vec{\sigma}_1)],\end{aligned}\quad (3)$$

with eigenvalues +1 and -1, respectively, for the operator P_{12} . Thus, it seems that every energy level of the two-electron H must be two-fold degenerate to all orders in perturbation theory, because the energy eigenfunctions can be either symmetric or antisymmetric. Even more, any linear combination of the symmetric and antisymmetric functions will have the same energy. Thus,

$$\Psi = c_s \psi^{(s)} + c_a \psi^{(a)}, \quad \text{with} \quad |c_s|^2 + |c_a|^2 = 1, \quad (4)$$

is an equally acceptable energy eigenfunction of our H . This function, however, leads to a tremendous dilemma. For this last Ψ , with arbitrary c_s and c_a , the probability one electron is at position \vec{r}_0 , with spin alignment $\vec{\sigma}_0$, and the other electron is at position \vec{r}'_0 , with spin alignment $\vec{\sigma}'_0$, is given by

$$\begin{aligned}P(\vec{r}_0, \vec{\sigma}_0; \vec{r}'_0, \vec{\sigma}'_0) &= |\Psi(\vec{r}_0, \vec{\sigma}_0; \vec{r}'_0, \vec{\sigma}'_0)|^2 + |\Psi(\vec{r}'_0, \vec{\sigma}'_0; \vec{r}_0, \vec{\sigma}_0)|^2 \\ &= |c_s \psi^{(s)} + c_a \psi^{(a)}|^2 + |c_s \psi^{(s)} - c_a \psi^{(a)}|^2 \\ &= 2(|c_s|^2 |\psi^{(s)}|^2 + |c_a|^2 |\psi^{(a)}|^2).\end{aligned}\quad (5)$$

We must add the probability the electron we have labeled 1 is at \vec{r}_0 with spin alignment given by $\vec{\sigma}_0$, and electron 2 is at the primed position with primed spin alignment, to the probability the electron we have labeled 2 is at position \vec{r}_0 with spin alignment given by $\vec{\sigma}_0$, because we cannot distinguish electrons 1 and 2. Also, this probability, a physically measurable quantity, seems to be dependent on c_s and c_a . Because c_s can vary between 0 and 1, it seems this physically measurable quantity has an essentially arbitrary predicted value. Consider, in particular, the special case in which both electrons are situated at the same position, \vec{r}_0 , and both have the same spin alignment given by $\vec{\sigma}_0$. In this case $\psi^{(a)} = 0$, so in this case this probability would be $2|c_s|^2 |\psi^{(s)}|^2$. Because c_s can vary between 0 and 1, this probability could seemingly be anything between 0 and a maximum of $2|\psi^{(s)}|^2$. The way out of this seeming dilemma is furnished by nature herself! An additional property of nature exists, first discovered empirically. The states of a system of n identical particles are either all totally symmetric or all totally antisymmetric.

The totally symmetric states are symmetric under any pair exchange and hence under any number of pair exchanges or any permutation of the n particle indices. This symmetry holds for systems of identical particles with integer spins; that is, $s = 0, 1, 2, \dots$. Such particles are known as Bose–Einstein particles or as bosons.

The totally antisymmetric states change sign under any pair exchange and, hence, any odd permutation of the particle indices involving an odd number of pair exchanges, while they do not change sign under even permutations of the particle indices, involving an even number of pair exchanges. This case applies to systems of identical particles with $\frac{1}{2}$ -integral spin, $s = \frac{1}{2}, \frac{3}{2}, \frac{5}{2}, \dots$. Such particles are known as Fermi–Dirac particles or as fermions.

Because electrons have $s = \frac{1}{2}$, they are fermions and belong to the antisymmetric case. The antisymmetry, however, applies to the total wave function. A two-electron system could have a two-particle orbital wave function symmetric under the pair exchange operator applied to orbital states, provided it is multiplied by an antisymmetric two-particle spin function, or vice versa. Because our Hamiltonian is spin-independent in first approximation (where we can neglect spin-orbit and spin magnetic-moment-spin magnetic moment interactions), we would expect a product of purely orbital and purely spin functions to be a good approximation. Let us look at the two-particle spin function first. Let us, in particular, couple the two single-particle spins s to resultant two-particle spin, S . Later, we shall specialize to the electron case with $s = \frac{1}{2}$. For the moment, let s be arbitrary.

$$\psi(\vec{s}_1, \vec{s}_2)_{M_S}^S = \sum_{m_{s_a}, m_{s_b}} \psi_{m_{s_a}}(\vec{s}_1) \psi_{m_{s_b}}(\vec{s}_2) \langle sm_{s_a} sm_{s_b} | SM_S \rangle. \quad (6)$$

Now, act on this ψ with the operator P_{12}^s , where the superscript s indicates we permute indices only on spin functions

$$P_{12}^s \psi(\vec{s}_1, \vec{s}_2)_{M_S}^S = \sum_{m_{s_a}, m_{s_b}} \psi_{m_{s_a}}(\vec{s}_2) \psi_{m_{s_b}}(\vec{s}_1) \langle sm_{s_a} sm_{s_b} | SM_S \rangle. \quad (7)$$

Now, in the sum over the indices, m_{s_a}, m_{s_b} , let us rename the dummy indices, $m_{s_a} \leftrightarrow m_{s_b}$, and let us then rewrite the product of the two single-particle spin functions in reverse order, to obtain

$$P_{12}^s \psi(\vec{s}_1, \vec{s}_2)_{M_S}^S = \sum_{m_{s_a}, m_{s_b}} \psi_{m_{s_a}}(\vec{s}_1) \psi_{m_{s_b}}(\vec{s}_2) \langle sm_{s_b} sm_{s_a} | SM_S \rangle. \quad (8)$$

Next, we make use of the symmetry property of the Clebsch–Gordan coefficient

$$\langle sm_{s_b} sm_{s_a} | SM_S \rangle = (-1)^{2s-S} \langle sm_{s_a} sm_{s_b} | SM_S \rangle \quad (9)$$

to obtain

$$P_{12}^s \psi(\vec{s}_1, \vec{s}_2)_{M_S}^S = (-1)^{2s-S} \psi(\vec{s}_1, \vec{s}_2)_{M_S}^S. \quad (10)$$

Thus, with $s = \frac{1}{2}$ -integer, so $2s =$ odd integer, two-particle spin functions, with $S = 0, 2, \dots$, even integer, are antisymmetric, whereas two-particle spin functions, with $S = 1, 3, \dots$, odd integer, are symmetric. For the special case of electrons, with $s = \frac{1}{2}$, the two-particle state with $S = 0$ is antisymmetric, whereas the two-particle states with $S = 1$ are symmetric. The antisymmetric two-particle spin states, with $S = 0$, must now be matched with a symmetric two-particle orbital state; similarly, the symmetric two-particle spin states, with $S = 1$, must be matched with antisymmetric two-particle orbital states. For two-electron states with $n_a l_a \neq n_b l_b$, we can always construct both a symmetric and an antisymmetric two-particle orbital state of good two-particle orbital angular momentum, L, M_L

$$\begin{aligned} \psi_{n_a l_a, n_b l_b}(\vec{r}_1, \vec{r}_2)_{M_L}^L &= \sum_{m_a, m_b} \left[\psi_{n_a l_a m_a}(\vec{r}_1) \psi_{n_b l_b m_b}(\vec{r}_2) \right. \\ &\quad \left. \pm \psi_{n_b l_b m_b}(\vec{r}_1) \psi_{n_a l_a m_a}(\vec{r}_2) \right] \langle l_a m_a l_b m_b | LM_L \rangle \end{aligned}$$

$$= \sum_{m_a, m_b} \left[\psi_{n_a l_a m_a}(\vec{r}_1) \psi_{n_b l_b m_b}(\vec{r}_2) \langle l_a m_a l_b m_b | L M_L \rangle \right. \\ \left. \pm \psi_{n_b l_b m_b}(\vec{r}_1) \psi_{n_a l_a m_a}(\vec{r}_2) (-1)^{l_a + l_b - L} \langle l_b m_b l_a m_a | L M_L \rangle \right], \quad (11)$$

where the upper sign refers to the orbitally symmetric and the lower sign to the orbitally antisymmetric two-particle functions. In the special case, when $n_a = n_b = n$ and $l_a = l_b = l$, we can rename the indices $m_a \leftrightarrow m_b$ in the second term of this equation because they are dummy summation indices. With $n_a = n_b = n$, and $l_a = l_b = l$, therefore, the symmetric and antisymmetric two-particle orbital states of good orbital angular momentum L , M_L become

$$\psi_{nl;nl}(\vec{r}_1, \vec{r}_2)_{M_L}^L = \sum_{m_a m_b} \psi_{nl m_a}(\vec{r}_1) \psi_{nl m_b}(\vec{r}_2) \left[1 \pm (-1)^{2l-L} \right] \langle l m_a l m_b | L M_L \rangle. \quad (12)$$

Because $2l =$ even integer, in this case, symmetric two-particle states survive only for states with even L [upper sign in eq. (12)], whereas antisymmetric two-particle states survive only for states with odd L [lower sign in eq. (12)]. Thus, in two-electron configurations with $n_a l_a = n_b l_b$, the only allowed states must have either $S = 0$ and $L =$ even integer, or $S = 1$ and $L =$ odd integer. For a two-electron configuration of type $(np)^2$ in a two-valence electron atom, the only possible energy states are

$${}^1 S_0, \quad {}^1 D_2, \quad \text{and} \quad {}^3 P_{0,1,2},$$

in standard spectroscopic notation, where S is identified through a left superscript $(2S + 1)$, L is identified by the spectroscopic letter, a capital letter because the state is not a one-electron state, and the possible J values are given by a right subscript. In the He atom, the ground state with $n_a l_a = n_b l_b = 10$, i.e., with ground-state configuration $(1s)^2$, must be a pure singlet state with $L = 0$, $S = 0$, i.e., a ${}^1 S_0$ state. Excited states with configurations such as $(1s, 2s)$ or $(1s, 2p)$ have both a singlet and a triplet component, with $L = 0$ and $L = 1$, respectively, as shown in Fig. 38.1. Because only the small fine structure terms in our Hamiltonian have a spin dependence, the singlet and triplet states are almost unconnected. In addition, electromagnetic transitions between singlet and triplet states are forbidden in zeroth (electric dipole approximation), because the transition operator is spin-independent. Thus, the singlet, $S = 0$ state atoms, the so-called para-helium atoms, and the triplet, $S = 1$ state atoms, the so-called ortho-helium atoms, essentially form a mixture of two gases; transitions from singlet to triplet states being extremely rare. Finally, configurations such as $(2s)^2$ or $(2p)^2$ are not included in Fig. 38.1 because they can be expected to lie above the first ionization threshold.

A Perturbation Theory for a Two-Electron Atom

To get a very rough idea of the energy spectrum for He (or once ionized Li, twice ionized Be, etc), let us neglect all spin-dependent fine structure terms in the Hamiltonian of eq. (1) and, even further, try to consider the Coulomb repulsion

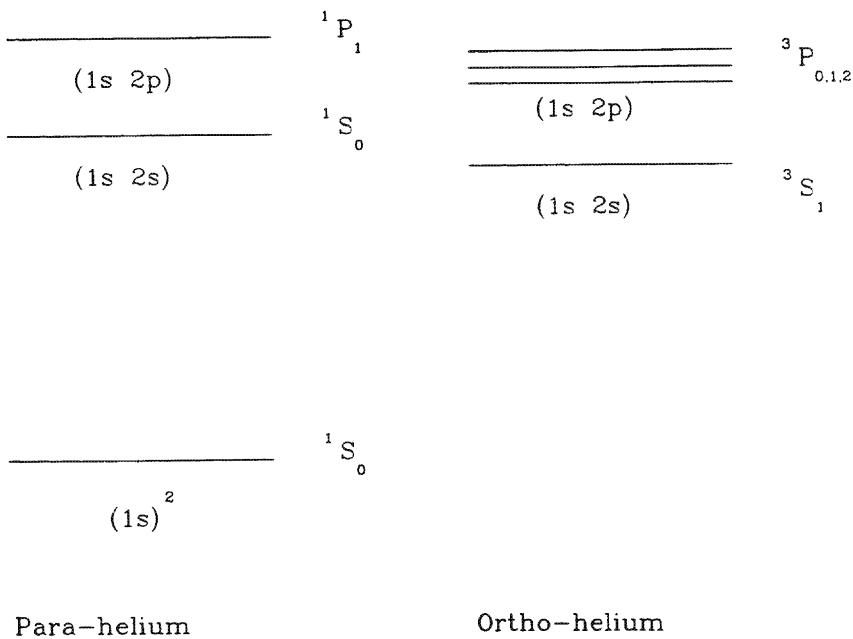


FIGURE 38.1. He atom spectrum.

term, e^2/r_{12} , as a first order perturbation. In eq. (1), the variables r_1, r_2 are the physical coordinates. Let us again introduce dimensionless r_1 and r_2 . Because we will now find it useful to separate the Z dependence of the various terms, let us make the substitutions

$$\vec{r}_{\text{phys},i} = \frac{1}{Z} \frac{\hbar^2}{\mu e^2} \vec{r}_i, \quad H_{\text{phys.}} = \frac{\mu e^4}{\hbar^2} H, \quad (13)$$

where all quantities without the subscript, phys., such as \vec{r}_1 and \vec{r}_2 are now dimensionless quantities, i.e., physical quantities given in atomic units. Then,

$$H = H^{(0)} + H^{(1)} = Z^2 \left(-\frac{1}{2} \nabla_1^2 - \frac{1}{r_1} - \frac{1}{2} \nabla_2^2 - \frac{1}{r_2} \right) + Z \frac{1}{r_{12}}. \quad (14)$$

With energies given in units of $\mu e^4/\hbar^2$, we get the dimensionless zeroth-order energy

$$E^{(0)} = -Z^2 \left(\frac{1}{2n_a^2} + \frac{1}{2n_b^2} \right), \quad (15)$$

and the first-order corrections (albeit very rough corrections!) to this energy would be given by the diagonal matrix elements of $H^{(1)}$. If, for the moment, we use the shorthand notation $a \equiv n_a l_a m_a$ and $b \equiv n_b l_b m_b$, the zeroth-order state vectors for

the two-electron system are

$$\begin{aligned} \frac{1}{\sqrt{2}}(|ab\rangle + |ba\rangle) &|S = 0, M_S = 0\rangle, \\ \frac{1}{\sqrt{2}}(|ab\rangle - |ba\rangle) &|S = 1, M_S\rangle, \end{aligned} \quad (16)$$

where the notation assumes the orbital quantum number, a or b , which appears first in the ket, refers to the particle with label 1 and that which appears second refers to particle with label 2. Because our $H^{(1)} = Z/r_{12}$ is spin-independent, no off-diagonal terms connect $S = 0$ states to $S = 1$ states. The spin states simply furnish a spin-space orthonormality integral. No spin dependence of the matrix elements exists. Therefore,

$$E^{(1)} = \frac{1}{2} \left(\left[\langle ab | H^{(1)} | ab \rangle + \langle ba | H^{(1)} | ba \rangle \right] \pm \left[\langle ab | H^{(1)} | ba \rangle + \langle ba | H^{(1)} | ab \rangle \right] \right). \quad (17)$$

Now, use

$$\begin{aligned} \langle ba | H^{(1)} | ba \rangle &= \langle ba | P_{12}^{-1} P_{12} H^{(1)} P_{12}^{-1} P_{12} | ba \rangle \\ &= \langle ab | P_{12} H^{(1)} P_{12}^{-1} | ab \rangle = \langle ab | H^{(1)} | ab \rangle, \end{aligned} \quad (18)$$

with a similar relation for $\langle ba | H^{(1)} | ab \rangle$, so

$$E^{(1)} = \langle ab | H^{(1)} | ab \rangle \pm \langle ab | H^{(1)} | ba \rangle = D_{ab} \pm X_{ab}, \quad (19)$$

where D_{ab} stands for the direct integral in which the order of the quantum numbers ab is the same in both bra and ket, whereas X_{ab} stands for the exchange integral in which the order of the quantum numbers ab is exchanged in the ket relative to the order in the bra. The upper sign (+) refers to the singlet or $S = 0$ states, whereas the lower sign (-) refers to the triplet $S = 1$ states. Because our $H^{(1)} = +Z/r_{12}$ is a positive (repulsive) interaction term, we can expect both D_{ab} and X_{ab} to be positive numbers. Thus, we would expect the triplet states to lie somewhat below the singlet states, as shown in Fig. 38.1. This is a special case of Hund's rule. In a many-electron atom, we would expect the state with the largest possible number of electron pairs coupled to spin $S = 1$ to lie lowest in energy. Thus, the lowest state should be the state with highest possible total spin S .

Finally, our final energies are spin-dependent, even though our Hamiltonian was spin-independent, the spin dependence coming from the symmetry of the two-electron orbital functions. The antisymmetric two-particle orbital functions have a smaller probability of bringing the two electrons close together. Hence, in these states, the Coulomb repulsion term between the two electrons is less effective. The resultant apparent spin-dependence of the Hamiltonian could be taken into account by introducing an effective spin-dependent Hamiltonian,

$$H_{ab}^{(1)} = D_{ab} - X_{ab} \frac{(1 + \vec{\sigma}_1 \cdot \vec{\sigma}_2)}{2}, \quad (20)$$

where we have used

$$P_{12}^{\sigma} = \frac{1}{2}(1 + \vec{\sigma}_1 \cdot \vec{\sigma}_2) = \frac{1}{2}(1 + 4\vec{s}_1 \cdot \vec{s}_2) = \frac{1}{2}(1 + 2[S(S+1) - \frac{3}{4} - \frac{3}{4}]), \quad (21)$$

which has eigenvalue +1 for an $S = 1$, or spin-symmetric state and eigenvalue -1 for an $S = 0$ or spin-antisymmetric state.

To actually carry out the direct and exchange integrals, we will expand $1/r_{12}$ in spherical harmonics

$$\begin{aligned} \frac{1}{|\vec{r}_1 - \vec{r}_2|} &= \frac{1}{\sqrt{r_1^2 + r_2^2 - 2r_1 r_2 \cos \theta_{12}}} \\ &= \sum_{k=0}^{\infty} \frac{r_2^k}{r_1^{k+1}} P_k(\cos \theta_{12}), \quad \text{for } r_2 < r_1, \\ &= \sum_{k=0}^{\infty} \frac{r_1^k}{r_2^{k+1}} P_k(\cos \theta_{12}), \quad \text{for } r_1 < r_2. \end{aligned} \quad (22)$$

We shall further use the addition theorem for spherical harmonics

$$P_k(\cos \theta_{12}) = \frac{4\pi}{(2k+1)} \sum_q Y_{kq}^*(\theta_1, \phi_1) Y_{kq}(\theta_2, \phi_2). \quad (23)$$

The direct term, D_{ab} , is made up of terms of the form

$$\begin{aligned} D_{ab} &= Z \sum_{k=0}^{\infty} \sum_q \frac{4\pi}{(2k+1)} \int_0^{\infty} dr_1 r_1^2 R_{n_a l_a}^2(r_1) \\ &\quad \times \left[\int_0^{r_1} dr_2 r_2^2 \frac{r_2^k}{r_1^{k+1}} R_{n_b l_b}^2(r_2) + \int_{r_1}^{\infty} dr_2 r_2^2 \frac{r_1^k}{r_2^{k+1}} R_{n_b l_b}^2(r_2) \right] \\ &\quad \times \int \int d\Omega_1 Y_{l_a(m_a-q)}^*(\theta_1, \phi_1) Y_{kq}^*(\theta_1, \phi_1) Y_{l_a m_a}(\theta_1 \phi_1) \\ &\quad \times \int \int d\Omega_2 Y_{l_b(m_b+q)}^*(\theta_2, \phi_2) Y_{kq}(\theta_2, \phi_2) Y_{l_b m_b}(\theta_2, \phi_2), \end{aligned} \quad (24)$$

weighted by the appropriate Clebsch-Gordan coefficients for the coupling $[l_a \times l_b]LM$. The angular integrals will in general greatly restrict the number of terms in the k sum. For the low-lying states of He, in particular, with one of the $n_a l_a$ or $n_b l_b = 10$, in general, just a single k term will exist. For the He ground state, for example, with $n_a l_a = n_b l_b = 10$, the angular integrals give

$$\int \int d\Omega Y_{00}^*(\theta, \phi) Y_{kq}(\theta, \phi) Y_{00}(\theta, \phi) = \delta_{k0} \delta_{q0} \frac{1}{\sqrt{4\pi}}, \quad (25)$$

so the energy, $E^{(1)}$, which is here given by the direct integral, gives

$$E^{(1)} = Z \int_0^{\infty} dr_1 r_1^2 R_{10}^2(r_1) \left[\int_0^{r_1} dr_2 r_2^2 \frac{1}{r_1} R_{10}^2(r_2) + \int_{r_1}^{\infty} dr_2 r_2^2 \frac{1}{r_2} R_{10}^2(r_2) \right]. \quad (26)$$

With $R_{10}(r) = 2e^{-r}$, and

$$\int_0^{r_1} dr_2 4r_2^2 e^{-2r_2} = \left[e^{-2r} (-2r^2 - 2r - 1) \right]_0^{r_1}, \quad (27)$$

and

$$\int_{r_1}^{\infty} dr_2 4r_2 e^{-2r_2} = - \left[e^{-2r} (2r + 1) \right]_{r_1}^{\infty}, \quad (28)$$

we get

$$\begin{aligned} E^{(1)} &= Z \left(4 \int_0^{\infty} dr_1 r_1 e^{-2r_1} - 4 \int_0^{\infty} dr_1 (r_1^2 + r_1) e^{-4r_1} \right) \\ &= Z \left(1! - \frac{2!}{16} - \frac{1!}{4} \right) = \frac{5}{8} Z. \end{aligned} \quad (29)$$

Thus, including this “first-order” correction term, the He atom ground-state energy would be (in atomic units $\mu e^4/\hbar^2$)

$$E = E^{(0)} + E^{(1)} = -Z^2 + \frac{5}{8} Z, \quad (30)$$

with $Z = 2, 3, \dots$ for He, once ionized Li, \dots . For He, therefore, we get

$$E \approx -4 + \frac{5}{4} = -2.75. \quad (31)$$

This result compares with the experimental value of -2.90351 . Considering the highly approximate nature of our calculation, this is not a bad result, but clearly improvements are necessary. This need for improvement will lead us to our final perturbation technique, the variational method. Before we discuss this perturbation technique, we need to make a few remarks about n identical-particle systems, with $n > 2$.

n-Identical Particle States

For the two-particle system, it was easy to make two-particle wavefunctions either symmetric or antisymmetric under exchange of particle indices. Moreover, it was easy to write the full two-particle wave functions as products of two-particle orbital and two-particle spin functions. For *n*-particle systems, however, it is in principle straightforward to make a totally symmetric or a totally antisymmetric wave function by acting on a product of *n* single-particle functions, with a symmetrizer or an antisymmetrizer operator, provided the single-particle functions include *all* variables, orbital and spin variables (and perhaps other internal variables, if they exist), appropriate for the *n*-particle system. We will denote the symmetrizer by \mathcal{S} and the antisymmetrizer by \mathcal{A} . For the two-particle system, we can construct symmetric and antisymmetric 2-particle functions via

$$\begin{aligned}\psi^{(s)}(\vec{r}_1, \sigma_1; \vec{r}_2, \vec{\sigma}_2) &= \left[\mathcal{S} = (1 + P_{(12)}) \right] \psi_a(\vec{r}_1, \vec{\sigma}_1) \psi_b(\vec{r}_2, \vec{\sigma}_2), \\ \psi^{(a)}(\vec{r}_1, \vec{\sigma}_1; \vec{r}_2, \vec{\sigma}_2) &= \left[\mathcal{A} = (1 - P_{(12)}) \right] \psi_a(\vec{r}_1, \vec{\sigma}_1) \psi_b(\vec{r}_2, \vec{\sigma}_2),\end{aligned}\quad (1)$$

where *a* and *b* now stand for all single-particle quantum numbers, e.g., $a \equiv n_a l_a m_{l_a} m_{s_a}$. To generalize this to *n*-particle systems, the symmetrizer must include, besides the identity operation, a sum over all possible permutation operators for the *n*-particle system. That is,

$$\mathcal{S} = \sum_P P, \quad (2)$$

where the sum includes all $n!$ possible permutation operators, *P*, including the identity operation, 1. For example, for $n = 3$,

$$\mathcal{S} = (1 + P_{(12)} + P_{(13)} + P_{(23)} + P_{(123)} + P_{(132)}), \quad (3)$$

where $P_{(ij)}$ are pair exchange operators, which exchange the indices i and j on both orbital and spin variables. The permutation operator $P_{(123)}$ designates the cyclic interchange of labels (123) in the order $1 \rightarrow 2, 2 \rightarrow 3, 3 \rightarrow 1$. This interchange could be achieved by first making the pair exchange $1 \leftrightarrow 3$ followed by the pair exchange $2 \leftrightarrow 3$; i.e., $P_{(123)} = P_{(23)}P_{(13)}$. We could just as well have expressed $P_{(123)}$ by $P_{(123)} = P_{(13)}P_{(12)}$, or in many other ways, e.g., $P_{(123)} = P_{(13)}P_{(23)}P_{(12)}P_{(13)}$. $P_{(123)}$ will, however, always involve a product of an even number of pair exchanges. In general, the $n!$ permutations of n labels involve $\frac{1}{2}n!$ even permutations, including the identity operation, and $\frac{1}{2}n!$ odd permutations. All even permutations can be expressed in terms of products of an even number of pair exchanges, and all odd permutations can be expressed in terms of products of an odd number of pair exchanges. For $n = 4$, the 24 permutation operators include the identity operation, six pair exchanges of type $P_{(ij)}$, three double pair exchanges of type $P_{(ij)}P_{(kl)}$, eight cyclic interchanges of type $P_{(ijk)}$ in which one label remains invariant, and six cyclic interchanges of all four labels of type $P_{(ijkl)}$, where the latter are odd permutations.

To build a totally symmetric n -particle state, for an n -boson system, we simply act with the symmetrizer, S , on a product of n single particle states. If the latter are given in Dirac ket notation, e.g.,

$$|aaaaabbccc\cdots\rangle,$$

where $a \equiv n_a l_a m_{l_a} m_{s_a}$; i.e., the quantum numbers for a include all orbital and all other (internal) quantum numbers, such as the spin quantum number m_s . In this example, the particles labeled 1, 2, 3, 4, 5 are all in the same quantum state, a , whereas particles labeled 6 and 7 are in quantum state, b , and particles labeled 8, 9, 10 are in quantum state, c , and so on. The operator S acting on such a state does not give a normalized state vector, but it is straightforward to construct the normalized totally symmetric state vector,

$$\sqrt{\frac{(n_1!n_2!n_3!\cdots)}{n!}} S |aaaaabbccc\cdots\rangle, \quad (4)$$

where we have assumed n_1 particles exist in quantum state a , n_2 particles exist in quantum state b , n_3 particles exist in quantum state c , and on on. Note, in particular, that all n bosons could be in the same quantum state. Also, in eq. (4) the symmetrizer, S , now includes only permutations that exchange particles in different quantum states, e.g., $P_{(16)}$ but not $P_{(12)}$.

For n -fermion states, we construct the n -particle states in the same way using an n -particle antisymmetrizer, A ,

$$A = \sum_P (-1)^{\sigma(P)} P, \quad \text{with} \quad \sigma(P) = \text{even (odd)} \\ \text{for } P = \text{even (odd)}. \quad (5)$$

For $n = 3$, e.g.,

$$A = [1 - P_{(12)} - P_{(13)} - P_{(23)} + P_{(123)} + P_{(132)}]. \quad (6)$$

Now, normalized states are constructed via

$$\frac{1}{\sqrt{n!}} \mathcal{A} |abc\dots\rangle. \quad (7)$$

In particular, all single-particle quantum states must now be different; i.e. $a \neq b \neq c \neq \dots$. Otherwise, the state vector would be annihilated by the antisymmetrizer \mathcal{A} . In coordinate representation, the totally antisymmetric state can also be expressed through an $n \times n$ determinant, the so-called Slater determinant,

$$\psi^{(a)} = \frac{1}{\sqrt{n!}} \begin{vmatrix} \psi_a(1) & \psi_b(1) & \psi_c(1) & \dots & \psi_k(1) \\ \psi_a(2) & \psi_b(2) & \psi_c(2) & \dots & \psi_k(2) \\ \psi_a(3) & \psi_b(3) & \psi_c(3) & \dots & \psi_k(3) \\ \dots & \dots & \dots & \dots & \dots \\ \psi_a(n) & \psi_b(n) & \psi_c(n) & \dots & \psi_k(n) \end{vmatrix}, \quad (8)$$

where the particle indices, (i) , are shorthand for $(\vec{r}_i, \vec{\sigma}_i)$. This n -particle wave function is totally antisymmetric. An odd permutation of particle indices corresponds to an odd permutation of rows of the determinant and therefore changes the sign of the determinant. Similarly, an even permutation of indices corresponds to an even permutation of rows of the determinant and does not change the sign of the determinant.

Even though we have succeeded in constructing n -particle wave functions of the appropriate totally symmetric or totally antisymmetric character, these functions may not be easy to work with. Later in the course (Chapters 78 and 79) we shall develop special techniques to deal with n -boson or n -fermion systems, involving single-boson or single-fermion creation and annihilation operators, with special commutation or anticommutation relations, respectively. The boson creation and annihilation operators are very similar to harmonic oscillator creation and annihilation operators. The fermion creation and annihilation operators will be particularly useful in quantum field theory, and we shall meet them there.

A final remark: For the n -electron atom, we would find it very convenient to separate the n -particle wave function into a product of an n -particle orbital function and an n -particle spin function because our Hamiltonian has only a very weak dependence on spin. For $n = 2$, this separation was trivial and led to orbitally symmetric spin singlet states and orbitally antisymmetric spin triplet states. For $n = 3$, this separation is already much more complicated. States with $S = \frac{3}{2}$ have totally symmetric three-particle spin functions. This fact is immediately apparent for the three-particle spin state with $S = \frac{3}{2}$ and $M_S = \frac{3}{2}$. It follows for the states with lower values of M_S because the three-particle M_S -lowering operator, $S_- = S_-(1) + S_-(2) + S_-(3)$, is totally symmetric, i.e., invariant under any permutation of particle indices. For these three-particle quartet spin states with $S = \frac{3}{2}$, it is trivial to combine this totally symmetric spin state with a totally antisymmetric orbital state. The three orbital quantum numbers $n_a l_a m_{l_a}$, $n_b l_b m_{l_b}$, and $n_c l_c m_{l_c}$ must differ in at least one of the three quantum numbers, in this totally antisymmetric orbital state. Next, it is impossible to make a totally antisymmetric three-particle spin state, because the single-particle spin states have only two available quantum

states, $m_s = \pm \frac{1}{2}$. We would require three different single-particle spin states to make a totally antisymmetric three-particle spin function. Three-particle spin functions, with $S = \frac{1}{2}$, thus, must have a mixed intermediate symmetry, neither totally antisymmetric nor totally symmetric. They must be combined with three-particle orbital functions also of such a mixed symmetry. Actually two types of intermediate-symmetry three-particle functions exist, and the two orbital and two spin functions must be combined in proper linear combination to make a totally antisymmetric total three-particle function. Already, for $n = 3$, this is no longer a completely trivial problem. For elegant techniques of handling such problems, we will find it advantageous to use the detailed properties of the permutation group of n objects. For a more detailed description of the possible intermediate symmetries for $n = 3$ and $n = 4$ in terms of the so-called Young tableaux, see the introductory part of Chapter 78.

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The Variational Method

Our final perturbation technique is the variational technique, which is particularly well-suited for finding approximations to ground-state energies and wave functions. We shall apply it, in particular, to find approximations to the ground-state energy and wave functions for the He atom.

The variational method employs the following functional: Let the solutions of an energy eigenvalue problem be part of a function space, part or all of our Hilbert space, and let ψ be a particular function of that space. Then, we define the functional, a function of functions ψ to be varied, through

$$E([\psi]) = \frac{\langle \psi | H | \psi \rangle}{\langle \psi | \psi \rangle}, \quad (1)$$

where $|\psi\rangle$ is square-integrable, but not necessarily normalized to unity; i.e., $\langle \psi | \psi \rangle$ is finite (nonzero), but not necessarily normalized to unity. Also $E([\psi])$ gives the average energy of the system in the state $|\psi\rangle$. The variational method is based on the following theorem.

Theorem: Any state vector, $|\psi\rangle$, for which the average energy, considered as a functional of the vectors of the full state vector space, is stationary is an eigenvector of the discrete spectrum of H ; and the corresponding energy eigenvalue is the stationary value of $E([\psi])$.

If we could actually carry out a variation of ψ , starting with some assumed value of ψ and varying ψ by small steps by rotating ψ by small amounts in the infinite-dimensional Hilbert space, such that we could end by finding the true minimum of the functional, we would attain the ground state eigenvector and eigenvalue exactly. Similarly, a local minimum or maximum would give us excited-state eigenvectors and eigenvalues. In actual practice, of course, we cannot do this

even with modern computers. The way the method is actually used is to restrict the variation of ψ , not to the set of all functions of the full space, but to a judiciously chosen subset of functions, perhaps a finite number of eigenfunctions of a closely related exactly soluble problem, which we guess to be the most important subspace of our full space. Alternatively, we might restrict the functions ψ to those of a specific analytical form that we guess to be good candidates. (Our physical intuition comes into play here!) These analytical functions should contain a few undetermined (variation) parameters, which are fixed at the values making the variation $\delta E = 0$. If we denote these functions, Φ , and vary $E([\Phi])$ such that $\delta E([\Phi]) = 0$, we may get a good approximation to the exact energy if $E([\Phi_0])$ and $E([\psi_0])$ differ by only a small amount.

A Proof of the Variational Theorem

To prove the variational principle theorem, let us put $E([\psi])$ in the form

$$E([\psi])\langle\psi|\psi\rangle = \langle\psi|H|\psi\rangle \quad (2)$$

and make the variation to give

$$\delta E\langle\psi|\psi\rangle + E\langle\delta\psi|\psi\rangle + E\langle\psi|\delta\psi\rangle = \langle\delta\psi|H|\psi\rangle + \langle\psi|H|\delta\psi\rangle, \quad (3)$$

or

$$\langle\psi|\psi\rangle\delta E = \langle\delta\psi|(H - E)|\psi\rangle + \langle\psi|(H - E)|\delta\psi\rangle. \quad (4)$$

Hence, we see: If $|\psi\rangle$ is an exact solution of $(H - E)|\psi\rangle = 0$, and if $\langle\psi|\psi\rangle$ is finite and nonzero, $\delta E = 0$.

Also, If $\delta E = 0$,

$$\langle\delta\psi|(H - E)|\psi\rangle + \langle\psi|(H - E)|\delta\psi\rangle = 0. \quad (5)$$

Now, the variation of $|\psi\rangle$ and the variation of $\langle\psi|$ are not independent, but because our vector space is a complex vector space and the variation of $|\psi\rangle$ is completely arbitrary, we could vary the pure real and pure imaginary parts of $|\psi\rangle$ separately and independently of each other. Equivalently, we could vary first $|\psi\rangle$ to give eq. (5), and then vary $i|\psi\rangle$ to give

$$-i\langle\delta\psi|(H - E)|\psi\rangle + i\langle\psi|(H - E)|\delta\psi\rangle = 0. \quad (6)$$

Eqs. (5) and (6), together, then yield: If $\delta E = 0$,

$$\begin{aligned} \langle\delta\psi|(H - E)|\psi\rangle &= 0 \\ \langle\psi|(H - E)|\delta\psi\rangle &= 0 \end{aligned} \quad (7)$$

separately, leading to the conclusion $|\psi\rangle$ is an exact eigenvector of H with eigenvalue E .

B Bounds on the Accuracy of the Variational Method

Because, in actual practice, we cannot vary the $|\psi\rangle$ of the full vector space, but will vary instead the $|\Phi\rangle$ of a highly restricted subspace of our vector space, it will be very useful to try to get a bound on the variational values of the energy obtained by this technique. We will show, in the subspace of the $|\Phi\rangle$, the variation of the $|\Phi\rangle$, which gives $\delta E([\Phi]) = 0$, leads to an $E([\Phi])$ such that

$$E([\Phi]) \geq E_0, \quad (8)$$

where E_0 is the exact value of the ground-state energy. To prove this, calculate

$$E([\Phi]) - E_0 = \frac{\langle \Phi | (H - E_0) | \Phi \rangle}{\langle \Phi | \Phi \rangle} = \sum_{\text{all } n} \frac{\langle \Phi | (H - E_0) | n \rangle \langle n | \Phi \rangle}{\langle \Phi | \Phi \rangle}, \quad (9)$$

where we have merely inserted the unit operator, $\sum_{\text{all } n} |n\rangle \langle n|$, into the equation and $|n\rangle$ is the exact eigenvector of H with eigenvalue E_n . The sum in this equation may include an integral over continuous energy values if the spectrum of eigenvalues E contains both a discrete part and a continuum. From the above, we get

$$E([\Phi]) - E_0 = \sum_n (E_n - E_0) \frac{\langle \Phi | n \rangle \langle n | \Phi \rangle}{\langle \Phi | \Phi \rangle} = \sum_n (E_n - E_0) \frac{|\langle n | \Phi \rangle|^2}{\langle \Phi | \Phi \rangle} \geq 0. \quad (10)$$

Thus, we know the sign of the error made in the variational technique, although the magnitude of the error is difficult to estimate, which is one of the drawbacks of the technique. However, we can proceed as follows: If we have found an approximate $E([\Phi_1])$ by varying the parameters in the set of functions Φ_1 to obtain an $E([\Phi_1])$, and if we subsequently take a more sophisticated (and hopefully better) set of trial functions, Φ_2 , perhaps with a larger number of variational parameters, then if $E([\Phi_2]) < E([\Phi_1])$, we know $E([\Phi_2])$ is a better approximation to the ground-state energy. In principle, this process could be continued to further improve our approximation. The absolute value of the error in the final approximation, however, may still be quite uncertain.

C An Example: The Ground-State Energy of the He Atom

The first step of the calculation involves a good choice of functions, Φ . Here, the ingenuity of the calculator comes to the fore. We want a family of Φ , simple enough for ease of calculation, yet complicated enough to get an accurate result. In our perturbation calculation for the He atom, our zeroth-order wave function, a simple product of hydrogenic 1s wave functions, took no account of the presence of the “second” electron. This electron partially shields the nucleus with charge Z from the “first” electron, so this one effectively sees a charge λZ rather than the full charge Z . Here, the shielding factor λ could be introduced as a very simple variational parameter. Thus, the zeroth-order single-particle wave functions,

$\psi_{n=1,l=0}^{(0)}$ of perturbation theory could be replaced by single-particle functions

$$\phi(\lambda) = R(r_i)Y_{00}(\theta_i, \phi_i) = \left(\frac{\lambda Z}{a_0}\right)^{\frac{3}{2}} 2e^{-\lambda Z r_{\text{phys},i}/a_0} \frac{1}{\sqrt{4\pi}}. \quad (11)$$

If we introduce, the dimensionless r_i , as in Chapter 38, viz. $r_{\text{phys},i} = \frac{a_0}{Z}r_i$, in terms of these dimensionless r_i , we will build the variational trial function from single-particle functions

$$\phi(\lambda) = \lambda^{\frac{3}{2}} 2e^{-\lambda r_i} \frac{1}{\sqrt{4\pi}}, \quad (12)$$

so the two-particle variational functions are

$$\Phi(\lambda) = 4\lambda^3 e^{-\lambda r_1 - \lambda r_2} \frac{1}{4\pi}. \quad (13)$$

We have chosen the $\Phi(\lambda)$ such that the normalization is $\langle \Phi(\lambda) | \Phi(\lambda) \rangle = 1$ (because it was extremely easy to do so!). Now, using the Hamiltonian, $H^{(0)} + H^{(1)}$ in the form of eq. (14) of Chapter 38, we have

$$\begin{aligned} & \langle \Phi(\lambda) | H | \Phi(\lambda) \rangle \\ &= 2Z^2 \langle \phi(\lambda) | T_{s.p.} | \phi(\lambda) \rangle + 2Z^2 \langle \phi(\lambda) | V_{s.p.} | \phi(\lambda) \rangle + Z \langle \Phi(\lambda) | \frac{1}{r_{12}} | \Phi(\lambda) \rangle, \end{aligned} \quad (14)$$

where the single-particle expectation values for the single-particle kinetic energy operator, $T_{s.p.}$, and the single-particle potential energy operator, $V_{s.p.}$, follow from

$$\begin{aligned} \langle \phi(\lambda) | T_{s.p.} | \phi(\lambda) \rangle &= -\frac{1}{2} \langle \phi(\lambda) | \frac{\partial^2}{\partial r^2} + \frac{2}{r} \frac{\partial}{\partial r} | \phi(\lambda) \rangle = \frac{\lambda^2}{2(1)^2}, \\ \langle \phi(\lambda) | V_{s.p.} | \phi(\lambda) \rangle &= -\langle \phi(\lambda) | \frac{1}{r} | \phi(\lambda) \rangle = -\lambda \frac{1}{(1)^2}, \end{aligned} \quad (15)$$

where we have simply made the substitutions, $r = r' / (\lambda)$ in the operators in these equations and have made the transformation $\lambda r = r'$ in the single-particle functions, $\phi(\lambda)$, to relate the integrals to the standard hydrogenic expectation value results, $\langle T_{s.p.} \rangle = +\frac{1}{2n^2}$, and $\langle \frac{1}{r} \rangle = \frac{1}{n^2}$, with $n = 1$. In the same way, we get

$$Z \langle \Phi(\lambda) | \frac{1}{r_{12}} | \Phi(\lambda) \rangle = \frac{5}{8} Z \lambda, \quad (16)$$

where we have again made the substitution $\lambda r_{12} = r'_{12}$ to convert the integral to the form evaluated through eq. (30) of Chapter 38. Thus,

$$E([\Phi(\lambda)]) = \langle \Phi(\lambda) | H | \Phi(\lambda) \rangle = \lambda^2 Z^2 - 2\lambda Z^2 + \frac{5}{8} \lambda Z. \quad (17)$$

With

$$\frac{\partial E(\lambda)}{\partial \lambda} = 2\lambda Z^2 - 2Z^2 + \frac{5}{8} Z = 0, \quad (18)$$

we get

$$\lambda = 1 - \frac{5}{16Z}, \quad (19)$$

or for He, with $Z = 2$, $\lambda Z = Z - \frac{5}{16} = 1.6875$, which is a reasonable value for the shielded nuclear charge. With this value of λ , the variational approximation, $E([\Phi(\lambda)])$, is

$$E([\Phi(\lambda)]) = -Z^2 + \frac{5}{8}Z - \frac{25}{256} = -\left(Z - \frac{5}{16}\right)^2. \quad (20)$$

For He, with $Z = 2$, this gives $E = -2.8477$. Recall the experimental value was $E = -2.90351$. Considering the extreme simplicity of our trial function, with a single variational parameter, this is a marked improvement over the first-order perturbation theory result of Chapter 38.

To make an improvement over the simple one-parameter variational wave function used here, Hylleraas in (1928) used a six-parameter variational function of the type

$$\Phi = e^{-\lambda(r_1+r_2)}(1 + c_1u + c_2t^2 + c_3s + c_4s^2 + c_5u^2)\frac{1}{4\pi}, \quad (21)$$

with $u = r_{12}$, $s = (r_1+r_2)$, $t = (r_1-r_2)$, defined in terms of the dimensionless coordinates, r_i , Φ being a function of the six variational parameters, λ , c_1 , c_2 , c_3 , c_4 , c_5 . These trial Φ are now not normalized. Variation of the six parameters in these Φ led to an $E([\Phi]) = -2.90362$. This result violates our theorem, $E([\phi]) \geq E_0(\text{exact})$, $E([\Phi])_{\text{Hylleraas}} < E_{\text{exp.}}$. Recall $E_{\text{exp.}} = -2.90351$. Hylleraas did not, however, include the spin-dependent fine structure terms $H_{f.s.}$ in his calculation. These terms are of order $\alpha^2 = (1/137)^2$ times the dominant terms in H and would have to be included if we want to compare with experimental results to the order of the 4th decimal place.

D The Ritz Variational Method

So far, we have illustrated the variational method with the use of trial functions built in terms of a few physically motivated parameters. In Ritz's use of the variational technique, the trial function is built in terms of an expansion in a finite number of zeroth-order eigenfunctions of a simpler related problem, with known eigenvalues and eigenfunctions.

$$|\Phi\rangle = \sum_{n=0}^N |n\rangle \langle n| \Phi \rangle = \sum_{n=0}^N c_n |n\rangle, \quad (22)$$

where the $N + 1$ parameters, c_n are now to be considered as the variational parameters, and it is now easy to choose these such that $\sum_n |c_n|^2 = 1$ and therefore $\langle \Phi | \Phi \rangle = 1$. Now,

$$\delta(\langle \Phi | H | \Phi \rangle) = 0, \quad (23)$$

subject to the subsidiary condition

$$\langle \Phi | \Phi \rangle = 1 = \sum_n |c_n|^2, \quad (24)$$

yields

$$\delta \left(\sum_{n,m}^N \langle \Phi | m \rangle \langle m | H | n \rangle \langle n | \Phi \rangle \right) = \delta \left(\sum_{n,m}^N c_m^* c_n \langle m | H | n \rangle \right) = 0, \quad (25)$$

subject to the subsidiary condition, arising from the normalization constraint

$$\delta \left(\sum_{n,m}^N c_m^* \delta_{mn} c_n \right) = 0. \quad (26)$$

Multiplying this second constraint equation by the Lagrange multiplier, named suggestively $-E$, and adding this to the first (variational) equation, we get

$$\begin{aligned} & \sum_{n,m}^N \left[\delta c_m^* (\langle m | H | n \rangle - E \delta_{mn}) c_n + c_m^* (\langle m | H | n \rangle - E \delta_{nm}) \delta c_n \right] = 0 \\ &= \sum_{n,m}^N \left[\delta c_m^* (\langle m | H | n \rangle - E \delta_{nm}) c_n + \delta c_m (\langle m | H | n \rangle^* - E \delta_{mn}) c_n^* \right] = 0, \end{aligned} \quad (27)$$

where we have used the hermitian character of the matrix elements of H and have renamed $n \leftrightarrow m$ in the second term of this equation. Now, the c_n are complex numbers, so we can vary separately the real and imaginary parts of c_n and combine these variations such that, separately, the real and imaginary parts of the above equation can be set equal to zero. This process leads to

$$\begin{aligned} & \sum_{n,m}^N \delta c_m^* (\langle m | H | n \rangle - E \delta_{nm}) c_n = 0, \\ & \sum_{n,m}^N \delta c_m (\langle m | H | n \rangle^* - E \delta_{nm}) c_n^* = 0. \end{aligned} \quad (28)$$

Because we can vary the individual c_n separately, we can set all $\delta c_k = 0$, except for one particular δc_m , leading to

$$\sum_n^N (\langle m | H | n \rangle - E \delta_{nm}) c_n = 0. \quad (29)$$

This relation is the usual eigenvalue–eigenvector equation for a finite-dimensional basis. The eigenvalues E_i , with eigenvectors given by the $c_n^{(i)}$ with $i = 0, 1, \dots, N$ are the variational approximate eigenvalues and eigenvectors. If our original basis was a “good guess,” we might expect the lowest few eigenvalues to be good approximations. Improved approximations might then be obtained by expanding the basis from an N -dimensional one to one of slightly higher dimensionality, and if our original guess was indeed a good one, this process should converge to the exact eigenvalues.

Part V

Scattering Theory

Introduction to Scattering Theory

A Potential Scattering

Until now, most of our applications have involved bound states of a quantum system. Now, in starting scattering theory, we shall be dealing with states in the continuum. We shall start by considering the scattering of a structureless point particle of mass, m , and incident momentum, \vec{p} , from a fixed scattering center via an interaction describable by a potential, $V(\vec{r})$, or the equivalent one-body problem for the relative motion of two structureless point particles of masses, m_1 and m_2 , and reduced mass, $m_1 m_2 / (m_1 + m_2)$, which again interact via a potential, $V(\vec{r})$, where \vec{r} is now the relative motion vector, $\vec{r} = \vec{r}_1 - \vec{r}_2$.

Before starting, let us make some remarks about possible generalizations as follows.

1. The particles may have spin, and a rearrangement of spin alignments may occur during the scattering process, if the interaction between the particles include spin-dependent forces.
2. The particles may not be treatable as point particles. They may be composites, made of several constituent particles. During the collision process, excitations of internal degrees of freedom of the particles may then occur (inelastic collisions), or rearrangement collisions, where constituent particles from projectile may be transferred to target or vice versa may occur.
3. Shortcomings may exist of the simple potential description of the scattering process. This difficulty may lead to nonlocal potentials. Also, in scattering of particles at relativistic energies, a simple potential description may not be possible. We shall restrict ourselves to nonrelativistic energies.

The scattering process is described by the *Scattering Cross Section*.

We assume we have an incoming beam of particles of definite fixed \vec{v} , or momentum \vec{p} , approximated by a plane wave, with specified incoming flux, that is, a fixed number of incoming particles per cm^2 per second, (initial condition). We want to calculate the probability particles are scattered into an element of solid angle, $d\Omega$, about some direction θ, ϕ , relative to the initial direction fixed by \vec{p} . (See Fig. 41.1.) It is assumed the detector detecting the scattered particles is at a distance r from the scattering center, where r is large compared with the size of the scattering quantum system. The scattering cross section is defined by

$$d\sigma = \frac{\text{number of particles scattered/sec into } d\Omega \text{ at } \theta, \phi}{\text{number of particles/cm}^2/\text{sec in incoming beam}} = I(\theta, \phi)d\Omega, \quad (1)$$

where

$$\frac{d\sigma}{d\Omega} = \text{differential scattering cross section,}$$

and

$$\sigma = \int_{\theta=0}^{\pi} \int_{\phi=0}^{2\pi} d\Omega \left(\frac{d\sigma}{d\Omega} \right) = \text{total scattering cross section.}$$

For the relative motion of the two-body problem, we need to discuss the transformation from the laboratory coordinates, \vec{r}_1 and \vec{r}_2 , to the center of mass coordinates. If we sit on the center of mass, the scattering process is describable by the relative motion vector, $\vec{r}_{\text{rel.}} \equiv \vec{r}$, where

$$\vec{r} = \vec{r}_1 - \vec{r}_2, \quad \vec{R}_{\text{c.m.}} = \frac{(m_1 \vec{r}_1 + m_2 \vec{r}_2)}{(m_1 + m_2)}, \quad (2)$$

with

$$\frac{\vec{p}}{\mu} = \dot{\vec{r}}_1 - \dot{\vec{r}}_2 = \vec{v}_1 - \vec{v}_2 = \frac{\vec{p}_1}{m_1} - \frac{\vec{p}_2}{m_2}, \quad \vec{P}_{\text{c.m.}} = \vec{p}_1 + \vec{p}_2. \quad (3)$$

In the laboratory, particle 1, the projectile, will have an initial momentum, $(m_1 \vec{v}_1)_0$, whereas particle 2, the target particle, will have an initial momentum of zero. After the scattering process, particle 1 will have a final momentum, $m_1 \vec{v}_1$, making an angle $\theta_{\text{lab.}}$ with the initial momentum direction, whereas particle 2 will recoil with momentum $m_2 \vec{v}_2$ at an angle θ_2 with respect to the initial momentum direction. (See Fig. 41.2.) We shall denote momentum and position vectors in the center of mass system with a prime. In the center of mass system, the initial momentum of particle 2 must be $(\vec{p}_2)'_0 = -(\vec{p}_1)'_0$. Similarly for the final momenta, $\vec{p}_2' = -\vec{p}_1'$. For true point particles, the scattering process is elastic, leading to $|\vec{p}_1'| = |(\vec{p}_1)'_0|$. The final momentum vector in the center of mass system has the same magnitude as the initial momentum vector, but makes an angle θ relative to the initial momentum direction. The transformation

$$\vec{r}_1 = \vec{r}_1' + \vec{R}_{\text{c.m.}} \quad (4)$$

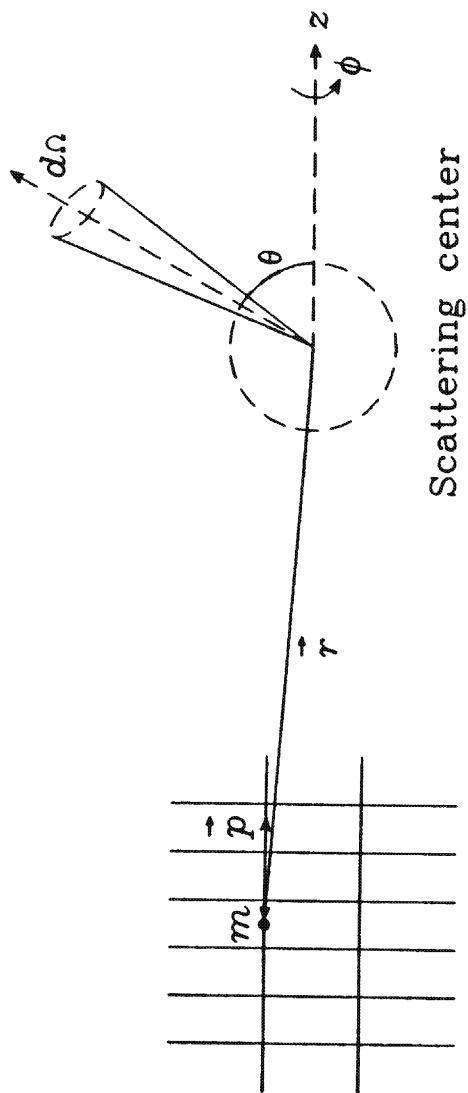


FIGURE 41.1.

leads to

$$\vec{v}'_1 = \vec{v}'_1 + \dot{\vec{R}}_{\text{c.m.}} = \vec{v}'_1 + \frac{(m_1 \vec{v}_1 + m_2 \vec{v}_2)}{(m_1 + m_2)}, \quad (5)$$

and

$$\vec{v}'_1 = \frac{m_2}{(m_1 + m_2)} (\vec{v}_1 - \vec{v}_2), \quad (6)$$

or

$$\vec{p}'_1 = m_1 \vec{v}'_1 = \mu (\vec{v}_1 - \vec{v}_2). \quad (7)$$

Similarly, using $(\vec{v}_2)_0 = 0$, we have

$$(\vec{p}_1)'_0 = \mu (\vec{v}_1)_0, \quad (8)$$

and because $|\vec{p}'_1| = |(\vec{p}_1)'_0|$, we have

$$|(\vec{v}_1 - \vec{v}_2)| = |(\vec{v}_1)_0|. \quad (9)$$

Now, from eq. (5) and Fig. 41.3,

$$\tan \theta_{\text{lab.}} = \frac{v'_1 \sin \theta}{(v'_1 \cos \theta + |\dot{\vec{R}}_{\text{c.m.}}|)} = \frac{\sin \theta}{(\cos \theta + \frac{m_1}{m_2})}, \quad (10)$$

where we have used

$$\frac{|\dot{\vec{R}}_{\text{c.m.}}|}{v'_1} = \frac{m_1 |(\vec{v}_1)_0|}{(m_1 + m_2)} \times \frac{(m_1 + m_2)}{m_2 |(\vec{v}_1 - \vec{v}_2)|} = \frac{m_1}{m_2}. \quad (11)$$

Now, the number of particles per second going into the detector, as seen by observers in the laboratory, or the center of mass system is one and the same number

$$d\sigma = I_{\text{lab.}}(\theta_{\text{lab.}}, \phi_{\text{lab.}}) \sin \theta_{\text{lab.}} d\theta_{\text{lab.}} d\phi_{\text{lab.}} = I(\theta, \phi) \sin \theta d\theta d\phi, \quad (12)$$

so the differential cross sections, as seen in the laboratory and the center of mass frames

$$\left(\frac{d\sigma}{d\Omega} \right)_{\text{lab.}} = I_{\text{lab.}}(\theta_{\text{lab.}}, \phi_{\text{lab.}}), \quad \left(\frac{d\sigma}{d\Omega} \right)_{\text{c.m.}} = I(\theta, \phi), \quad (13)$$

are related by

$$\left(\frac{d\sigma}{d\Omega} \right)_{\text{lab.}} = \left(\frac{d\sigma}{d\Omega} \right)_{\text{c.m.}} \frac{\sin \theta d\theta}{\sin \theta_{\text{lab.}} d\theta_{\text{lab.}}} = \left(\frac{d\sigma}{d\Omega} \right)_{\text{c.m.}} \frac{d(\cos \theta)}{d(\cos \theta_{\text{lab.}})}. \quad (14)$$

With

$$\cos \theta_{\text{lab.}} = \frac{(\cos \theta + \frac{m_1}{m_2})}{\sqrt{(1 + \frac{m_1^2}{m_2^2} + 2 \frac{m_1}{m_2} \cos \theta)}}, \quad (15)$$

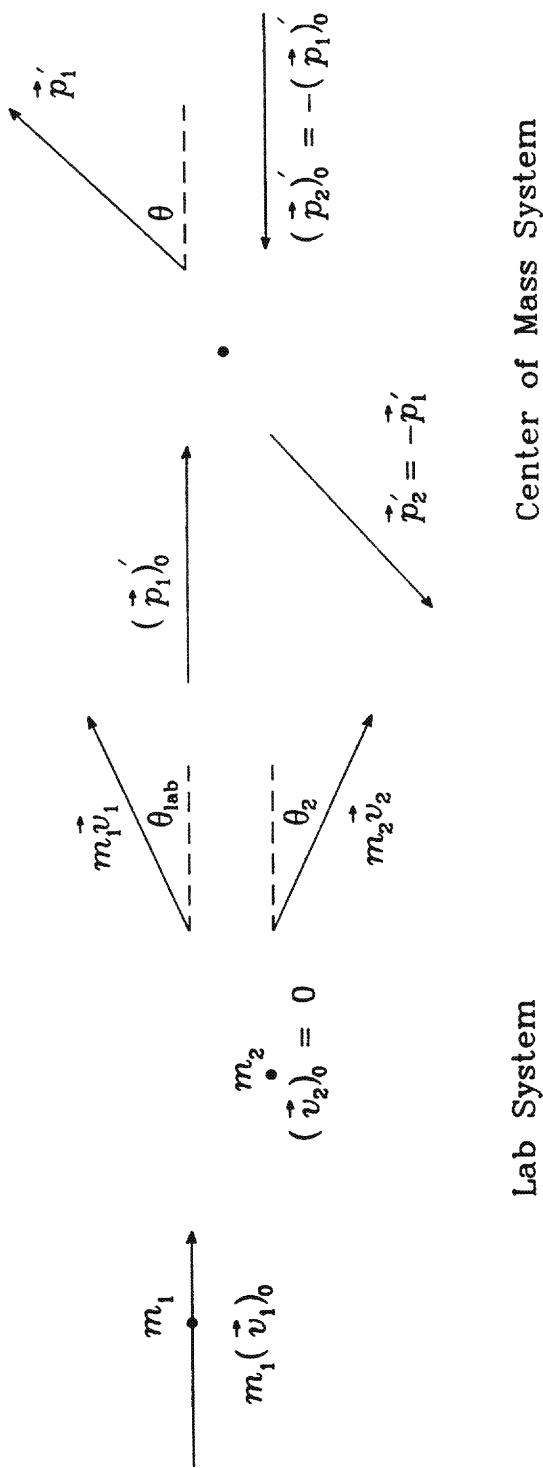


FIGURE 41.2.

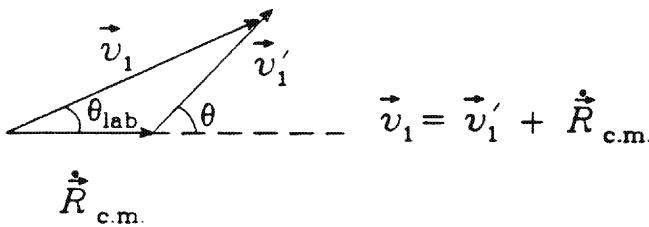


FIGURE 41.3.

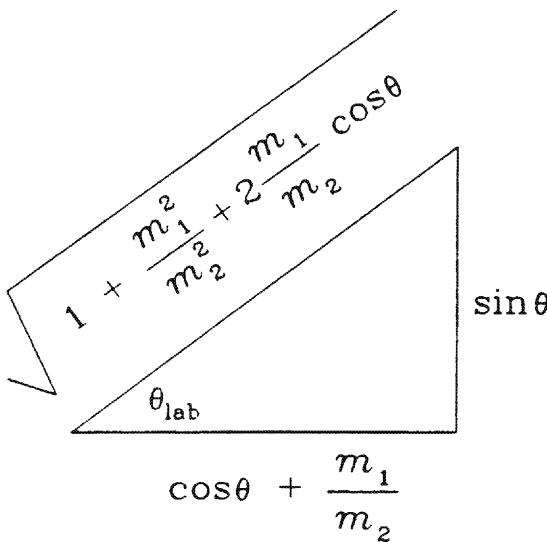


FIGURE 41.4.

(see Fig. 41.4), we get

$$d(\cos \theta_{\text{lab}}) = d(\cos \theta) \times \frac{(1 + \frac{m_1}{m_2} \cos \theta)}{\left(1 + \frac{m_1^2}{m_2^2} + 2 \frac{m_1}{m_2} \cos \theta\right)^{\frac{3}{2}}}. \quad (16)$$

This equation leads to

$$\left(\frac{d\sigma}{d\Omega}\right)_{\text{lab.}} = \left(\frac{d\sigma}{d\Omega}\right)_{\text{c.m.}} \frac{\left(1 + \frac{m_1^2}{m_2^2} + 2 \frac{m_1}{m_2} \cos \theta\right)^{\frac{3}{2}}}{\left(1 + \frac{m_1}{m_2} \cos \theta\right)}. \quad (17)$$

Having established this relationship between the differential scattering cross sections in the laboratory and the center of mass systems, we shall henceforth work entirely in the center of mass system, and calculate differential cross sections only in the center of mass system.

To solve the scattering problem, we need to find solutions to the Schrödinger equation

$$\nabla^2 \psi + \frac{2\mu}{\hbar^2} (E - V(\vec{r})) \psi = 0, \quad (18)$$

where ψ is a function of the relative coordinate vector \vec{r} for the two-body system. Moreover, the solutions ψ we seek must satisfy the boundary conditions of the physical situation: Asymptotically, as $r \rightarrow \infty$, ψ must be of the form, $\psi = \text{incoming plane wave} + \text{spherical outgoing wave}$ starting from the scattering center; that is, as $r \rightarrow \infty$,

$$\psi = e^{i\vec{k}\cdot\vec{r}} + f(\theta, \phi) \frac{e^{ikr}}{r}, \quad (19)$$

where $\vec{k} = \vec{p}/\hbar$. The function, $f(\theta, \phi)$, is known as the scattering amplitude. The flux for the incoming wave, $\psi_{\text{inc.}} = e^{i\vec{k}\cdot\vec{r}}$, is

$$\frac{\hbar}{2\mu i} (\psi_{\text{inc.}}^* \vec{\nabla} \psi_{\text{inc.}} - \psi_{\text{inc.}} \vec{\nabla} \psi_{\text{inc.}}^*) = \frac{\hbar}{2\mu i} (i\vec{k} - (-i\vec{k})) = \frac{\hbar\vec{k}}{\mu} = \frac{\vec{p}}{\mu} = \vec{v}. \quad (20)$$

Similarly, the flux of the outgoing scattered wave, normal to the surface of the detector, at a distance, $r \rightarrow \infty$, is

$$\frac{\hbar}{2\mu i} (\psi_{\text{out}}^* \frac{\partial \psi_{\text{out}}}{\partial r} - \psi_{\text{out}} \frac{\partial \psi_{\text{out}}^*}{\partial r}) = \frac{\hbar k}{\mu} \frac{|f(\theta, \phi)|^2}{r^2} + \text{Order}\left(\frac{1}{r^3}\right), \quad (21)$$

leading to

$$d\sigma = \frac{\left(\frac{\hbar k}{\mu} \times \frac{|f(\theta, \phi)|^2}{r^2} \times r^2 d\Omega \right)}{\frac{\hbar k}{\mu}}, \quad (22)$$

so

$$\frac{d\sigma}{d\Omega} = |f(\theta, \phi)|^2. \quad (23)$$

A note about the normalization of our ψ is perhaps in order. Above we have normalized the incoming plane wave such that the incoming flux had magnitude, $\hbar k/\mu = v \equiv v_{\text{rel.}}$. This normalization factor, however, drops out in the expression for the cross section. A second possibility might have been to normalize the incoming plane wave to unit flux, in which case we could have used

$$\psi_{\text{inc.}} = \frac{e^{i\vec{k}\cdot\vec{r}}}{\sqrt{v}}. \quad (24)$$

Since, \vec{k} , and hence \vec{p} , has a continuous spectrum, we could also have normalized the incoming plane wave according to the standard coordinate space representation

$$u_{\vec{k}}(\vec{r}) \equiv \langle \vec{r} | \vec{k} \rangle = \frac{e^{i\vec{k}\cdot\vec{r}}}{(2\pi)^{\frac{3}{2}}}, \quad (25)$$

so these plane wave states have the standard Dirac delta function orthonormality property, $\langle \vec{k}' | \vec{k} \rangle = \delta(\vec{k}' - \vec{k})$. Alternatively, we could have used the coordinate space function

$$u_{\vec{p}}(\vec{r}) \equiv \langle \vec{r} | \vec{p} \rangle = \frac{e^{i\vec{p}\cdot\vec{r}/\hbar}}{(2\pi\hbar)^{\frac{3}{2}}}, \quad (26)$$

so $\langle \vec{p}' | \vec{p} \rangle = \delta(\vec{p}' - \vec{p})$.

Finally, we could have used a box normalization for our plane wave by imagining that all of our quantum systems are located in a cubical “laboratory” where the cube has a side of length L , hence, volume, L^3 ; where L is a macroscopic quantity; and where all wave functions must be zero at the surface of the cube. This means that we will replace the continuous spectrum for \vec{k} with a very finely spaced discrete spectrum, with

$$k_x = \frac{2\pi}{L} n_1, \quad k_y = \frac{2\pi}{L} n_2, \quad k_z = \frac{2\pi}{L} n_3, \quad (27)$$

where the n_i are integers (positive or negative). [This condition means the wavelengths of our discrete set of states are such that our cube of side L must contain an integral (rather than a $\frac{1}{2}$ -integral) number of wavelengths, so we are using so-called periodic boundary conditions.] With this type of plane wave state, our plane wave functions are normalized according to

$$u_{\vec{n}}(\vec{r}) = \frac{e^{i\vec{k}_{\vec{n}} \cdot \vec{r}}}{\sqrt{L^3}} = \frac{e^{i\vec{k}_{\vec{n}} \cdot \vec{r}}}{\sqrt{\text{Vol.}}}, \quad (28)$$

where the orthonormality integral is now given by

$$\langle \vec{k}_{\vec{n}'} | \vec{k}_{\vec{n}} \rangle = \delta_{n_1 n'_1} \delta_{n_2 n'_2} \delta_{n_3 n'_3} \quad (29)$$

in terms of ordinary Kronecker deltas. Because no quantum-mechanical result for a system of atomic or subatomic size can depend on the size or shape of the macroscopic “laboratory,” the Volume = L^3 , must drop out of all meaningful final results that must be independent of L . This form of the plane wave state, therefore, has its uses, and we shall occasionally use it as a pedagogic device. For the moment, however, we shall stick with the normalization of eq. (19).

To solve the relative motion problem and find solutions of the form of eq. (19), it will be useful to expand both the incoming plane wave and the scattering amplitude, $f(\theta, \phi)$, in spherical harmonics. Choosing our z axis along the direction of the incoming \vec{k} ,

$$e^{i\vec{k}\cdot\vec{r}} = e^{ikr \cos\theta} = \sum_l c_l R_l(r) P_l(\cos\theta), \quad (30)$$

where it will be useful to write the radial functions in terms of the dimensionless variable kr and convert to the one-dimensionalized radial functions, $u_l(r)$, with $R_l(kr) = u_l(kr)/kr$. The radial equation for the free waves is then given by

$$\frac{d^2 u_l}{dr^2} + (k^2 - \frac{l(l+1)}{r^2}) u_l(r) = 0, \quad \text{with} \quad k^2 = \frac{2\mu E}{\hbar^2}, \quad (31)$$

or, with $kr = \rho$,

$$\frac{d^2 u_l}{d\rho^2} + \left(1 - \frac{l(l+1)}{\rho^2}\right) u_l(\rho) = 0. \quad (32)$$

To recognize this equation, it will be useful to make the transformation, $u_l(\rho) = \sqrt{\rho} v_l(\rho)$ (although we will not actually use the v_l to find the general solutions). The differential equation in the $v_l(\rho)$ becomes

$$\rho^2 \frac{d^2 v_l}{d\rho^2} + \rho \frac{dv_l}{d\rho} + [\rho^2 - (l + \frac{1}{2})^2] v_l(\rho) = 0. \quad (33)$$

This is recognized as the Bessel equation with index $n = \pm(l + \frac{1}{2})$. The solutions for $R_l(kr) = u_l(\rho)/\rho$ are then (with an additional normalization factor, $\sqrt{\frac{\pi}{2}}$),

$$\frac{u_l(\rho)}{\rho} = \sqrt{\frac{\pi}{2\rho}} J_{(l+\frac{1}{2})}(\rho) \equiv j_l(\rho), \quad (34)$$

and

$$\frac{u_{-(l+1)}(\rho)}{\rho} = \sqrt{\frac{\pi}{2\rho}} J_{-(l+\frac{1}{2})}(\rho) \equiv n_l(\rho)(-1)^{l+1}, \quad (35)$$

where we have made use of the invariance of the quantity $l(l+1)$ under the transformation, $l \rightarrow -(l+1)$, hence, $(l + \frac{1}{2}) \rightarrow -(l + \frac{1}{2})$. In the above equations, the j_l and n_l are standard spherical Bessel functions and spherical Neumann functions, respectively. [The phase factor $(-1)^{l+1}$, as well as the normalization factor $\sqrt{\frac{\pi}{2}}$, are needed to get the “standard” functions.]

B Spherical Bessel Functions

To get the needed properties of the spherical Bessel and Neumann functions, we shall use the equation for the $u_l(\rho)$ in the form

$$\left(-\frac{d^2}{d\rho^2} + \frac{l(l+1)}{\rho^2}\right) u_l(\rho) = 1 u_l(\rho) \quad (36)$$

and use the factorization method of Chapter 7 to study the solutions. The factors are

$$O_{\pm}(l) = \left(\mp \frac{d}{d\rho} + \frac{l}{\rho}\right), \quad (37)$$

so

$$\begin{aligned} O_+(l) O_-(l) u_l &= \left(-\frac{d^2}{d\rho^2} + \frac{l(l+1)}{\rho^2}\right) u_l = [\lambda - \mathcal{L}(l)] u_l, \\ O_-(l+1) O_+(l+1) u_l &= \left(-\frac{d^2}{d\rho^2} + \frac{l(l+1)}{\rho^2}\right) u_l = [\lambda - \mathcal{L}(l+1)] u_l. \end{aligned} \quad (38)$$

Comparing with eq. (36), we see that $\lambda = 1$ and $\mathcal{L}(l) = 0$. Hence, the possible l values can range from $+\infty$ to $-\infty$. Of course, the possible l values are further

restricted to be integers by the angular functions of eq. (30). The negative integers, which yield the functions $u_{-(l+1)}$, and hence the spherical Neumann functions, are acceptable through the invariance of the quantity $l(l+1)$ under the transformation $l \rightarrow -(l+1)$. To get the starting function, for the l step processes, we look at the equation for $l = 0$

$$-\frac{d^2 u_0}{d\rho^2} = u_0, \quad (39)$$

so u_0 could be either $\sin \rho$ or $\cos \rho$. Note, however, that u_0 is identified with j_0 through $j_0 = u_0/\rho$, and since the $j_l(\rho)$ are the solutions regular at the origin, $\rho = 0$, we must choose $u_0 = \sin \rho$; hence, $j_0 = \sin \rho/\rho$. From this, we get

$$\begin{aligned} j_1 &= \frac{1}{\rho} O_+(1) u_0 = \frac{1}{\rho} \left(-\frac{d}{d\rho} + \frac{1}{\rho} \right) \sin \rho = -\frac{\cos \rho}{\rho} + \frac{\sin \rho}{\rho^2}, \\ -n_0 &= \frac{1}{\rho} O_-(0) u_0 = \frac{1}{\rho} \frac{d}{d\rho} \sin \rho = \frac{\cos \rho}{\rho}. \end{aligned} \quad (40)$$

Continuing this process, we can get the j_l and n_l for higher l . We list a few:

$$\begin{aligned} j_0 &= \frac{\sin \rho}{\rho}, \\ j_1 &= -\frac{\cos \rho}{\rho} + \frac{\sin \rho}{\rho^2}, \\ j_2 &= -\frac{\sin \rho}{\rho} - 3\frac{\cos \rho}{\rho^2} + 3\frac{\sin \rho}{\rho^3}, \end{aligned} \quad (41)$$

and

$$\begin{aligned} n_0 &= -\frac{\cos \rho}{\rho}, \\ n_1 &= -\frac{\sin \rho}{\rho} - \frac{\cos \rho}{\rho^2}, \\ n_2 &= \frac{\cos \rho}{\rho} - 3\frac{\sin \rho}{\rho^2} - 3\frac{\cos \rho}{\rho^3}. \end{aligned} \quad (42)$$

The j_l are regular at the origin, whereas the n_l are not. A general expression in terms of $l+1$ terms with alternating sin and cos functions can also be obtained from the repeated step-up/down operations (see mathematical appendix):

$$\begin{aligned} j_l(\rho) &= \sum_{k=0}^l \frac{\sin[\rho - \frac{\pi}{2}(l-k)]}{\rho^{k+1}} \frac{(l+k)!}{k!(l-k)!2^k}, \\ n_l(\rho) &= -\sum_{k=0}^l \frac{\cos[\rho - \frac{\pi}{2}(l-k)]}{\rho^{k+1}} \frac{(l+k)!}{k!(l-k)!2^k}. \end{aligned} \quad (43)$$

The approximate values in the limit $\rho \rightarrow \infty$ (which we shall need!) are

$$\begin{aligned} j_l(\rho) &\rightarrow \frac{\sin[\rho - \frac{\pi}{2}l]}{\rho}, \\ n_l(\rho) &\rightarrow -\frac{\cos[\rho - \frac{\pi}{2}l]}{\rho}. \end{aligned} \quad (44)$$

Finally (see mathematical appendix), the power series expansions for the spherical Bessel functions are

$$\begin{aligned} j_l(\rho) &= \sum_{k=0}^{\infty} \frac{(-1)^k 2^l (l+k)!}{k! (2l+2k+1)!} \rho^{l+2k} = \frac{2^l l!}{(2l+1)!} \rho^l + \dots, \\ n_l(\rho) &= -\frac{1}{\rho^{l+1}} \sum_{k=0}^{\infty} \frac{(2l-2k)!}{2^l (l-k)!} \rho^{2k} = -\frac{1}{\rho^{l+1}} \frac{(2l)!}{2^l l!} + \dots. \end{aligned} \quad (45)$$

With these properties of the spherical Bessel functions, we can return to eqs. (19) and (30). In particular, because $e^{ikr \cos \theta}$ is regular at the origin, only the solutions j_l regular at the origin can occur in the expansion of eq. (30), so that

$$e^{i\vec{k}\cdot\vec{r}} = e^{ikr \cos \theta} = \sum_{l=0}^{\infty} c_l j_l(kr) P_l(\cos \theta). \quad (46)$$

To determine the coefficients c_l in this expansion, we use the orthogonality of the Legendre polynomials

$$c_l j_l(kr) = \frac{(2l+1)}{2} \int_0^\pi d\theta \sin \theta e^{ikr \cos \theta} P_l(\cos \theta). \quad (47)$$

To evaluate the c_l through this integral, it is sufficient to take the limit $kr \rightarrow 0$, and note only the l^{th} term in the power series expansion of the exponential term in the integral can make a contribution to the integral, so

$$c_l \frac{2^l l! (kr)^l}{(2l+1)!} = \frac{(2l+1)}{2} \frac{(ikr)^l}{l!} \int_0^\pi d\theta \sin \theta \cos^l \theta P_l(\cos \theta). \quad (48)$$

The θ -integral can now be done via the orthonormality integral of the Legendre polynomials, and the relation

$$\cos^l \theta = \frac{2^l (l!)^2}{(2l)!} P_l(\cos \theta) + b_{l-2} P_{l-2}(\cos \theta) + \dots \quad (49)$$

Note that the leading, i.e., highest power, term in the expansion of $P_l(x)$ in powers of x can be obtained most easily from the Rodrigues formula

$$P_l(x) = \frac{1}{2^l l!} \frac{d^l}{dx^l} (x^2 - 1)^l = \frac{1}{2^l l!} \frac{d^l}{dx^l} x^{2l} + \dots = \frac{(2l)!}{2^l (l!)^2} x^l + \dots \quad (50)$$

The integral of eq. (48) then yields

$$c_l \frac{2^l l! (kr)^l}{(2l+1)!} = \frac{(ikr)^l}{l!} \frac{2^l (l!)^2}{(2l)!}, \quad \text{hence } c_l = i^l (2l+1), \quad (51)$$

so

$$e^{ikr \cos \theta} = \sum_{l=0}^{\infty} i^l (2l+1) j_l(kr) P_l(\cos \theta). \quad (52)$$

Mathematical Appendix to Chapter 41. Spherical Bessel Functions

The spherical Bessel functions, $j_l(\rho)$, can be obtained from $j_0(\rho)$, via repeated application of the step-up relation

$$j_{l+1} = \frac{u_{l+1}}{\rho} = \frac{1}{\rho} \left(-\frac{d}{d\rho} + \frac{(l+1)}{\rho} \right) u_l. \quad (1)$$

It will be convenient to define

$$y_l(\rho) \equiv \frac{j_l}{\rho^l} = \frac{u_l}{\rho^{l+1}}, \quad (2)$$

so

$$y_{l+1} = \frac{1}{\rho^{l+2}} \left(-\frac{d}{d\rho} + \frac{(l+1)}{\rho} \right) u_l = \frac{1}{\rho^{l+2}} \left(-\frac{d}{d\rho} + \frac{(l+1)}{\rho} \right) (\rho^{l+1} y_l) = -\frac{1}{\rho} \frac{dy_l}{d\rho}. \quad (3)$$

Similarly, if we define a second y_l via

$$y_l(\rho) \equiv \frac{n_l}{\rho^l} = \frac{u_{-(l+1)}}{\rho^{l+1}} (-1)^{l+1}, \quad (4)$$

then

$$\begin{aligned} y_{l+1} &= \frac{(-1)^{l+2}}{\rho^{l+2}} \left(\frac{d}{d\rho} - \frac{(l+1)}{\rho} \right) u_{-(l+1)} \\ &= \frac{(-1)^{l+2}}{\rho^{l+2}} \left(\frac{d}{d\rho} - \frac{(l+1)}{\rho} \right) ((-1)^{l+1} \rho^{l+1} y_l) = -\frac{1}{\rho} \frac{dy_l}{d\rho}. \end{aligned} \quad (5)$$

Therefore, for both the spherical Bessel and Neumann functions, y_l can be obtained from y_0 by the successive action of l operations

$$-\frac{1}{\rho} \frac{d}{d\rho}.$$

If we define the l -independent operator

$$\mathcal{D} \equiv \frac{1}{\rho} \frac{d}{d\rho}, \quad (6)$$

then

$$y_l(\rho) = (-1)^l \mathcal{D}^l y_0(\rho). \quad (7)$$

[$y_0(\rho)$ is $(\sin \rho / \rho)$ for the spherical Bessel functions and it is $-(\cos \rho / \rho)$ for the spherical Neumann functions.] We can simplify the operator \mathcal{D} with a change of variable

$$\rho = \sqrt{2t}, \quad t = \frac{1}{2} \rho^2, \quad (8)$$

so

$$\mathcal{D} = \frac{1}{\rho} \frac{d}{d\rho} = \frac{d}{dt} \quad (9)$$

and, then,

$$y_l(\sqrt{2t}) = (-1)^l \frac{d^l}{dt^l} y_0(\sqrt{2t}). \quad (10)$$

We shall now express this function, involving an l^{th} derivative of y_0 , in terms of a contour integral via the Cauchy integral formula for the l^{th} derivative

$$\frac{d^l f(z)}{dz^l} = \frac{l!}{2\pi i} \oint \frac{f(\zeta) d\zeta}{(\zeta - z)^{l+1}} \quad (11)$$

or, in language appropriate to our y_l ,

$$y_l(\sqrt{2t}) = \frac{(-1)^l l!}{2\pi i} \oint \frac{y_0(\sqrt{2\tau})}{(\tau - t)^{l+1}} d\tau. \quad (12)$$

Because our functions y_0 must have a branch cut ending on the singularity at $\tau = 0$, and we are interested in functions y_l at real positive values of t . The point $\tau = t$ must be on the positive real axis in the complex τ -plane, and the contour around this point must avoid the branch cut. We can achieve this result by locating the branch cut on the negative real axis in the τ -plane. (See Fig. 41.5).

It will be useful to calculate first the y_l for the spherical Hänkel functions, which are defined by

$$h_l^{(1)}(\rho) = j_l(\rho) + i n_l(\rho), \quad (13)$$

$$h_l^{(2)}(\rho) = j_l(\rho) - i n_l(\rho), \quad (14)$$

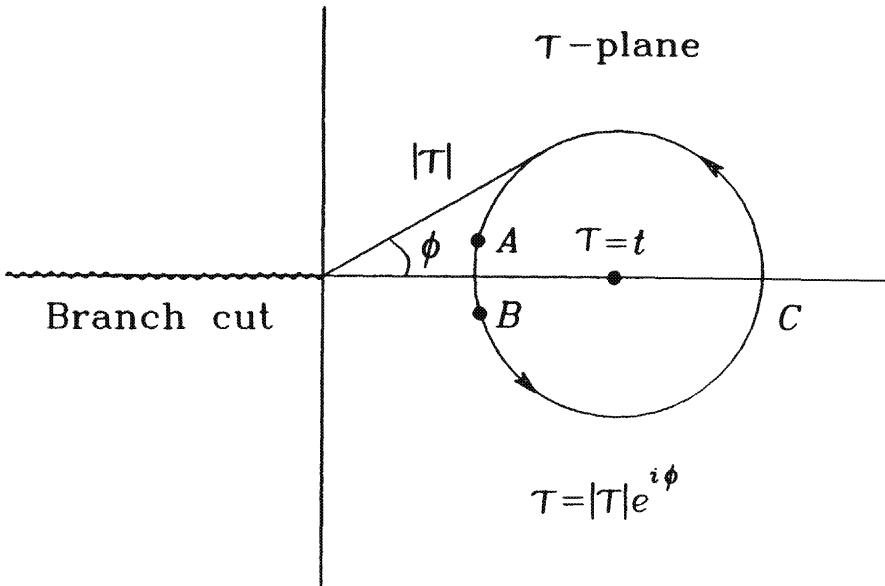


FIGURE 41.5. Contour for eq. (16).

in particular, with

$$h_0^{(1)}(\rho) = -\frac{i}{\rho} e^{i\rho}, \quad h_0^{(2)}(\rho) = +\frac{i}{\rho} e^{-i\rho}. \quad (15)$$

For these equations then

$$y_l(\sqrt{2t}) = \frac{(-1)^l l! (\mp i)}{2\pi i} \oint_C d\tau \frac{e^{\pm i\sqrt{2\tau}}}{\sqrt{2\tau}(\tau-t)^{l+1}}, \quad (16)$$

where the contour, C , is that of Fig. 41.5 and the upper(lower) case refers to the y_l for $h_l^{(1)}$ ($h_l^{(2)}$). To actually carry out the contour integral, it will be convenient to make additional transformations.

For $h_l^{(1)}$, let

$$[2\tau]^{\frac{1}{2}} = -\rho z, \quad \frac{d\tau}{[2\tau]^{\frac{1}{2}}} = -\rho dz. \quad (17)$$

This transformation maps the point $\tau = t$ of the τ plane into the point $z = -1$ in the z plane, and the contour, C , of the τ plane into a contour, C_1 , in the left half of the complex z plane. [See Fig. 41.6 (a).] This equation leads to the contour integral expression

$$\frac{h_l^{(1)}(\rho)}{\rho^l} = \frac{(-1)^l l!}{2\pi} \oint_{C_1} \frac{dz \rho e^{-i\rho z}}{\left(\frac{\rho^2 z^2}{2} - \frac{\rho^2}{2}\right)^{l+1}}, \quad (18)$$

so

$$h_l^{(1)}(\rho) = \frac{(-1)^l 2^l l!}{\pi \rho^{l+1}} \oint_{C_1} \frac{e^{-i\rho z} dz}{[(z-1)(z+1)]^{l+1}}. \quad (19)$$

Conversely, for $h_l^{(2)}$, we make the substitution

$$[2\tau]^{\frac{1}{2}} = +\rho z, \quad \frac{d\tau}{[2\tau]^{\frac{1}{2}}} = \rho dz. \quad (20)$$

This transformation will now map the point $\tau = t$ of the τ plane into the point $z = +1$ in the complex z plane, and the contour, C , of the τ plane into a contour, C_2 , now in the right half of the complex z plane. [See Fig. 41.6 (b).] With this transformation, we get

$$h_l^{(2)}(\rho) = \frac{(-1)^l 2^l l!}{\pi \rho^{l+1}} \oint_{C_2} \frac{e^{-i\rho z} dz}{[(z-1)(z+1)]^{l+1}}. \quad (21)$$

The integrals are the same for both spherical Hänkel functions. Only the contours are different, going about the points $z = -1$ for $h_l^{(1)}$, and $z = +1$ for $h_l^{(2)}$. To evaluate the contour integrals, we merely use the residue theorem. For example, to evaluate the contour integral for $h_l^{(1)}$, we need to expand the function

$$\frac{e^{-i\rho z}}{(z-1)^{l+1}}$$

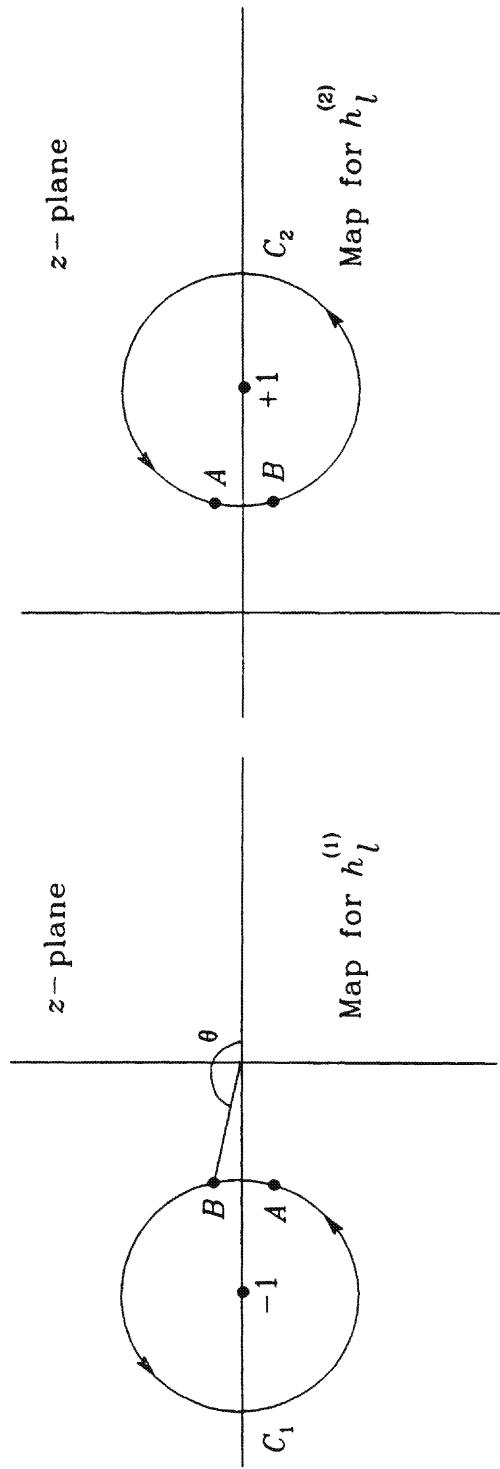


FIGURE 41.6. Contours for eqs. (18) and (21).

in powers of $(z + 1)$. The contour integral will be $2\pi i \times$ the coefficient of the $(z + 1)^l$ term in this expansion. We need

$$e^{-i\rho z} = e^{i\rho} e^{-i\rho(z+1)} = \sum_{n=0}^{\infty} e^{i\rho} \frac{(-i\rho)^n}{n!} (z+1)^n \quad (22)$$

$$\begin{aligned} \frac{1}{(z-1)^{l+1}} &= \frac{1}{(z+1-2)^{l+1}} = \frac{1}{(-2)^{l+1}[1-\frac{1}{2}(z+1)]^{l+1}} \\ &= \sum_{k=0}^{\infty} \frac{1}{(-2)^{l+1}} \frac{(l+1)_k}{k!} \frac{(z+1)^k}{2^k} = \sum_{k=0}^{\infty} \frac{(l+k)!}{(-2)^{l+1} l! k! 2^k} (z+1)^k, \end{aligned} \quad (23)$$

so

$$\frac{e^{-i\rho z}}{(z-1)^{l+1}} = \sum_{n=0}^{\infty} \sum_{k=0}^{\infty} e^{i\rho} \frac{(-i\rho)^n}{n!} \frac{(l+k)!}{l! k! (-1)^{l+1} 2^{l+1+k}} (z+1)^{n+k}. \quad (24)$$

The coefficient of the $(z+1)^l$ term has contributions only from terms with $n = l-k$, and terms with $k = 0$ to $k = l$. Thus, the contour integral has the value

$$2\pi i \sum_{k=0}^l e^{i\rho} \frac{\rho^{l-k} (-i\rho)^{l-k} (l+k)!}{l! k! (l-k)! (-1)^{l+1} 2^{l+1+k}}, \quad (25)$$

so

$$h_l^{(1)}(\rho) = \sum_{k=0}^l \frac{e^{i(\rho-(l+1-k)\frac{\pi}{2})}}{\rho^{k+1}} \frac{(l+k)!}{k!(l-k)! 2^k}. \quad (26)$$

In the same fashion, the contour integral about C_2 can be evaluated to give

$$h_l^{(2)}(\rho) = \sum_{k=0}^l \frac{e^{-i(\rho-(l+1+k)\frac{\pi}{2})}}{\rho^{k+1}} \frac{(l+k)!}{k!(l-k)! 2^k}. \quad (27)$$

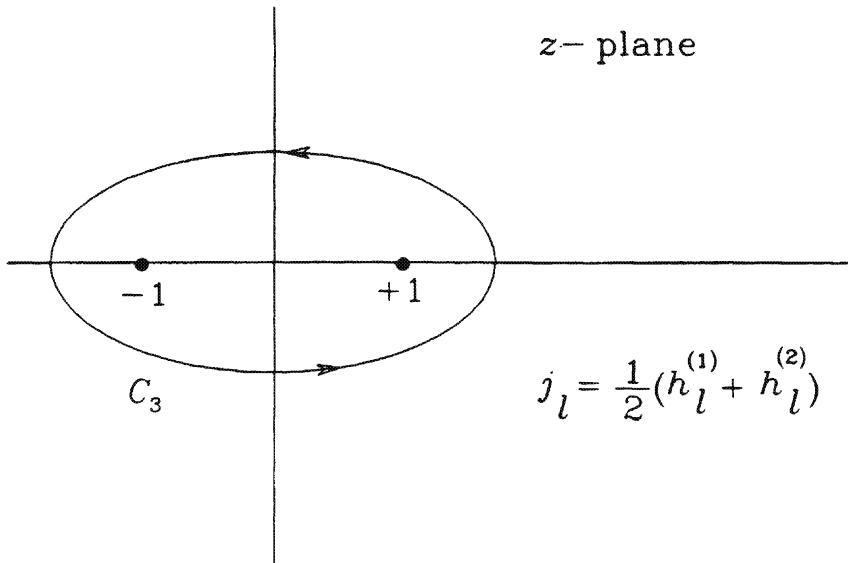
Combining these via eqs. (13) and (14), we get the expressions for $j_l(\rho)$ and $n_l(\rho)$ given through eq. (43) of the main body of Chapter 41.

Finally, we can also use the contour integral expressions to evaluate the infinite power series expansions for the spherical Bessel and Neumann functions. Again, using eqs. (13) and (14) with eqs. (18) and (20), we can express j_l and n_l via similar contour integrals. For example,

$$j_l(\rho) = \frac{(-1)^l l! 2^l}{2\pi \rho^{l+1}} \oint_{C_3} \frac{e^{-i\rho z} dz}{[(z-1)(z+1)]^{l+1}}, \quad (28)$$

where the contour, C_3 , now encircles both the points $z = -1$ and $z = +1$ (see Fig. 41.7). The similar expression for $n_l(\rho)$ would involve a contour, C_4 , shown in Fig. 41.8.

To evaluate the contour integral for j_l , make a new transformation, $z' = \rho z$, which transforms the singular points $z = \pm 1$ of the z plane into $z' = \pm \rho$ in the z'

FIGURE 41.7. Contour for $j_l(\rho)$, eq. (28).

plane. This process gives

$$\begin{aligned}
 j_l(\rho) &= \frac{(-1)^l l! 2^l \rho^l}{2\pi} \oint_{C_3} \frac{e^{-iz'} dz'}{[(z' - \rho)(z' + \rho)]^{l+1}} \\
 &= \frac{(-1)^l l! 2^l \rho^l}{2\pi} \oint_{C_3} \frac{e^{-iz'} dz'}{z'^{(2l+2)} \left(1 - \frac{\rho^2}{z'^2}\right)^{l+1}} \\
 &= \frac{(-1)^l l! 2^l \rho^l}{2\pi} \sum_{k=0}^{\infty} \frac{\rho^{2k} (l+k)!}{l! k!} \oint_{C_3} \frac{e^{-iz'} dz'}{z'^{(2l+2+2k)}}. \tag{29}
 \end{aligned}$$

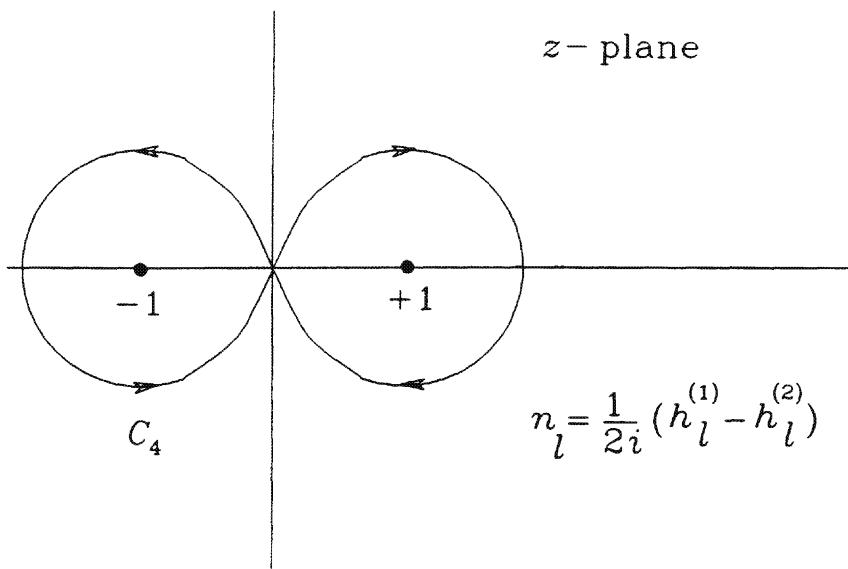
The contour integral in this expression is again evaluated by the residue theorem and has the value

$$2\pi i \times \frac{(-i)^{2l+2k+1}}{(2l+2k+1)!} = \frac{2\pi (-1)^{l+k}}{(2l+2k+1)!},$$

yielding

$$j_l(\rho) = \sum_{k=0}^{\infty} \frac{(-1)^k 2^l (l+k)!}{k! (2l+2k+1)!} \rho^{l+2k}, \tag{30}$$

which was quoted in eq. (45) of the main body of Chapter 41. The corresponding expression for n_l can be obtained from the corresponding contour integral over the contour C_4 of Fig. 41.8. In this case, it may be more efficient to evaluate the contour integral only for the dominant $1/\rho^{l+1}$ term, and then obtain the remaining terms of the infinite series via a two-term recursion formula for the c_k in the expan-

FIGURE 41.8. Contour for $n_l(\rho)$.

sion, $n_l(\rho) = \sum_k c_k \rho^{2k-l-1}$. This recursion formula follows from the differential equation for the n_l by standard techniques.

42

The Rayleigh–Faxen–Holtzmark Partial Wave Expansion: Phase Shift Method

We shall now solve the scattering problem, that is, find solutions for the Schrödinger equation [eq. (18) of Chapter 41] in the form of eq. (19) of Chapter 41 for a spherically symmetric $V(r)$ that goes to zero faster than $1/r^2$ as $r \rightarrow \infty$. [Note: For such a potential, the effective $V(r)$ approaches the pure centrifugal term for sufficiently large r . Also, we exclude for the moment the case of scattering via a Coulomb potential with a $V(r)$ that goes to zero only as $1/r$ at large r . Our assumed $V(r)$ would be good for the scattering of neutrons from complex nuclei, but the scattering of charged particles from nuclei, e.g., the scattering of protons or alpha particles from nuclei, would require a slightly more complicated treatment.]

We shall expand the solution to the relative motion equation

$$\nabla^2\psi + \frac{2\mu}{\hbar^2}(E - V(r))\psi = 0 \quad (1)$$

in a series similar to that of the expansion of the incoming plane wave of Chapter 41

$$\psi = \sum_{l=0}^{\infty} \frac{w_l(kr)}{(kr)} P_l(\cos \theta). \quad (2)$$

This equation is the partial wave expansion. The ψ are independent of the azimuthal angle, ϕ . This axial symmetry is dictated by the spherical symmetry of $V(r)$ and the axial symmetry about the direction of the incoming beam. In the above, the l^{th} partial wave solution is determined by the radial function, $R_l(kr) \equiv w_l(kr)/(kr)$, which is a solution of the one-dimensionalized wave equation

$$\frac{d^2w_l}{dr^2} + \left(k^2 - \frac{2\mu}{\hbar^2}V(r) - \frac{l(l+1)}{r^2} \right) w_l = 0. \quad (3)$$

As $r \rightarrow \infty$, $V(r) \rightarrow 0$, such that $V_{\text{effective}} \rightarrow V_{\text{centrifugal}}$. Thus, $w_l(kr) \rightarrow$ is a linear combination of the free-wave radial solutions $(kr)j_l(kr)$ and $(kr)n_l(kr)$. From their asymptotic form [see eq. (44) of Chapter 41], this is a linear combination of $\sin(kr - \frac{l\pi}{2})$ and $\cos(kr - \frac{l\pi}{2})$, so, as $r \rightarrow \infty$,

$$\begin{aligned} w_l(kr) &\rightarrow a_l \sin(kr - \frac{l\pi}{2} + \delta_l(k)), \\ \frac{w_l(kr)}{(kr)} &\rightarrow \frac{a_l}{2ikr} \left(e^{ikr} (-i)^l e^{i\delta_l} - e^{-ikr} (i)^l e^{-i\delta_l} \right). \end{aligned} \quad (4)$$

Here, a_l is the amplitude of the l^{th} partial wave, and δ_l , an energy (k)-dependent quantity, is its phase shift. To find the differential scattering cross section, we need to compare these partial wave solutions with the expected asymptotic form of our solution

$$\psi = e^{i\vec{k}\cdot\vec{r}} + f(\theta) \frac{e^{ikr}}{r}. \quad (5)$$

Expanding, $f(\theta)$, through

$$f(\theta) = \sum_{l=0}^{\infty} f_l P_l(\cos \theta), \quad (6)$$

and using eq. (52) of the last chapter to expand the plane wave, we have, as $r \rightarrow \infty$,

$$\begin{aligned} \psi &\rightarrow \sum_l \left(i^l (2l+1) \frac{\sin(kr - \frac{\pi}{2}l)}{kr} + f_l \frac{e^{ikr}}{r} \right) P_l(\cos \theta) \\ &\rightarrow \sum_l \left(\frac{e^{ikr}}{r} \left(f_l + \frac{(2l+1)}{2ik} \right) - \frac{e^{-ikr}}{r} \frac{(-1)^l (2l+1)}{2ik} \right) P_l(\cos \theta). \end{aligned} \quad (7)$$

Comparing with eqs. (2) and (4),

$$a_l = i^l (2l+1) e^{i\delta_l} \quad \text{and} \quad f_l = \frac{(2l+1)}{2ik} (e^{2i\delta_l} - 1), \quad (8)$$

so

$$\begin{aligned} f(\theta) &= \sum_{l=0}^{\infty} \frac{i(2l+1)}{2k} (1 - e^{2i\delta_l(k)}) P_l(\cos \theta) \\ &= \sum_{l=0}^{\infty} e^{i\delta_l(k)} \frac{(2l+1)}{k} \sin \delta_l(k) P_l(\cos \theta), \end{aligned} \quad (9)$$

leading to

$$\begin{aligned} \frac{d\sigma}{d\Omega} &= |f(\theta)|^2 = \left| \sum_l \frac{(2l+1)}{2k} (1 - \eta_l) P_l(\cos \theta) \right|^2 \\ &= \left| \sum_l e^{i\delta_l} \frac{(2l+1)}{k} \sin \delta_l P_l(\cos \theta) \right|^2, \end{aligned} \quad (10)$$

where the common shorthand notation, $\eta_l = e^{2i\delta_l}$, has been used in the first form. Using the orthogonality integral

$$\int \int d\Omega P_l(\cos \theta) P_{l'}(\cos \theta) = \frac{4\pi}{(2l+1)} \delta_{ll'}, \quad (11)$$

these two expressions lead to expressions for the total cross section

$$\begin{aligned} \sigma &= \sum_l \frac{\pi}{k^2} (2l+1) |1 - \eta_l|^2 \\ &= \sum_l \frac{4\pi}{k^2} (2l+1) \sin^2 \delta_l. \end{aligned} \quad (12)$$

A number of remarks are in order, as follows.

1. For $V(r) \rightarrow 0$, $\delta_l(k) \rightarrow 0$. In this case, we are left only with the free incoming plane wave.

2. In the limit of very large k , in particular, for $\frac{\hbar^2 k^2}{2\mu} \gg |V_{\max}|$, again $\delta_l(k) \rightarrow 0$ as $k \rightarrow$ very large. Effectively, the potential again becomes insignificant compared with the energy of the incoming beam.

3. For an attractive $V(r)$, $\delta_l(k) > 0$. In this case, the wavelength becomes shorter in the small r region where the potential is effective, and the l^{th} partial wave is pulled into smaller values of r as a result (see Fig. 42.1). Say the first minimum of the l^{th} partial wave beyond the region where the true $V(r)$ is effectively zero occurs at a phase angle, χ_1 . Then, $(kr_{\text{with}} - \frac{\pi l}{2} + \delta_l) = (kr_{\text{without}} - \frac{\pi l}{2}) = \chi_1$, where r_{with} is the position of this minimum *with* the potential $V(r)$ turned on, whereas r_{without} is the position of this minimum *without* the potential, that is, for the free partial wave. Because $r_{\text{with}} < r_{\text{without}}$, $\delta_l(k) > 0$.

Similarly, for a repulsive $V(r)$, $\delta_l(k) < 0$.

4. The total scattering cross section, σ , is related to the imaginary part of the scattering amplitude, $f(\theta = 0)$. From the second form for $f(\theta)$ and σ above,

$$\sigma(k) = \frac{4\pi}{k} \Im[f(\theta = 0)]. \quad (13)$$

This form is a special case of the so-called Optical Theorem. It also leads to the Wick inequality for the elastic scattering cross section

$$\sigma_{\text{elastic}} \leq \frac{4\pi}{k} \sqrt{\frac{d\sigma}{d\Omega}(\theta = 0)}. \quad (14)$$

Note,

$$\frac{d\sigma}{d\Omega} = (\Im[f(\theta)])^2 + (\Re[f(\theta)])^2.$$

5. A relation exists between the maximum l for which $\delta_l(k)$ is appreciably different from zero and the magnitude k of the incoming wave. Thus, although our expressions for both $\frac{d\sigma}{d\Omega}$ and σ in general involve an infinite series in l , only a finite number of terms may be effective. Suppose the range of our $V(r)$ is r_0 ; i.e., $V(r) \approx 0$ for $r > r_0$. Classically, if a projectile particle comes in with an impact parameter, $b > r_0$, it will “miss” feeling the potential and not be scattered

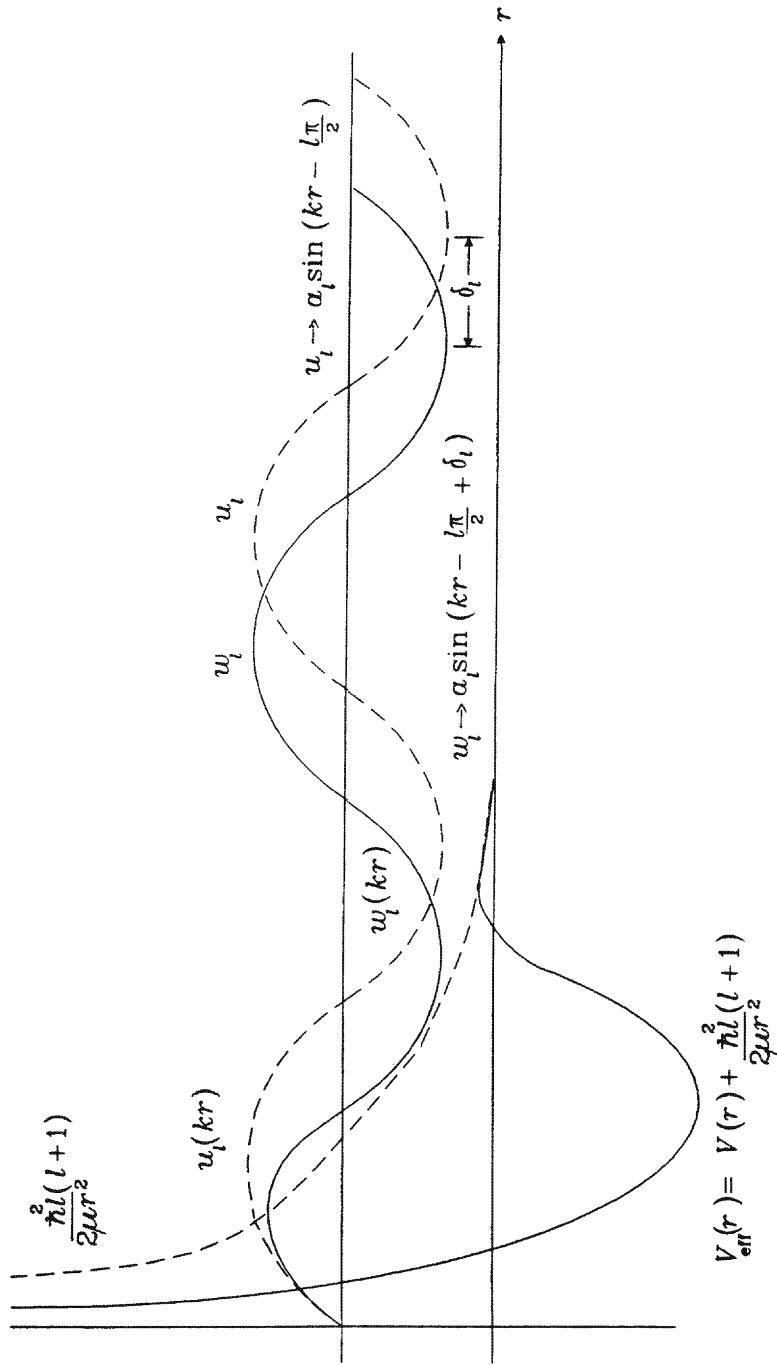


FIGURE 42.1. The l th partial wave solutions, u_l (plane wave), and w_l [with attractive $V(r)$].

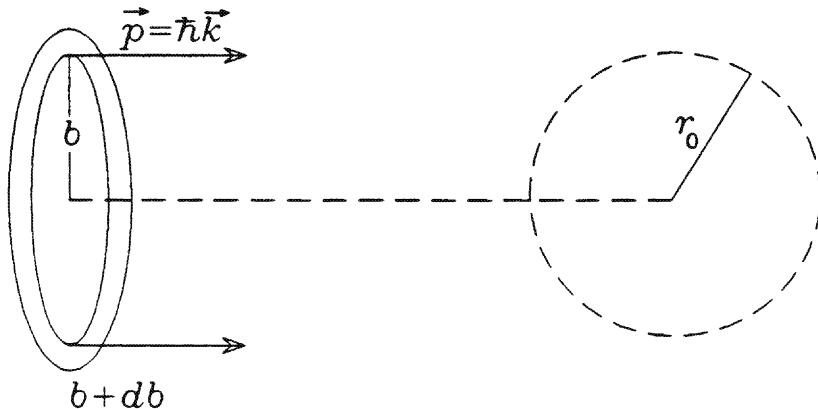


FIGURE 42.2. Semiclassical picture of the scattering process.

at all. (See Fig. 42.2.) Although the wave nature of the particle motion and the uncertainty relation washes out this relationship somewhat, it nevertheless still has approximate validity. The angular momentum of an incoming particle with impact parameter, b , is $\hbar kb$. Approximately,

$$\hbar kb \approx \hbar\sqrt{l(l+1)}, \quad b \approx \frac{l}{k}. \quad (15)$$

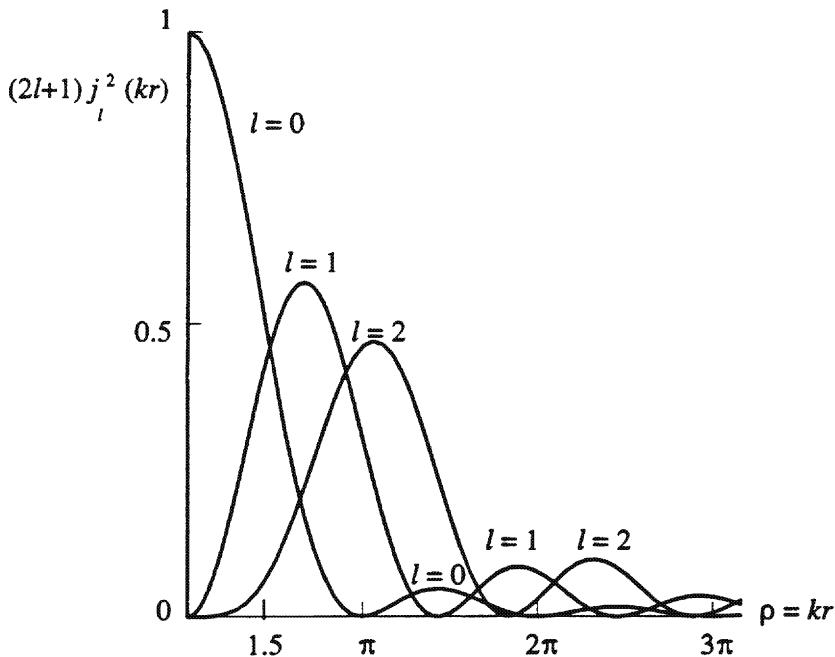
Because we expect strong scattering only for $b < r_0$, we expect δ_l will be appreciably different from zero only for $l \leq kr_0$, where this relation might be a particularly good approximation for large l , where semiclassical arguments are valid. Recalling $P_l(\cos \theta) = \sqrt{4\pi/(2l+1)}Y_{l0}$, the plane wave expansion in terms of normalized angular functions, Y_{lm} , is

$$e^{ikr \cos \theta} = \sum_l i^l \sqrt{4\pi(2l+1)} j_l(kr) Y_{l0}(\theta), \quad (16)$$

so the probability of finding the l^{th} partial wave component of the plane wave within a radius r_0 is proportional to the integrated value, from 0 to r_0 , of the function $(2l+1)j_l(kr)^2$. This function is plotted for the lower l values in Fig. 42.3. We see, e.g., if $kr_0 = 1.5$, only the $l = 0$ and $l = 1$ partial waves will have a large probability of penetrating into the effective range of the potential. In general, for very small k , that is, for extreme low energy scattering, only the $l = 0$ term will contribute to the differential scattering cross section. Because $P_0(\cos \theta) = 1$, independent of θ , the scattering will be isotropic. In this case,

$$f(\theta) \approx e^{i\delta_0} \frac{\sin \delta_0}{k}, \quad (17)$$

$$\frac{d\sigma}{d\Omega} = \frac{\sin^2 \delta_0}{k^2}, \quad \sigma = 4\pi \frac{\sin^2 \delta_0}{k^2}. \quad (18)$$

FIGURE 42.3. The functions $(2l+1)[j_l(kr)]^2$.

In the extreme low-energy limit, therefore, the cross section is proportional to the square of the wavelength. In this low-energy limit, the pertinent length is the wavelength of the incident beam, not the size of the scatterer.

If the energy is somewhat higher so both phase shifts, δ_1 and δ_0 , contribute, but assuming $\delta_1 \ll 1$, then

$$\begin{aligned} \frac{d\sigma}{d\Omega} &= \frac{\sin^2 \delta_0}{k^2} + \frac{6}{k^2} \cos(\delta_0 - \delta_1) \sin \delta_0 \sin \delta_1 \cos \theta + \dots \\ &\simeq \frac{1}{k^2} (\sin^2 \delta_0 + 3\delta_1 \sin 2\delta_0 \cos \theta + \dots) \\ &= A + B \cos \theta + \dots \end{aligned} \quad (19)$$

With $B \ll A$, the differential cross section is almost isotropic but does now have a weak $\cos \theta$ dependence.

6. The determination of the $\delta_l(k)$ from a known $V(r)$ is in principle straightforward and just a matter of calculation. Often, however, $V(r)$ is unknown and we would like to determine it from the observed differential cross sections at different energies. Although the $\delta_l(k)$ can be determined from the observed $\frac{d\sigma}{d\Omega}$, the determination of the $V(r)$ from these $\delta_l(k)$ is difficult. The “inverse” problem is tough.

7. Generalizations to scattering of complex projectile from complex target particles. So far, we have studied only the scattering of structureless point projectile

particles from structureless point target particles. If we name projectile particle, a , and target particle, A , we have in general three possibilities, as follows.

(1) $a + A \rightarrow a + A$, the elastic scattering process.

(2) $a + A \rightarrow a + A'$. Particle A is in an excited state after the scattering process and the final kinetic energy of the relative motion is less than the initial kinetic energy. This is an inelastic scattering process.

(3) $a + A \rightarrow b + B$. This is a rearrangement collision. The ejectiles are different from the initial projectile and target particles. In such a process, the number of outgoing particles could also be greater than two.

The different processes are labeled by a “channel” index: α for the elastic process (1) and $\beta = \beta_1 + \beta_2 + \dots$ for the processes of type (2) and (3). For the case of structureless point particles, we could have written our solution, as $r \rightarrow \infty$, in the form

$$\psi \rightarrow \sum_l \frac{i\sqrt{\pi(2l+1)v_\alpha}}{k_\alpha} i^l Y_{l0}(\theta, \phi) \left(I_l(k_\alpha r) - \eta_{l,\alpha} O_l(k_\alpha r) \right), \quad (20)$$

where the incoming and outgoing l^{th} partial wave relative motion functions are now given in the unit flux normalization, [see eq. (24) of Chapter 41], and

$$I_l(k_\alpha r) = \frac{1}{\sqrt{v_\alpha}} \frac{e^{-i(k_\alpha r - \frac{\pi l}{2})}}{r}, \quad O_l(k_\alpha r) = \frac{1}{\sqrt{v_\alpha}} \frac{e^{i(k_\alpha r - \frac{\pi l}{2})}}{r}. \quad (21)$$

For the case of complex projectile and target, this process can now be generalized. Now, as $r \rightarrow \infty$,

$$\psi \rightarrow \sum_l \frac{i\sqrt{\pi(2l+1)v_\alpha}}{k_\alpha} \sum_\beta (\mathcal{I}_{l,\alpha} - \eta_{l,\beta} \mathcal{O}_{l,\beta}), \quad (22)$$

where the sum over β includes the elastic term, $\beta = \alpha$, and all other β_i , and the outgoing and incoming wave functions must now include, besides the asymptotic outgoing and incoming relative motion functions, the appropriate internal wave functions for the particles a , A , or b , and B .

$$\begin{aligned} \mathcal{I}_{l,\alpha} &= i^l Y_{l0}(\theta, \phi) I_l(k_\alpha r) \psi_{\text{internal}}(\xi_a) \psi_{\text{internal}}(\xi_A), \\ \mathcal{O}_{l,\beta} &= i^l Y_{l0}(\theta, \phi) O_l(k_\beta r) \psi_{\text{internal}}(\xi_b) \psi_{\text{internal}}(\xi_B), \end{aligned} \quad (23)$$

where the ξ_a, ξ_A, \dots , stand for the needed internal variables of the various particles. Now,

$$\begin{aligned} \sigma_{\text{total}} &= \sigma_{\text{elastic}} + \sigma_{\text{reaction}} \\ &= \sigma_\alpha + \sum_{\beta \neq \alpha} \sigma_\beta \\ &= \frac{\pi}{k_\alpha^2} \sum_l \sum_{\text{all } \beta} (2l+1) |\delta_{\alpha\beta} - \eta_{l,\beta}|^2 \\ &= \frac{\pi}{k_\alpha^2} \sum_l (2l+1) \left(|1 - \eta_{l,\alpha}|^2 + \sum_{\beta \neq \alpha} |\eta_{l,\beta}|^2 \right). \end{aligned} \quad (24)$$

Later, we shall see the conservation of probability, the so-called unitarity condition, will require

$$(|\eta_{l,\alpha}|^2 + \sum_{\beta \neq \alpha} |\eta_{l,\beta}|^2) = 1. \quad (25)$$

Previously, we saw for the case of pure elastic scattering, e.g., at low energies, where all inelastic processes and rearrangement collisions are energetically forbidden, $\eta_{l,\alpha} = e^{2i\delta_{l,\alpha}}$. Now, in general, $|\eta_{l,\beta}| \leq 1$. The unitarity condition severely restricts the values of the l^{th} partial cross sections, σ_l . Fig. 42.4 gives a plot of the possible values of $\sigma_{\text{elastic},l}$ versus $\sigma_{\text{reaction},l}$, both in units of $\pi(2l+1)/k_\alpha^2$.

A final remark: Eqs. (20) and (22) can also be used for the case of scattering by a Coulomb potential, provided the r dependence in the exponential factors in the incoming and outgoing relative motion functions, $I_l(kr)$ and $O_l(kr)$, are replaced by slightly more complicated r -dependent functions.

Mathematical Appendix to Chapter 42

Continuum Solutions for the Coulomb Problem

In the main body of Chapter 42, we restricted our discussion to potentials that go to zero faster than $1/r^2$ as $r \rightarrow \infty$. This, therefore, excluded the important case of the Coulomb potential, $V(r) = Z_1 Z_2 e^2 / r$, needed for the scattering of point charges from point charges. We shall be interested, in particular, in the asymptotic form of the l^{th} partial wave solutions, w_l , in the limit $r \rightarrow \infty$, to obtain the analogues of the incoming and outgoing wave solutions, $I_l(kr)$ and $O_l(kr)$.

For the Coulomb potential, the one-dimensionalized wave equation is given by

$$\frac{d^2 w_l}{dr^2} + \left(k^2 - \frac{2\mu}{\hbar^2} \frac{Z_1 Z_2 e^2}{r} - \frac{l(l+1)}{r^2} \right) w_l = 0, \quad (1)$$

$$\frac{d^2 w_l}{dr^2} + \left(k^2 - \frac{2\gamma k}{r} - \frac{l(l+1)}{r^2} \right) w_l = 0, \quad (2)$$

where we have introduced the Coulomb parameter

$$\gamma = \frac{\mu e^2 Z_1 Z_2}{\hbar^2 k} = \frac{\mu c e^2}{\hbar k \hbar c} Z_1 Z_2 = \frac{c}{v} \alpha Z_1 Z_2. \quad (3)$$

In addition, it will be useful to introduce the new variable

$$\rho = ikr, \quad (4)$$

so

$$-\frac{d^2 w_l}{d\rho^2} + \left(1 - \frac{2i\gamma}{\rho} + \frac{l(l+1)}{\rho^2} \right) w_l = 0. \quad (5)$$

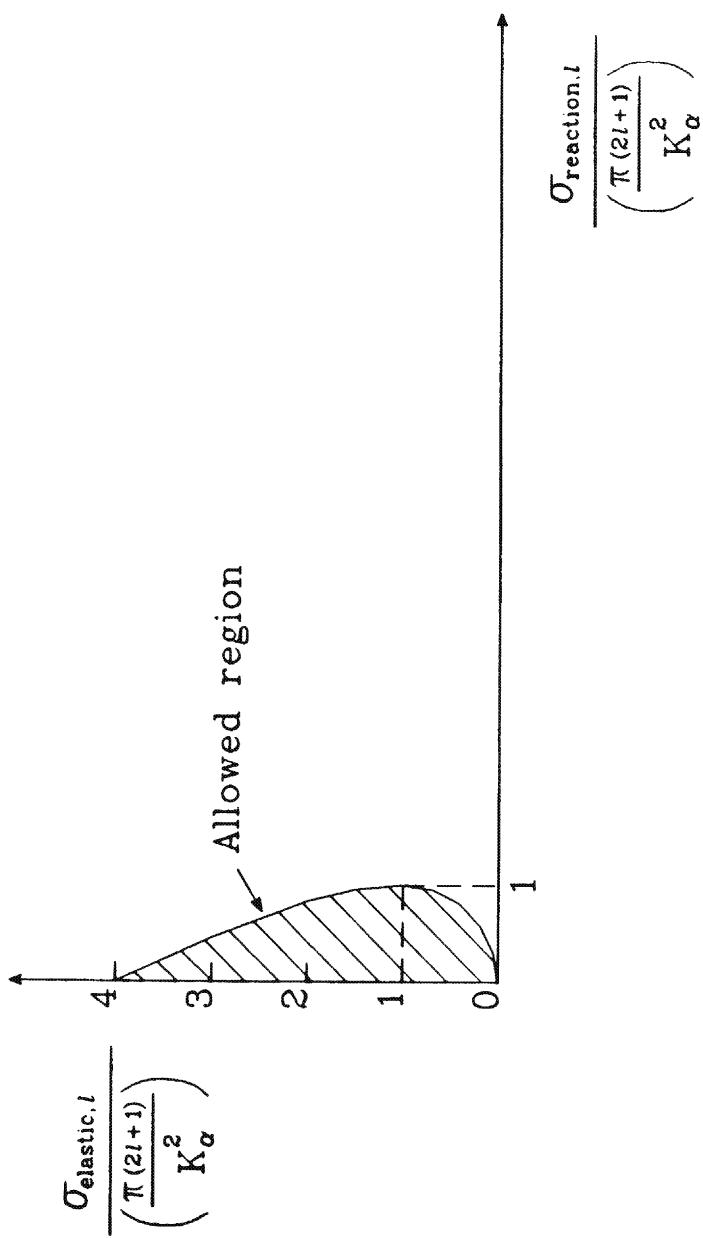


FIGURE 42.4. The domain of allowed $\sigma_{\text{elastic},l}$ vs. $\sigma_{\text{reaction},l}$.

Factoring out the asymptotic behavior of the w_l at $\rho = 0$ and $\rho = \infty$, we need solutions of the form

$$w_l = \rho^{l+1} e^\rho v_l(\rho), \quad (6)$$

where we restrict ourselves for the moment to the solution regular at $r = 0$ and v_l satisfies the differential equation

$$\rho v_l'' + (2l + 2 + 2\rho)v_l' + 2(l + 1 + i\gamma)v_l = 0. \quad (7)$$

With the further substitution,

$$t = -2\rho = -2ikr, \quad (8)$$

this solution can be put in the standard form

$$\begin{aligned} t \frac{d^2 v_l}{dt^2} + (2l + 2 - t) \frac{dv_l}{dt} - (l + 1 + i\gamma)v_l &= 0, \\ tv_l'' + (c - t)v_l' - av_l &= 0, \end{aligned} \quad (9)$$

where $c \equiv (2l + 2)$ and $a \equiv (l + 1 + i\gamma)$. This is the standard form of the differential equation for the hypergeometric function of type, ${}_1F_1(a; c; t)$, the so-called confluent hypergeometric function [in a notation in which the Gaussian hypergeometric function would have been named a ${}_2F_1(a, b; c; t)$]. Substituting an infinite power series solution of the form

$$v_l = \sum_{n=0}^{\infty} c_n t^n, \quad (10)$$

we are led to a two-term recursion formula for the c_n ,

$$\frac{c_n}{c_{n-1}} = \frac{(a + n - 1)}{n(c + n - 1)}, \quad (11)$$

which, with the choice $c_0 = 1$, leads to

$$c_n = \frac{a(a + 1) \cdots (a + n - 1)}{n!c(c + 1) \cdots (c + n - 1)} = \frac{(a)_n}{n!(c)_n} = \frac{\Gamma(a + n)}{n!\Gamma(a)} \frac{\Gamma(c)}{\Gamma(c + n)}, \quad (12)$$

where the c_n have been expressed in terms of Γ functions. Note, $\Gamma(a + 1) = a\Gamma(a)$ and, for the integer $c = (2l + 2)$, $\Gamma(2l + 2) = (2l + 1)!$. We then have

$$w_l(kr) = (ikr)^{l+1} (e^{ikr}) {}_1F_1(a; c; -2ikr), \quad \text{with } a = (l + 1 + i\gamma), \quad c = (2l + 2). \quad (13)$$

For our purposes, it will be useful to express the confluent hypergeometric function in terms of a contour integral

$${}_1F_1(a; c; t) = \frac{\Gamma(c)}{2\pi i} \oint_C \frac{dz e^z}{z^{c-a}(z-t)^a} = \frac{\Gamma(c)}{2\pi i} \oint_C \frac{dz e^z}{z^c \left(1 - \frac{t}{z}\right)^a}, \quad (14)$$

where the contour, C , in the complex z plane surrounds the branch cut from $z = 0$ to $z = t$, where the complex number t is $t = -2ikr$ in our case. The contour will

be chosen such that $|\frac{t}{z}| < 1$, so we can make the expansion, which will be used to establish eq. (13),

$${}_1F_1(a; c; t) = \frac{\Gamma(c)}{2\pi i} \sum_{n=0}^{\infty} \frac{(a)_n}{n!} t^n \oint_C \frac{dze^z}{z^{c+n}} = \Gamma(c) \sum_{n=0}^{\infty} \frac{(a)_n}{n!} \frac{t^n}{(c+n-1)!}, \quad (15)$$

where we have evaluated the contour integral by the residue theorem, bearing in mind $c = (2l + 2)$ is an integer. Using $(a)_n = \Gamma(a + n)/\Gamma(a)$ for the complex number, a , and $(c + n - 1)! = \Gamma(c + n)$ for the integer, $c + n$, we get

$${}_1F_1(a; c; t) = \sum_{n=0}^{\infty} \frac{\Gamma(a+n)}{\Gamma(a)} \frac{\Gamma(c)}{\Gamma(c+n)} \frac{t^n}{n!}, \quad (16)$$

which establishes the contour integral form for ${}_1F_1(a; c; t)$. It will now be useful to deform the contour C , as shown in Fig. 42.5, where the new deformed contour integral can effectively be decomposed into the two loop integrals over contours C_1 and C_2 ,

$${}_1F_1(a; c; -2ikr) = \frac{\Gamma(c)}{2\pi i} \sum_{n=1,2} \oint_{C_n} \frac{dze^z}{z^c (1 + \frac{2ikr}{z})^a}. \quad (17)$$

If we further make the substitution, $z = krz'$, so

$${}_1F_1(a; c; -2ikr) = \frac{\Gamma(c)}{2\pi i (kr)^{c-1}} \sum_{n=1,2} \int_{C_n} \frac{dz' e^{krz'}}{z'^c (1 + \frac{2i}{z'})^a}, \quad (18)$$

in the new contour integrals, C_1 and C_2 (see the final form of these contours in Fig. 42.5), only the circular parts of the new contours about the points $z' = 0$ and $z' = -2i$ contribute to the contour integrals in the limit $kr \rightarrow \infty$, because the real part of z' is negative on the straight-line portions of the final forms of C_1 and C_2 , so $e^{krz'} \rightarrow 0$ as $r \rightarrow \infty$. Now, to do the contour integrals for the circular parts of the contours C_1 and C_2 , surrounding the points $z' = 0$ and $z' = -2i$, in the limit $kr \rightarrow \infty$, let us rename $krz' = z$, so for the first integral, for the contour C_1 , we have

$$\begin{aligned} I_1 &= \frac{\Gamma(c)}{2\pi i} \lim_{r \rightarrow \infty} \oint_{C_1} \frac{dze^z}{z^c (1 + \frac{2ikr}{z})^a} \\ &= \frac{\Gamma(c)}{2\pi i} \lim_{r \rightarrow \infty} \frac{1}{(2ikr)^a} \oint_{C_1} \frac{dze^z}{z^{c-a} (1 - \frac{iz}{2kr})^a} \\ &= \frac{\Gamma(c)}{2\pi i} \frac{1}{(2ikr)^a} \oint_{C_1} \frac{dze^z}{z^{c-a}} = \frac{\Gamma(c)}{(2ikr)^a \Gamma(c-a)}, \end{aligned} \quad (19)$$

where we have replaced the contour, C_1 , by a small circle around the point $z = 0$ and we have used

$$\frac{1}{2\pi i} \oint \frac{dze^z}{z^{c-a}} = \frac{1}{\Gamma(c-a)}. \quad (20)$$

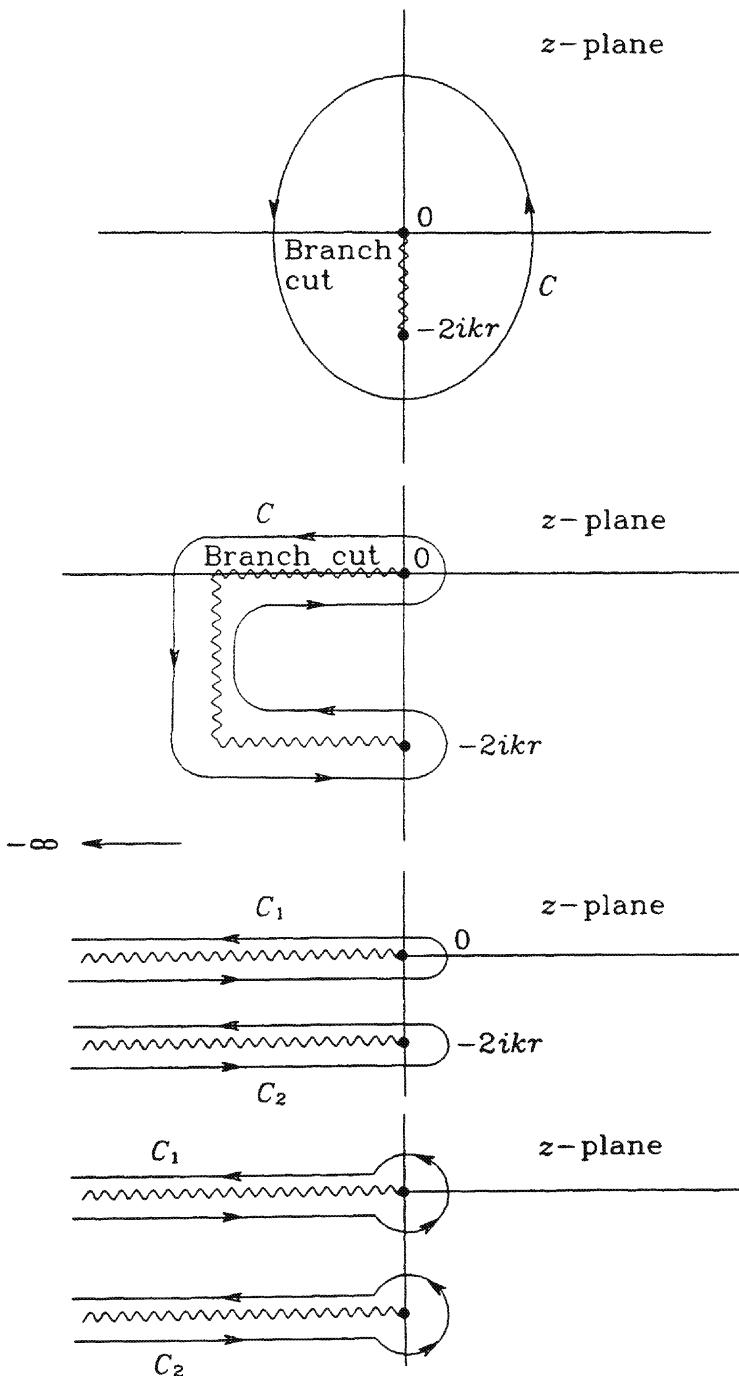


FIGURE 42.5. Contour integral for the confluent hypergeometric function and the deformed contours used to evaluate the integral.

Substituting for $c = (2l + 2)$, and $a = (l + 1 + i\gamma)$, we have, in the limit $r \rightarrow \infty$,

$$I_1 = \frac{(2l + 1)!}{\Gamma(l + 1 - i\gamma)} \frac{1}{(2ikr)^{l+1+i\gamma}}. \quad (21)$$

Similarly,

$$\begin{aligned} I_2 &= \frac{\Gamma(c)}{2\pi i} \lim_{r \rightarrow \infty} \oint_{C_2} \frac{dze^z}{z^{c-a}(z + 2ikr)^a} \\ &= e^{-2ikr} \frac{\Gamma(c)}{2\pi i} \oint_{C_2} \frac{d(z + 2ikr)e^{(z+2ikr)}}{(z + 2ikr - 2ikr)^{c-a}(z + 2ikr)^a} \\ &= \lim_{r \rightarrow \infty} \frac{e^{-2ikr}}{(-2ikr)^{c-a}} \frac{\Gamma(c)}{2\pi i} \oint_{C_2} \frac{dze^z}{z^a \left(1 - \frac{z}{2ikr}\right)^{c-a}} \\ &= \frac{e^{-2ikr}}{(-2ikr)^{c-a}} \frac{\Gamma(c)}{2\pi i} \oint_{C_2} \frac{dze^z}{z^a} = \frac{e^{-2ikr}}{(-2ikr)^{c-a}} \frac{\Gamma(c)}{\Gamma(a)}. \end{aligned} \quad (22)$$

Now, the contour, C_2 , is a small circle around the point $z = -2ikr$ in the first line of this equation. This contour has then been transformed into a small circle about the point $z = 0$ in subsequent lines of this equation. Therefore, in the limit $r \rightarrow \infty$, this second contour integral gives

$$I_2 = \frac{e^{-2ikr}}{(-2ikr)^{l+1-i\gamma}} \frac{(2l + 1)!}{\Gamma(l + 1 + i\gamma)}. \quad (23)$$

Thus, we have for the solution, regular at the origin,

$$\begin{aligned} \lim_{r \rightarrow \infty} w_l &= \lim_{r \rightarrow \infty} (ikr)^{l+1} (e^{ikr}) {}_1F_1((l + 1 + i\gamma); (2l + 2); -2ikr) \\ &= \frac{(2l + 1)! e^{\frac{\gamma\pi}{2}}}{2^{l+1}} \left(\frac{e^{ikr}}{(2kr)^{i\gamma} \Gamma(l + 1 - i\gamma)} + \frac{(-1)^{l+1} e^{-ikr}}{(2kr)^{-i\gamma} \Gamma(l + 1 + i\gamma)} \right) \\ &= \frac{i^l (2l + 1)! e^{\frac{\gamma\pi}{2}}}{2^{l+1} |\Gamma(l + 1 + i\gamma)|} \left(e^{i(kr - \frac{\pi}{2}l - \gamma \ln(2kr) + \sigma_l)} - e^{-i(kr - \frac{\pi}{2}l - \gamma \ln(2kr) + \sigma_l)} \right). \end{aligned} \quad (24)$$

In the last step, we have used

$$\frac{1}{(2kr)^{\pm i\gamma}} = e^{\mp i\gamma \ln(2kr)}, \quad (25)$$

and

$$\Gamma(l + 1 \pm i\gamma) = |\Gamma(l + 1 + i\gamma)| e^{\pm i\sigma_l}, \quad (26)$$

where σ_l is the argument of the complex number $\Gamma(l + 1 + i\gamma)$. (σ_l is a fairly standard mathematical notation for this quantity, not to be confused with a partial cross section!). Except for an overall constant

$$\frac{i^l (2l + 1)! e^{\frac{\gamma\pi}{2}}}{2^l |\Gamma(l + 1 + i\gamma)|},$$

as $r \rightarrow \infty$,

$$R_l(kr) = \frac{w_l(kr)}{ikr} \rightarrow \frac{\sin(kr - \frac{\pi}{2}l - \gamma \ln(2kr) + \sigma_l)}{kr}, \quad (27)$$

which, in the limit in which the Coulomb parameter, γ , can be set equal to zero, is the asymptotic form of $j_l(kr)$.

If we define a $w_l^{(1)}(kr)$ and a $w_l^{(2)}(kr)$, such that

$$\begin{aligned} \frac{(w_l^{(1)} - w_l^{(2)})}{(ikr)} &= (ikr)^l (e^{ikr}) {}_1F_1((l+1+i\gamma); (2l+2); -2ikr) \\ &= \frac{i^l (2l+1)! e^{\frac{\gamma\pi}{2}}}{2^l |\Gamma(l+1+i\gamma)|} \frac{F_l(kr)}{kr}, \end{aligned} \quad (28)$$

the Coulomb function, $F_l(kr)/(kr)$, is the analogue of $j_l(kr)$, with

$$\lim_{r \rightarrow \infty} F_l(kr) = \sin\left(kr - \frac{1}{2}\pi l - \gamma \ln(2kr) + \sigma_l\right). \quad (29)$$

Similarly, the linear combination

$$\frac{(w_l^{(1)} + w_l^{(2)})}{(kr)} = -\frac{i^l (2l+1)! e^{\frac{\gamma\pi}{2}}}{2^{l+1} |\Gamma(l+1+i\gamma)|} \frac{G_l(kr)}{kr}, \quad (30)$$

where the Coulomb function, $G_l(kr)/(kr)$, is the analogue of $-n_l(kr)$, with

$$\lim_{r \rightarrow \infty} G_l(kr) = \cos\left(kr - \frac{1}{2}\pi l - \gamma \ln(2kr) + \sigma_l\right). \quad (31)$$

[The $w_l^{(1)}$ and $w_l^{(2)}$ are the generalizations of the spherical Hänkel functions, $h_l^{(1)}$ and $h_l^{(2)}$.]

For Coulomb scattering, therefore, the generalizations of the outgoing and incoming waves of eq. (21), are

$$\begin{pmatrix} O_l^{\text{Coul.}}(kr) \\ I_l^{\text{Coul.}}(kr) \end{pmatrix} = \frac{(G_l(kr) \pm i F_l(kr))}{r \sqrt{v}}, \quad (32)$$

with asymptotic form

$$\lim_{r \rightarrow \infty} \begin{pmatrix} O_l^{\text{Coul.}}(kr) \\ I_l^{\text{Coul.}}(kr) \end{pmatrix} = \frac{e^{\pm i(kr - \frac{1}{2}\pi l - \gamma \ln(2kr) + \sigma_l)}}{r \sqrt{v}}. \quad (33)$$

It will also be important to give the radial Coulomb functions, regular at the origin, the proper normalization to make these part of a complete orthonormal set. For this purpose, it is sufficient to compare the asymptotic limits, as $r \rightarrow \infty$, of the plane wave solutions with the Coulomb functions in the high-energy limit in which the Coulomb parameter $\gamma \rightarrow 0$. Because we will use both Dirac delta function and box normalizations, we shall use $\mathcal{N} e^{i\vec{k} \cdot \vec{r}}$ for the plane wave solution, with $\mathcal{N} = (1/2\pi)^{\frac{3}{2}}$, or $\mathcal{N} = (1/\sqrt{\text{Vol}})$. The partial wave expansion is

$$\begin{aligned} \mathcal{N} e^{i\vec{k} \cdot \vec{r}} &= \mathcal{N} \sum_l i^l (2l+1) j_l(kr) P_l(\cos \Theta) \\ &= \mathcal{N} 4\pi \sum_{l,m} i^l j_l(kr) Y_{lm}^*(\theta_k, \phi_k) Y_{lm}(\theta, \phi) \\ &\rightarrow \mathcal{N} 4\pi \sum_{l,m} i^l \left[\frac{e^{i(kr - \frac{l\pi}{2})} - e^{-i(kr - \frac{l\pi}{2})}}{2ikr} \right] Y_{lm}^*(\theta_k, \phi_k) Y_{lm}(\theta, \phi), \end{aligned} \quad (34)$$

where Θ is the angle between the vectors \vec{r} and \vec{k} , and θ, ϕ are the polar and azimuth angles of the vector \vec{r} , and θ_k, ϕ_k are those of \vec{k} . This solution is to be compared with the partial wave expansion of the continuum Coulomb wave function

$$\begin{aligned}\psi_{\text{Coul.}}(r, \theta, \phi) &= \sum_{l,m} R_l(kr) Y_{lm}(\theta, \phi) \\ &= \sum_{l,m} A_{lm}(ikr)^l e^{ikr} [{}_1F_1((l+1+i\gamma); (2l+2); -2ikr)] Y_{lm}(\theta, \phi) \\ &\rightarrow \sum_{l,m} A_{lm} \frac{i^l (2l+1)! e^{\frac{\gamma\pi}{2}}}{2^l |\Gamma(l+1+i\gamma)|} \\ &\times \left[\frac{e^{i(kr-\frac{\pi}{2}l-\gamma\ln(2kr)+\sigma_l)} - e^{-i(kr-\frac{\pi}{2}l-\gamma\ln(2kr)+\sigma_l)}}{2ikr} \right] Y_{lm}(\theta, \phi).\end{aligned}\quad (35)$$

Comparing these expressions, we see that

$$A_{lm} = \mathcal{N} |\Gamma(l+1+i\gamma)| e^{-\frac{\gamma\pi}{2}} \frac{2^l}{(2l+1)!} 4\pi Y_{lm}^*(\theta_k, \phi_k), \quad (36)$$

so

$$\begin{aligned}\psi_{\text{Coul.}}(r, \theta, \phi) &= \sum_{l,m} \mathcal{N} |\Gamma(l+1+i\gamma)| e^{-\frac{\gamma\pi}{2}} 2^l 4\pi Y_{lm}^*(\theta_k, \phi_k) (ikr)^l e^{ikr} \\ &\times \frac{1}{2\pi i} \oint_C \frac{dz e^z}{z^{l+1-i\gamma} (z+2ikr)^{l+1+i\gamma}} Y_{lm}(\theta, \phi).\end{aligned}\quad (37)$$

In this expansion, $|\Gamma(l+1+i\gamma)|$ can be related to $|\Gamma(1+i\gamma)|$ via repeated use of the relation $\Gamma(1+z) = z\Gamma(z)$, and

$$|\Gamma(1+i\gamma)|^2 = i\gamma \Gamma(i\gamma) \Gamma(1-i\gamma) = \frac{\pi\gamma}{\sinh\pi\gamma}. \quad (38)$$

Here, the product of Γ functions has been expressed in terms of a beta function, B,

$$\begin{aligned}\Gamma(i\gamma)\Gamma(1-i\gamma) &= \Gamma(1)B(i\gamma, 1-i\gamma) = 2 \int_0^{\pi/2} d\theta \cos^{2i\gamma-1}\theta \sin^{1-2i\gamma}\theta \\ &= 2 \int_0^\infty \frac{ds s^{2i\gamma-1}}{(s^2+1)}.\end{aligned}\quad (39)$$

The s integral can be done by contour integration techniques.

An Application: Electric Dipole Moment Matrix Element Between the Hydrogen Ground State and a Continuum State

For the photoelectric effect in the hydrogen atom (to be discussed in detail in Chapter 64), we shall need the matrix element of the electric dipole operator, $e\vec{r}$, between the hydrogen atom ground state, $|n=1, l=0, m=0\rangle$, and a continuum state in which the electron is ejected with momentum, $\hbar\vec{k}$, in a direction given by angles, θ_k, ϕ_k , with respect to a laboratory-fixed unit vector, \vec{e} ; i.e., we shall need

the matrix element

$$\langle \vec{k} | (\vec{r} \cdot \vec{e}) | n = 1, l = 0, m = 0 \rangle.$$

If we choose \vec{e} to lie in the laboratory z direction, only the $l = 1, m = 0$ term in the partial wave decomposition of eq. (37) can make a contribution to the matrix element. Also, with $Z_1 = -1$ (electron) and $Z_2 = +1$ (proton), the Coulomb parameter, γ , is negative. It will therefore be convenient to change notation and let γ stand for the absolute value of the Coulomb parameter, [requiring a change of sign in eq. (37)]. Then,

$$\begin{aligned} & \langle \vec{k} | (\vec{r} \cdot \vec{e}_z) | n = 1, l = 0, m = 0 \rangle \\ &= \mathcal{N} |\Gamma(2 - i\gamma)| e^{+\frac{\gamma\pi}{2}} 2(4\pi) Y_{10}^*(\theta_k, \phi_k) \int d\Omega Y_{10}^*(\theta, \phi) \cos \theta Y_{00}(\theta, \phi) \\ & \quad \times \int_0^\infty dr r^3 e^{ikr} (ikr) \frac{2e^{-(r/a_0)}}{a_0^{\frac{3}{2}}} \frac{1}{2\pi i} \oint \frac{dze^z}{z^{2+i\gamma} (z + 2ikr)^{2-i\gamma}} \\ &= \mathcal{N} |\Gamma(2 - i\gamma)| e^{+\frac{\gamma\pi}{2}} 2\sqrt{(4\pi)} \cos \theta_k \int_0^\infty dr r^3 e^{ikr} (ikr) \frac{2e^{-(r/a_0)}}{a_0^{\frac{3}{2}}} \\ & \quad \times \frac{1}{2\pi i} \oint \frac{dze^z}{z^{2+i\gamma} (z + 2ikr)^{2-i\gamma}}, \end{aligned} \quad (40)$$

where a_0 is the Bohr radius. It will be convenient to make the transformation, $z = 2ikr(z' - \frac{1}{2})$, in the contour integral and the transformation, $r = a_0 r'$, in the radial integral. Performing the radial integral first

$$\int_0^\infty dr' r' e^{-r'} e^{2ika_0 r' z'} = \frac{1}{(1 - 2ika_0 z')^2}, \quad (41)$$

and using the identity

$$ka_0 = \frac{1}{\gamma},$$

the matrix element of $(\vec{r} \cdot \vec{e}_z)$ becomes

$$\frac{\mathcal{N} |\Gamma(2 - i\gamma)| e^{+\frac{\gamma\pi}{2}} \sqrt{4\pi} \cos \theta_k \gamma^4 a_0^{\frac{5}{2}}}{8} \frac{1}{2\pi i} \oint_C \frac{dz'}{(z' - \frac{1}{2})^{2+i\gamma} (z' + \frac{1}{2})^{2-i\gamma} (z' + \frac{i\gamma}{2})^2},$$

where the transformation $z = 2ikr(z' - \frac{1}{2})$ has transformed the counterclockwise contour C around the branch cut between $z = 0$ and $z = -2ikr$ in the z plane (see Fig. 42.5) into a counterclockwise contour around the branch cut between $z' = -\frac{1}{2}$ and $z' = +\frac{1}{2}$ in the z' plane (see Fig. 42.6). Besides this branch cut, there is now a singular point at $z' = -\frac{1}{2}i\gamma$. The integrand vanishes for large values of $|z'|$; and the contour C can be transformed into a clockwise contour, C' , around the singular point at $z' = -\frac{1}{2}i\gamma$. Residue theory shows this contour integral has the value

$$-\frac{d}{dz'} \left[(z' - \frac{1}{2})^{-2-i\gamma} (z' + \frac{1}{2})^{-2+i\gamma} \right]_{|z'|=-i\gamma/2} = \left(\frac{\gamma + i}{\gamma - i} \right)^{i\gamma} \frac{64i\gamma}{(\gamma^2 + 1)^3}$$

$$= e^{-2\gamma \tan^{-1}(1/\gamma)} \frac{64i\gamma}{(\gamma^2 + 1)^3}. \quad (42)$$

Also, using eq. (38), and

$$|\Gamma(2 - i\gamma)|^2 = (\gamma^2 + 1)|\Gamma(1 - i\gamma)|^2, \quad (43)$$

we get

$$\langle \vec{k} | \vec{r} \cdot \vec{e}_z | n = 1, l = 0, m = 0 \rangle = \\ \mathcal{N} \sqrt{4\pi} \cos \theta_k \left[\frac{(\gamma^2 + 1)\pi\gamma}{\sinh \pi\gamma} \right]^{\frac{1}{2}} e^{\frac{\gamma\pi}{2}} a_0^{\frac{5}{2}} \frac{8i\gamma^5}{(\gamma^2 + 1)^3} e^{-2\gamma \tan^{-1}(1/\gamma)}. \quad (44)$$

The square of the absolute value of this matrix element can be put into the following convenient form

$$|\langle \vec{k} | (\vec{r} \cdot \vec{e}_z) | 100 \rangle|^2 = 512\pi^2 \cos^2 \theta_k a_0^5 \mathcal{N}^2 \frac{\gamma^{11}}{(\gamma^2 + 1)^5} \frac{e^{-4\gamma \tan^{-1}(1/\gamma)}}{(1 - e^{-2\gamma\pi})}. \quad (45)$$

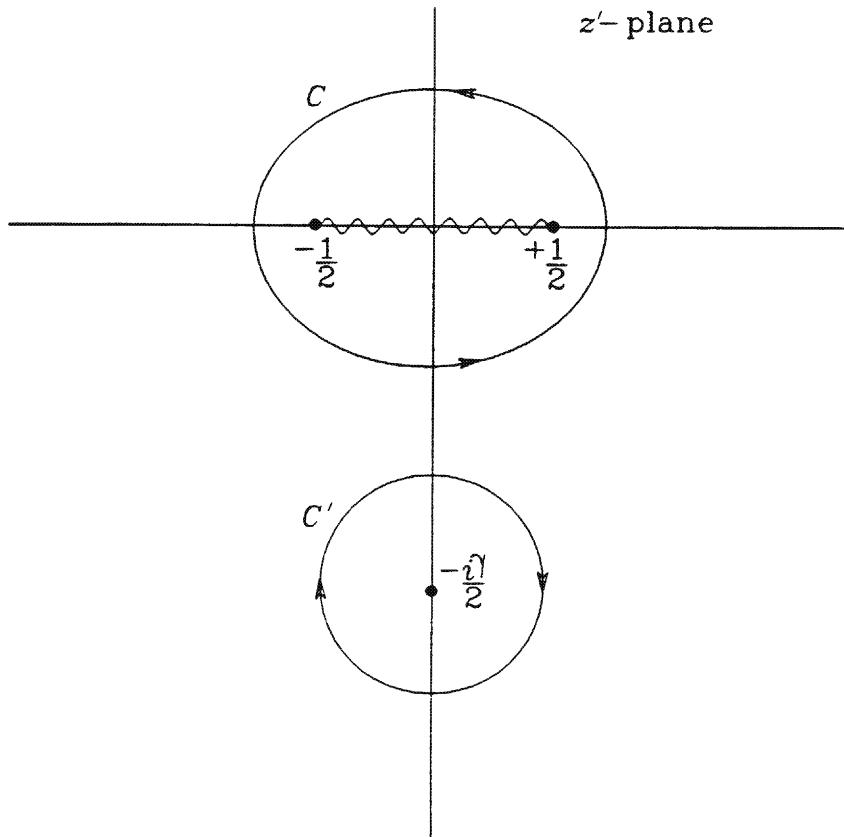


FIGURE 42.6. The z' plane contour integral.

43

A Specific Example: Scattering from Spherical Square Well Potentials

To solve a very specific example, let us look first at the scattering from a spherical square well potential, with

$$V(r) = V_0 \quad \text{for } r \leq a, \quad V(r) = 0 \quad \text{for } r > a, \quad (1)$$

(see Fig. 43.1), where the constant V_0 could be either negative (attractive potential) or positive (repulsive potential), including $V_0 = +\infty$, the so-called hard sphere case. The latter might be a good approximation for the scattering of noble gas atoms from noble gas atoms. In this case, classical scattering theory would be sufficient for gases at temperatures such that $\lambda \ll a$. Quantum theory would be needed only for $\lambda \simeq a$ or $\lambda > a$. For noble gas atoms with mass, m , at an absolute temperature, T ,

$$\begin{aligned} \frac{\lambda}{2\pi} = \frac{\hbar}{p} &\sim \frac{\hbar}{[mkT]^{\frac{1}{2}}} = \frac{\hbar c}{[mc^2 k T]^{\frac{1}{2}}} = \frac{1.97 \times 10^3 eV \times 10^{-8} cm}{[M(9.4 \times 10^9 eV) \times \frac{1}{40} eV \frac{T}{300}]^{\frac{1}{2}}} \\ &\approx \frac{7 \times 10^{-8} cm}{\sqrt{MT}}, \end{aligned} \quad (2)$$

where M is the mass number of the atom in atomic units. Thus, quantum theory is needed only for the lightest atoms, e.g., He with $M = 4$, at extremely low temperatures.

For the general $V(r)$, the asymptotic form of the solution, as $r \rightarrow \infty$, is

$$\begin{aligned} R_l(kr) &= \frac{w_l(kr)}{kr} \rightarrow i^l e^{i\delta_l} (2l+1) \frac{\sin(kr - \frac{\pi}{2}l + \delta_l)}{kr} \\ &= i^l e^{i\delta_l} (2l+1) (j_l(kr) \cos \delta_l - n_l(kr) \sin \delta_l), \end{aligned} \quad (3)$$

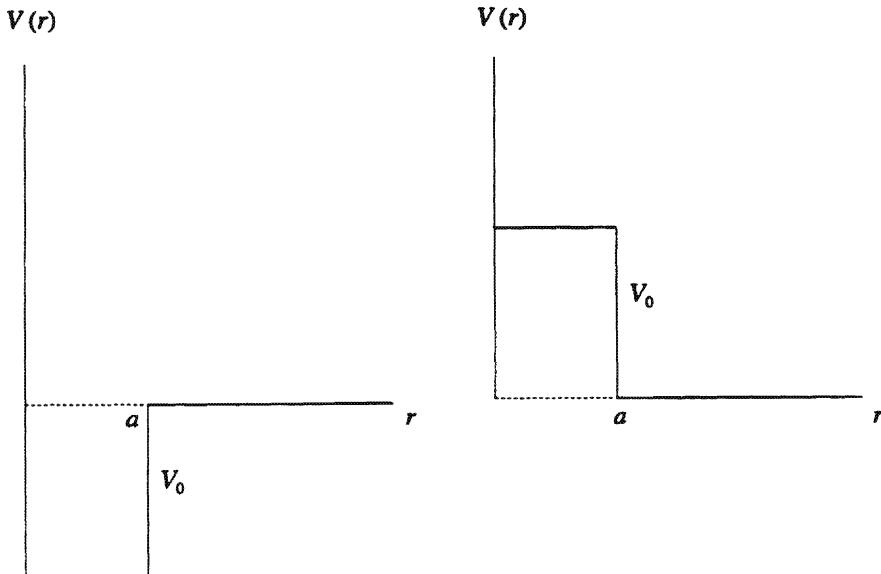


FIGURE 43.1. Square well potential scatterers.

where we have used the asymptotic forms for j_l and n_l , eq. (44) of Chapter 41. Now for the square well problem, the solution for $R_l(kr)$ is a linear combination of the free-wave radial functions, $j_l(kr)$ and $n_l(kr)$, for all values of $r \geq a$, so our solution for $r \geq a$ is

$$R_l(kr) = i^l e^{i\delta_l} (2l + 1) (j_l(kr) \cos \delta_l - n_l(kr) \sin \delta_l). \quad (4)$$

We shall also need, again in the region $r \geq a$,

$$\left(r \frac{dR_l}{dr} \right) = (kr) i^l e^{i\delta_l} (2l + 1) (j'_l(kr) \cos \delta_l - n'_l(kr) \sin \delta_l). \quad (5)$$

All of the information from the interior region will be related to the ratio, evaluated at the boundary $r = a$, of the quantity

$$\begin{aligned} \left[\frac{1}{R_l} r \frac{dR_l}{dr} \right]_{r=a} &\equiv \beta_l = (ka) \left[\frac{(j'_l \cos \delta_l - n'_l \sin \delta_l)}{(j_l \cos \delta_l - n_l \sin \delta_l)} \right]_{r=a} \\ &= (ka) \left[\frac{(j'_l + i n'_l) e^{2i\delta_l} + (j'_l - i n'_l)}{(j_l + i n_l) e^{2i\delta_l} + (j_l - i n_l)} \right]_{r=a}. \end{aligned} \quad (6)$$

Solving this for the phase shift,

$$e^{2i\delta_l} = - \left[\frac{(j_l - i n_l)}{(j_l + i n_l)} \left[\frac{1 - \frac{ka}{\beta_l} \left(\frac{j'_l - i n'_l}{j_l - i n_l} \right)}{1 - \frac{ka}{\beta_l} \left(\frac{j'_l + i n'_l}{j_l + i n_l} \right)} \right] \right]_{r=a}. \quad (7)$$

A Hard Sphere Scattering

For the hard sphere case, we must have $R_l(ka) = 0$, and $\frac{dR_l}{dr}$ must be finite at $r = a$. Thus, $\beta_l = \infty$, and

$$\begin{aligned} e^{2i\delta_l^{\text{H.Sph.}}} &= -\left[\frac{(j_l(ka) - i n_l(ka))}{(j_l(ka) + i n_l(ka))} \right] \\ &= \left[\frac{(n_l(ka) + i j_l(ka))}{(n_l(ka) - i j_l(ka))} \right] = \frac{e^{i\delta_l^{\text{H.Sph.}}}}{e^{-i\delta_l^{\text{H.Sph.}}}}, \end{aligned} \quad (8)$$

so

$$\tan \delta_l^{\text{H.Sph.}} = \frac{j_l(ka)}{n_l(ka)}. \quad (9)$$

For the low-energy limit [see eq. (45) of Chapter 41],

$$\tan \delta_l^{\text{H.Sph.}} = \frac{\frac{2^l l!}{(2l+1)!} (ka)^l \left(1 - \frac{(ka)^2}{2(2l+3)} + \dots\right)}{-\frac{(2l)!}{(ka)^{l+1} 2^l l!} \left(1 + \frac{(ka)^2}{2(2l-1)} + \dots\right)}. \quad (10)$$

Again, in the low-energy limit δ_0 dominates. Note that $\tan \delta_0^{\text{H.Sph.}} = -\tan(ka)$; and for all (ka)

$$\delta_0^{\text{H.Sph.}} = -(ka), \quad (11)$$

whereas, for $(ka) \ll 1$,

$$\delta_1^{\text{H.Sph.}} \simeq -\frac{(ka)^3}{3} + \dots \quad (12)$$

In the extreme low-energy limit, neglecting all but the $l = 0$ phase shift,

$$\frac{d\sigma}{d\Omega} = \frac{\sin^2 \delta_0}{k^2} = a^2, \quad \sigma = 4\pi a^2. \quad (13)$$

In next approximation, with $(ka) \ll 1$,

$$\begin{aligned} \frac{d\sigma}{d\Omega} &= \frac{1}{k^2} \left(\sin^2 \delta_0 + 3\delta_1 \sin 2\delta_0 \cos \theta + \dots \right) \\ &= a^2 \left(\left[1 - \frac{(ka)^2}{3}\right] + 2(ka)^2 \cos \theta \right). \end{aligned} \quad (14)$$

As (ka) increases, the differential cross section will show more and more angular oscillations, as more and more terms in the l sum contribute. Fig. 43.2 shows the θ dependence of the differential cross section for a very large value of (ka) , as well as the limit of extremely large (ka) . In this extreme short-wavelength limit, the differential cross section has the classical value, $\frac{a^2}{4}$, for all values of $\theta > \theta_{\min} \approx (\pi/(ka))$. The total cross section is

$$\sigma_{ka \rightarrow \infty} = 2\pi a^2, \quad (15)$$

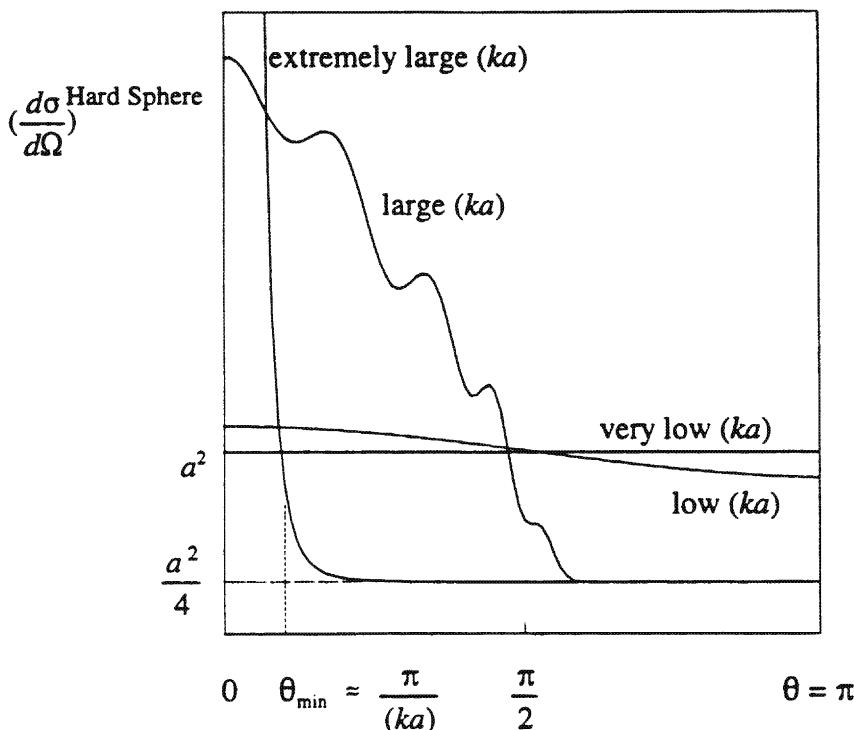


FIGURE 43.2. Hard sphere differential scattering cross sections.

that is, twice the classical value: one unit of πa^2 coming from the forward peak for $\theta < \theta_{\min}$; the second unit of πa^2 coming from all values of θ from the constant value of $\frac{a^2}{4}$ for $\frac{d\sigma}{d\Omega}$. The strong forward peak giving the extra factor of πa^2 comes from the wave description of even the classical limit. Our wave function now consists of essentially three components, a plane wave extending through *all* of space, a “true” scattered wave showing an isotropic scattering with equal probability in all directions, and a strongly forward-peaked wave interfering with the plane wave in the forward direction to make the geometrical shadow. (See Fig. 43.3.)

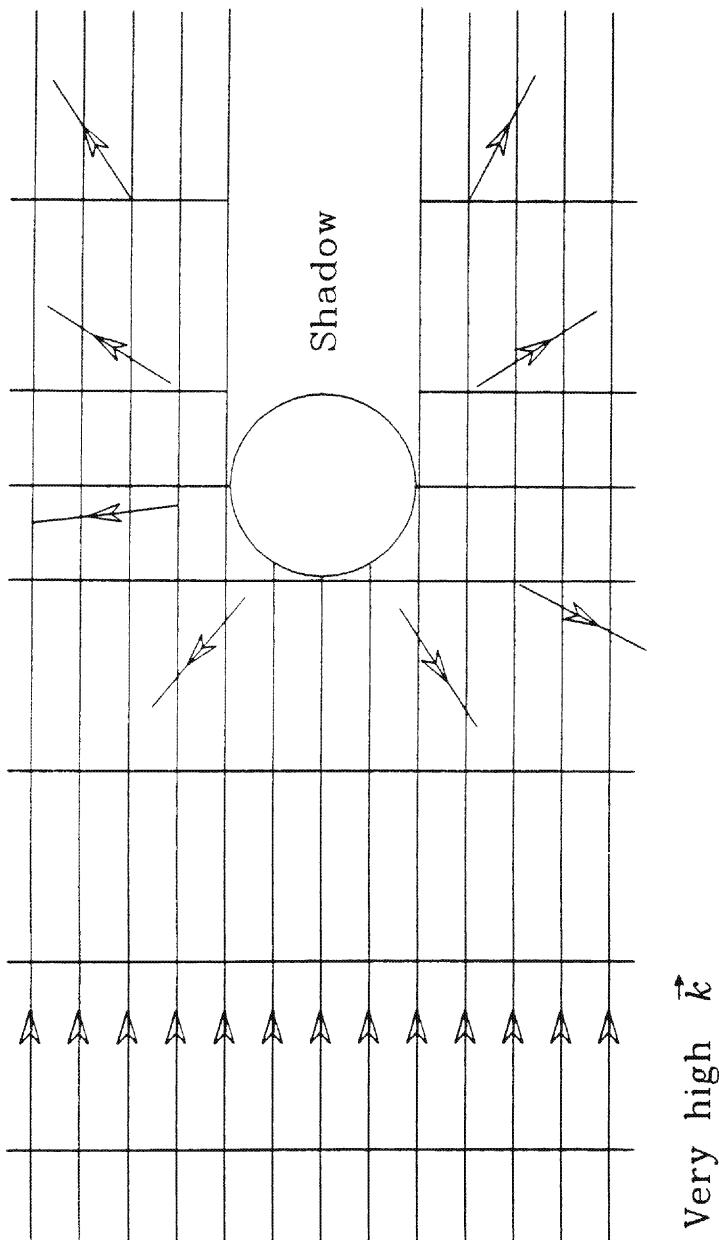


FIGURE 43.3. Hard sphere scattering, high k limit.

B The General Case: Arbitrary V_0

In the general case, we can express the phase shifts, δ_l , by

$$e^{2i\delta_l} = e^{2i\delta_l^{\text{H.Sph.}}} \frac{\beta_l - (ka) \left(\frac{j'_l - in'_l}{j_l - in_l} \right)_{r=a}}{\beta_l - (ka) \left(\frac{j'_l + in'_l}{j_l + in_l} \right)_{r=a}}, \quad (16)$$

that is, δ_l is determined exclusively from the quantity β_l . From the continuity of the wave function and its first derivative at $r = a$, we get

$$\beta_l = (k_0 a) \frac{j'(k_0 a)}{j_l(k_0 a)}, \quad \text{with} \quad k_0^2 = \frac{2\mu(E - V_0)}{\hbar^2}, \quad (17)$$

where we have also used the fact that the interior solution, for $r < a$, must be regular at the origin. Using the abbreviation for the quantity

$$(ka) \left(\frac{j'_l + in'_l}{j_l + in_l} \right)_{r=a} \equiv (\Delta_l + is_l), \quad (18)$$

we have

$$e^{2i\delta_l} = e^{2i\delta_l^{\text{H.Sph.}}} \frac{\beta_l - \Delta_l + is_l}{\beta_l - \Delta_l - is_l} = e^{2i\delta_l^{\text{H.Sph.}}} \left(1 + \frac{2is_l}{\beta_l - \Delta_l - is_l} \right). \quad (19)$$

The quantities Δ_l , s_l , and $e^{i\delta_l^{\text{H.Sph.}}}$ are all known functions of ka and completely independent of the strength of the potential. Moreover, they are all smooth functions of ka . For example, for $l = 0$,

$$\delta_0^{\text{H.Sph.}} = -ka, \quad \Delta_0 = -1, \quad s_0 = ka. \quad (20)$$

For $l = 1$,

$$e^{i\delta_1^{\text{H.Sph.}}} = e^{-ika} \frac{(1 + ika)}{[1 + (ka)^2]^{\frac{1}{2}}}, \quad \Delta_1 = -\frac{[2 + (ka)^2]}{[1 + (ka)^2]}, \quad s_1 = \frac{(ka)^3}{[1 + (ka)^2]}. \quad (21)$$

To express the differential and total cross sections as functions of $\delta_l^{\text{H.Sph.}}$, Δ_l , s_l , and β_l , it will be useful to use the identity

$$e^{i\delta_l} \sin \delta_l = \frac{i}{2} (1 - e^{2i\delta_l}) \quad (22)$$

to rewrite

$$e^{i\delta_l} \sin \delta_l = e^{i\delta_l^{\text{H.Sph.}}} \sin \delta_l^{\text{H.Sph.}} + \frac{s_l e^{2i\delta_l^{\text{H.Sph.}}}}{\beta_l - \Delta_l - is_l}. \quad (23)$$

This equation leads to an expression for the l^{th} partial cross section

$$\sigma_l = \frac{4\pi}{k^2} (2l+1) \left(\sin^2 \delta_l^{\text{H.Sph.}} + \frac{s_l^2 (1 - 2 \sin^2 \delta_l^{\text{H.Sph.}})}{(\beta_l - \Delta_l)^2 + s_l^2} + \frac{s_l (\beta_l - \Delta_l) \sin 2\delta_l^{\text{H.Sph.}}}{(\beta_l - \Delta_l)^2 + s_l^2} \right). \quad (24)$$

Because Δ_l , s_l , and $\delta_l^{\text{II,Sph.}}$, especially for low values of l , are mild functions of (ka) , any rapid changes in $\delta_l(k)$ with k , and hence σ_l with k , must be caused by a strong k dependence in β_l . In particular, β_l can go to infinity for particular values of k for which $R_l(ka) = 0$. This process leads us to the next topic.

Scattering Resonances: Low-Energy Scattering

A Potential Resonances

In the last chapter, the quantities, $\delta_l^{\text{H.Sph.}}$, Δ_l , and s_l , which determine the phase shift δ_l for a particular V_0 , are mild functions of the energy, E . If the quantity, β_l , is also a mild function of E , the phase shifts, δ_l , and the cross sections will be mild, smooth functions of the energy. Conversely, if a particular β_l has a very strong energy dependence, particularly at low E , the corresponding $\delta_l(k)$ may have an abrupt change over a short energy interval, and the cross section σ_l may have a sharp peak over a small energy interval, leading to a resonance in the scattering cross section.

If we expand β_l as a power series in E

$$\beta_l = c_l^{(0)} + c_l^{(1)}E + \dots, \quad (1)$$

neglecting E^2 and E^3 terms, which may be a good approximation at low energy, particularly if $c_l^{(1)}$ is large; then,

$$e^{2i(\delta_l - \delta_l^{\text{H.Sph.}})} = \frac{\beta_l - \Delta_l + is_l}{\beta_l - \Delta_l - is_l} = \frac{\frac{c_l^{(0)}}{c_l^{(1)}} + E - \frac{\Delta_l}{c_l^{(1)}} + i\frac{s_l}{c_l^{(1)}}}{\frac{c_l^{(0)}}{c_l^{(1)}} + E - \frac{\Delta_l}{c_l^{(1)}} - i\frac{s_l}{c_l^{(1)}}}. \quad (2)$$

Let

$$\left(\frac{c_l^{(0)}}{c_l^{(1)}} - \frac{\Delta_l}{c_l^{(1)}} \right) \equiv -E_0, \quad \frac{s_l}{c_l^{(1)}} \equiv -\frac{\Gamma}{2}. \quad (3)$$

$\Gamma \ll 1$ if $c_l^{(1)}$ is large (strong energy dependence of β_l) because s_l is small at low energies. (Recall, e.g., $s_0 = ka$, $s_1 = (ka)^3/[1 + (ka)^2]$.) With this notation, we have

$$e^{2i(\delta_l - \delta_l^{\text{H.Sph.}})} = \frac{E_0 - E + i\frac{1}{2}\Gamma}{E_0 - E - i\frac{1}{2}\Gamma}, \quad (4)$$

so

$$\tan(\delta_l - \delta_l^{\text{H.Sph.}}) = \frac{\Gamma}{2(E_0 - E)}. \quad (5)$$

In the vicinity of $E = E_0$, the phase shift δ_l may have wide excursions.

For example, for $E = E_0 \mp \frac{1}{2}\Gamma$, $\tan(\delta_l - \delta_l^{\text{H.Sph.}}) = \pm 1$,

while for $E = E_0 \mp 2\Gamma$, $\tan(\delta_l - \delta_l^{\text{H.Sph.}}) = \pm \frac{1}{4}$,

so δ_l changes by $\sim \frac{\pi}{2}$ over an energy interval Γ about E_0 , and changes by $\sim .85\pi$ over an energy interval 4Γ about E_0 . A change in $\delta_l \sim \pi$ over a small energy interval $\sim \Gamma$ signals a possible sharp rise and subsequent fall in σ . The resonance peak can be very narrow, if $\frac{1}{2}\Gamma = (s_l/c_l^{(1)})$ is very small. Fig. 44.1 shows an example in which β_0 has no spectacular E dependence near $E \sim 0$, so δ_0 is a smooth function of k . Conversely, δ_1 shows a sharp rise of $\sim \frac{1}{2}\pi$ to π at a small value of ka , leading to a resonance peak in σ . We note in passing our expression for δ_l in terms of its tangent determines δ_l only to within a multiple of π . The δ_l can be normalized, however, by the requirement $\delta_l \rightarrow 0$ as $E \rightarrow \infty$.

When expressed in terms of the parameters E_0 and Γ , the l^{th} partial cross section has the form

$$\sigma_l = \frac{4\pi}{k^2} (2l+1) \left(\frac{\left(\frac{\Gamma}{2}\right)^2 (1 - 2 \sin^2 \delta_l^{\text{H.Sph.}})}{(E - E_0)^2 + \left(\frac{\Gamma}{2}\right)^2} + \frac{\frac{\Gamma(E_0 - E)}{2} \sin 2\delta_l^{\text{H.Sph.}}}{(E - E_0)^2 + \left(\frac{\Gamma}{2}\right)^2} + \sin^2 \delta_l^{\text{H.Sph.}} \right) \quad (6)$$

The sharpness of the resonance peak is amplified at low energy by the $1/k^2$ factor of this expression. Also, for $(ka) \ll 1$, $\delta_l^{\text{H.Sph.}} \ll 1$, so the first of the three terms dominates. For $E = E_0 \pm \frac{1}{2}\Gamma$, therefore, $\sigma_l \approx \frac{1}{2}(\sigma_l)_{\text{max.}}$, so Γ gives the half-width of the resonance.

B Low-Energy Scattering for General $V(r)$: Scattering Length

As we have seen in the last two chapters, for very low-energy scattering, pure s wave ($l = 0$ -partial wave) scattering dominates, leading to an isotropic differential cross section. In the limit $k \rightarrow 0$, the differential equation for the $l = 0$ radial function goes over to

$$\frac{d^2 u_0}{dr^2} - \frac{2\mu}{\hbar^2} V(r) u_0 = 0. \quad (7)$$

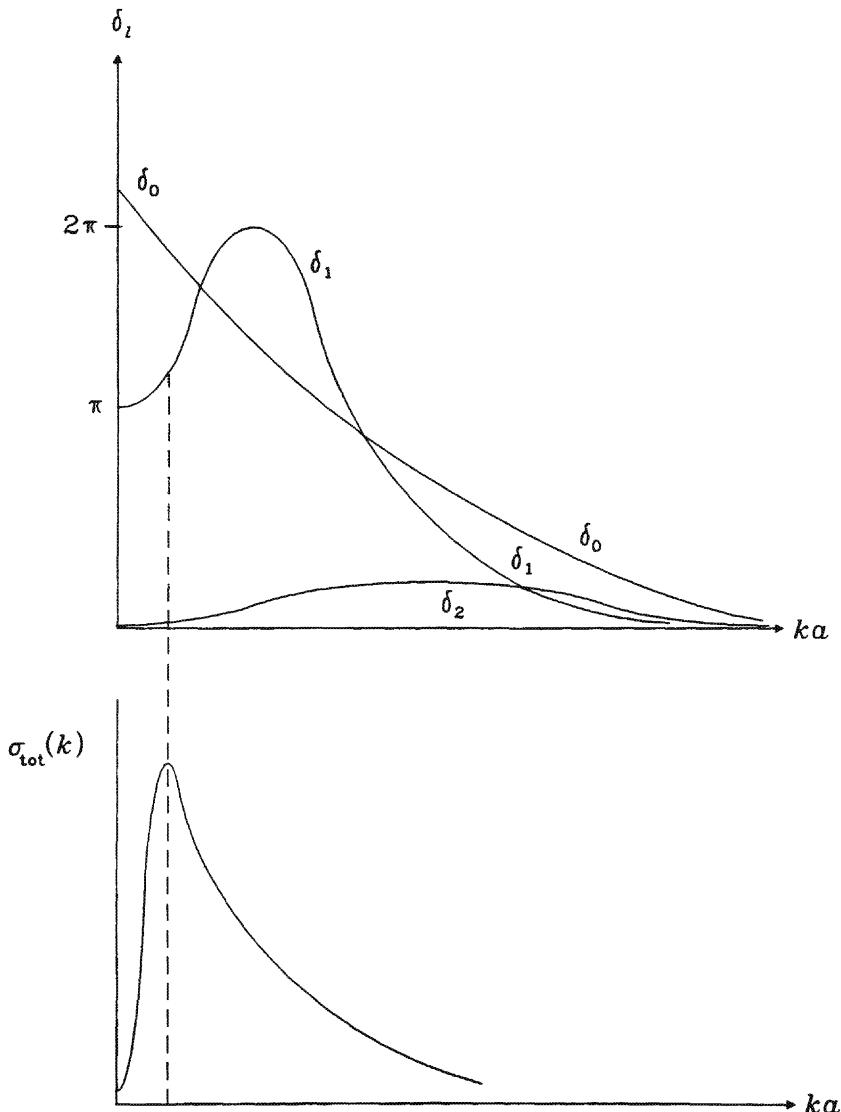


FIGURE 44.1. Scattering phase shifts and cross section for a potential with a low-energy p wave resonance.

Thus, for $r > r_0$, where r_0 is the range of the potential, this differential equation collapses to

$$\frac{d^2 u_0}{dr^2} = 0. \quad (8)$$

Thus, for $E = 0$, the solution u_0 for $r > r_0$ is a straight-line function

$$u_0(r) = A(r - a_{\text{sc.l.}}), \quad (9)$$

where the constant, $a_{\text{sc.l.}}$, is known as the “scattering length.” For finite but very small k , the solution u_0 for $r > r_0$ has the form

$$\begin{aligned} u_0 &= e^{i\delta_0} \sin(kr + \delta_0) = e^{i\delta_0} (\sin kr \cos \delta_0 + \cos kr \sin \delta_0) \\ &\approx e^{i\delta_0} k \cos \delta_0 \left(r - \left(\frac{\tan \delta_0}{-k} \right) \right), \end{aligned} \quad (10)$$

so

$$\tan \delta_0 = -ka_{\text{sc.l.}}, \quad (11)$$

and

$$\sigma = \frac{4\pi}{k^2} \sin^2 \delta_0 \approx \frac{4\pi}{k^2} \tan^2 \delta_0 \approx 4\pi a_{\text{sc.l.}}^2. \quad (12)$$

At very low energies, therefore, the cross section is given by the square of the scattering length. The scattering length can be both positive and negative, and its absolute value can be much larger than the range of the potential, r_0 . For example, if the interior solution for $r < r_0$ is such that the interior u_0 at $E = 0$ has a curvature toward the abscissa such that it has just begun to bend over beyond a maximum, at $r = r_0$ (see Fig. 44.2), the scattering length will be large and positive. If, conversely, the interior wave function has not quite reached a maximum at $r = r_0$, the scattering length will have a large negative value (see Fig. 44.4).

It is interesting to look at the neutron–proton system. The $n-p$ potential is a potential of the form shown in Fig. 44.3, with a well-defined r_0 of approximately 2 fm = 2×10^{-13} cm. The $n-p$ potential must be spin-dependent, however. Because neutron and proton have a spin of $\frac{1}{2}$, the two-particle spin, S , can be either $S = 1$, or $S = 0$. The $n-p$ system has only a single (barely)-bound state, at -2.2 MeV, with spin, $S = 1$, the bound state of the deuteron. No bound state exists with

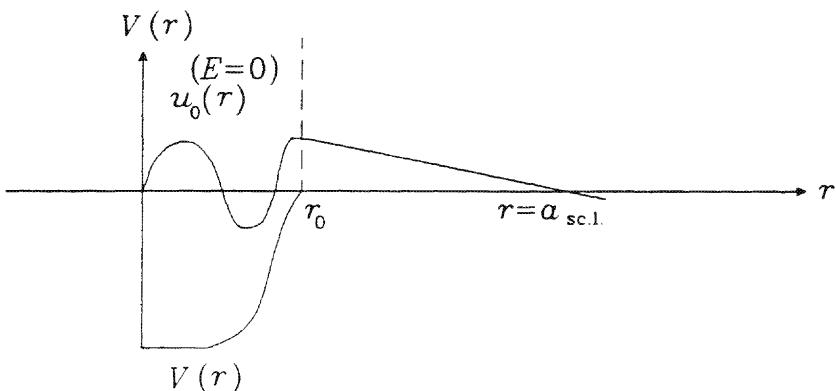


FIGURE 44.2. Potential with a positive scattering length.

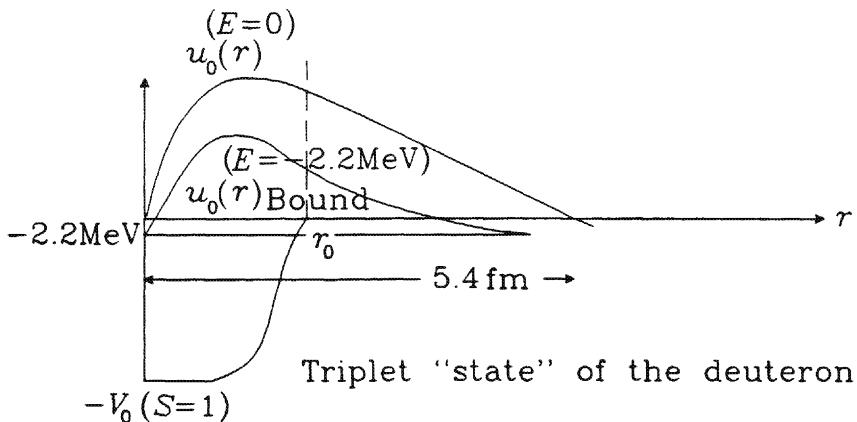


FIGURE 44.3. Low-energy proton-neutron scattering. The triplet $S = 1$ proton-neutron potential with its bound-state eigenfunction and its $E = 0$ function with positive scattering length.

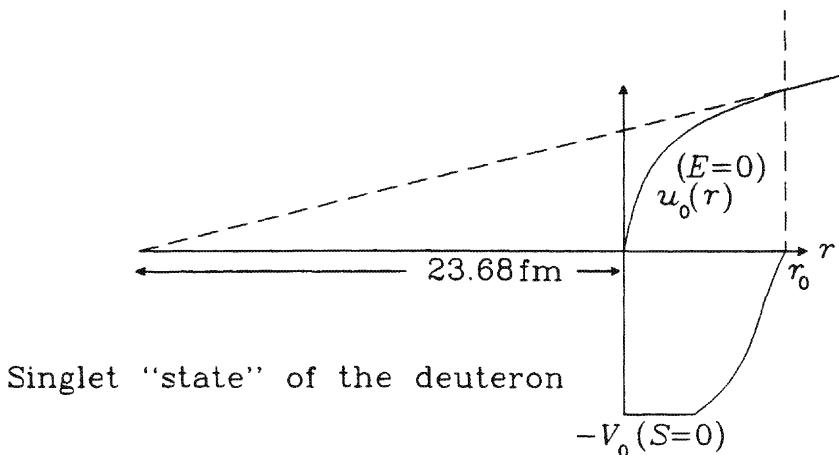


FIGURE 44.4. The singlet $S = 0$ proton-neutron potential with its $E = 0$ function with negative scattering length.

$S = 0$. From the analysis of the experimental low-energy cross sections, the $n-p$ system is found to have a positive scattering length in the triplet ($S = 1$) state and a negative scattering length in the singlet ($S = 0$) state

$$\begin{aligned} a_{\text{sc.l.}}^{S=1} &= +5.400 \pm .001 \text{ fm}, \\ a_{\text{sc.l.}}^{S=0} &= -23.677 \pm .029 \text{ fm}. \end{aligned} \quad (13)$$

The $S = 1$ bound state wave function of the deuteron at -2.2 MeV has enough curvature toward the abscissa in the interior region, so it has a negative slope at

$r = r_0$ and has bent over enough to fit onto a properly behaved exponentially decaying function for $r > r_0$. The wave function for $E = 0$ will have a slightly smaller effective wavelength in the interior region and will therefore also reach the point $r = r_0$ with a negative slope, leading to a positive scattering length. Conversely, the $S = 0$ potential is not sufficiently attractive, so even at $E = 0$ the interior wave function has not bent sufficiently and has not yet reached a maximum at $r = r_0$, so its slope is still positive at $r = r_0$, but is so small that there is a large negative scattering length. Also, the $n-p$ potential must have a significant spin dependence. Because the singlet scattering length is very large, we would expect an s wave scattering resonance in low-energy $n-p$ scattering.

Problems

1. For the spherical step potential

$$V = V_0, \quad 0 \leq r < a, \quad V = 0, \quad r > a$$

show

$$\tan \delta_l = \frac{k j_l(k_0 a) j'_l(ka) - k_0 j_l(ka) j'_l(k_0 a)}{k j_l(k_0 a) n'_l(ka) - k_0 j'_l(k_0 a) n_l(ka)},$$

where

$$k^2 = \frac{2\mu E}{\hbar^2}, \quad k_0^2 = \frac{2\mu}{\hbar^2}(E - V_0).$$

Give approximate values for δ_l for the cases:

- (a) For V_0 fixed, $E \rightarrow \infty$.
- (b) For $E > V_0$ (E, V_0 fixed), $l \rightarrow \infty$.
- (c) For $V_0 < 0$ (attractive potential), and $E \rightarrow 0$ (very low-energy scattering), find $\sigma(E)$.
- (d) For the special case (c), show values of $|V_0|a^2$ exist for which $\sigma = 0$ ($\delta_0 = \pi, 2\pi, \dots$); i.e., special conditions exist for which the target is completely transparent to the projectiles (Ramsauer–Townsend effect).
- (e) Investigate the special case (c) further when the attractive V_0 is just deep enough to have one bound state with a binding energy, $\epsilon \ll |V_0|$ (this is approximately true for the special case of low-energy neutron–proton scattering; the deuteron has a binding energy of only 2.2 MeV). Show, in this case,

$$\sqrt{\frac{2\mu a^2 |V_0|}{\hbar^2}} \approx \frac{\pi}{2} + \Delta, \quad (\Delta \ll 1).$$

Show first the bound state energies with $E = -\epsilon$ can be obtained from solutions to the transcendental equation

$$\xi \cot \xi = -\sqrt{\frac{2\mu a^2 |V_0|}{\hbar^2} - \xi^2}, \quad \text{where } \xi = \sqrt{\frac{2\mu a^2}{\hbar^2}(|V_0| - \epsilon)}.$$

Then show, in the special case of one bound state only, with $\epsilon \ll |V_0|$, the low-energy cross section is a function of the length parameter $\sqrt{\hbar^2/2\mu\epsilon}$ only. Find the scattering length as a function of this length parameter, assuming

$$a^2 \ll \frac{\hbar^2}{2\mu\epsilon}.$$

2. Potential Resonances. For an attractive square well potential of depth $|V_0|$, with

$$k_0 a = \sqrt{\frac{2\mu E a^2}{\hbar^2} + \frac{2\mu |V_0| a^2}{\hbar^2}} = \sqrt{(ka)^2 + \frac{2\mu |V_0| a^2}{\hbar^2}} \equiv \rho^2 = \sqrt{(ka)^2 + \rho_0^2},$$

investigate the possibility the $l = 1$ partial cross section can give rise to a resonant peak at low values of (ka) . Show, in particular, in the limit $(ka) \rightarrow 0$, the quantity $(\beta_1 - \Delta_1)$ has the value zero for $\rho = n\pi$. Investigate the special case, $n = 2$. Test this case by choosing a value of ρ_0 slightly less than 2π . For example, choose $\rho_0 = 6.20$. For this case, plot the phase shifts $\delta_0, \delta_1, \delta_2$ and the partial cross sections $\sigma_0, \sigma_1, \sigma_2$ as functions of (ka) , paying particular attention to the interval, $0 \leq ka \leq 1.5$.

3. For low-energy neutron-proton scattering, the neutron-proton interaction is approximated quite well by a square well with $V = -|V_0|$ for $r \leq a$; $V = 0$ for $r > a$. A reasonable estimate of the range of this potential would be $a = 2\text{fm}$. Use the experimentally observed triplet and singlet scattering lengths, $a_{\text{sc.l.}}^{S=1} = +5.400$ fm, $a_{\text{sc.l.}}^{S=0} = -23.677$ fm, to estimate the triplet and singlet well depths, $|V_0|$, and note their difference.

Plot the singlet scattering cross section, $\sigma_{S=0}$, for the range $E = 0 \rightarrow 0.2\text{MeV}$.

Integral Equation for Two-Body Relative Motion: Scattering Green's Functions in Coordinate Representation

Let us now solve the two-body relative motion scattering problem by integral equation techniques. Our main aim will be to find an approximation for the scattering cross sections valid in the limit of large energies. (Recall the partial wave expansion was useful mainly in the low energy limit, where only a few partial waves may make a significant contribution).

We want to find continuum solutions to

$$H\psi = E\psi, \quad \text{with} \quad H = H_0 + V(\vec{r}), \quad H_0 = -\frac{\hbar^2}{2\mu}\nabla^2, \quad (1)$$

where the plane wave solutions, the solutions for the equation for H_0 , are known

$$(E - H_0)\phi(\vec{r}) = 0. \quad (2)$$

A Box Normalization: Discrete Spectrum

For the moment, let us take box normalization, so the continuous spectrum is replaced by a finely discrete spectrum,

$$(E_n - H_0)\phi_n(\vec{r}) = 0, \quad (3)$$

with

$$\phi_n(\vec{r}) = \frac{e^{i(\vec{k}_n \cdot \vec{r})}}{\sqrt{L^3}}, \quad \vec{k}_n \equiv \vec{k}_{n_1 n_2 n_3}, \quad (4)$$

$$E_n = \frac{\hbar^2}{2\mu} k_n^2 = \frac{\hbar^2}{2\mu} \frac{4\pi^2}{L^2} (n_1^2 + n_2^2 + n_3^2), \quad (5)$$

$$\langle \phi_n | \phi_{n'} \rangle = \delta_{nn'} \equiv \delta_{n_1 n'_1} \delta_{n_2 n'_2} \delta_{n_3 n'_3}. \quad (6)$$

We now seek solutions, ψ , of the wave equation for the full H in the form of a Fourier series,

$$\psi = \sum_n c_n \phi_n. \quad (7)$$

In the wave equation

$$(E - H_0)\psi(\vec{r}) = V(\vec{r})\psi(\vec{r}) = f(\vec{r}), \quad (8)$$

we will also expand the source term, $f(\vec{r})$, in a Fourier series. (This source term carries the source of the scattering process.)

$$f(\vec{r}) = \sum_n a_n \phi_n, \quad (9)$$

with

$$a_n = \int d\vec{r}' \phi_n^*(\vec{r}') f(\vec{r}'), \quad (10)$$

where the integral is over the volume of our cubical laboratory of volume L^3 . Then,

$$(E - H_0) \sum_n c_n \phi_n = \sum_n (E - E_n) c_n \phi_n = \sum_n \int d\vec{r}' \phi_n^*(\vec{r}') \phi_n(\vec{r}) f(\vec{r}'). \quad (11)$$

Using the orthonormality of the ϕ_n

$$c_n = \int \frac{d\vec{r}' \phi_n^*(\vec{r}') f(\vec{r}')}{(E - E_n)}, \quad (12)$$

$$\psi(\vec{r}) = \int d\vec{r}' \sum_n \frac{\phi_n^*(\vec{r}') \phi_n(\vec{r})}{(E - E_n)} f(\vec{r}') = \int d\vec{r}' G(\vec{r}, \vec{r}') f(\vec{r}'), \quad (13)$$

where we have interchanged the integration and the infinite sum, assuming the infinite series has the proper convergence properties. (We have quietly assumed $E \neq E_n$, for any n .) Here, $G(\vec{r}, \vec{r}')$ is the Green's function for the scattering problem

$$G(\vec{r}, \vec{r}') = \sum_n \frac{\phi_n^*(\vec{r}') \phi_n(\vec{r})}{(E - E_n)}, \quad (14)$$

where

$$(E - H_0)G(\vec{r}, \vec{r}') = \sum_n \phi_n^*(\vec{r}') \phi_n(\vec{r}) = \delta(\vec{r} - \vec{r}'). \quad (15)$$

Also, by acting with $(E - H_0)$ on our integral expression for $\psi(\vec{r})$, we can check to make sure we regain the original wave equation,

$$(E - H_0)\psi(\vec{r}) = \int d\vec{r}' \sum_n \phi_n^*(\vec{r}') \phi_n(\vec{r}) V(\vec{r}') \psi(\vec{r}') = V(\vec{r})\psi(\vec{r}). \quad (16)$$

B Continuum Green's Function

Alternatively, we could have taken for our plane-wave states true continuum states

$$\phi_{\vec{k}}(\vec{r}) = \frac{e^{i\vec{k}\cdot\vec{r}}}{(2\pi)^{\frac{3}{2}}} = \langle \vec{r} | \vec{k} \rangle, \quad (17)$$

with Dirac delta-function orthonormality

$$\langle \vec{k}' | \vec{k} \rangle = \delta(\vec{k} - \vec{k}'). \quad (18)$$

It will now be convenient to write the wave equation in the form

$$\frac{2\mu}{\hbar^2}(E - H_0 - V(\vec{r}))\psi(\vec{r}) = 0 \longrightarrow (k^2 + \nabla^2 - U(\vec{r}))\psi(\vec{r}) = 0, \quad (19)$$

or

$$(k^2 + \nabla^2)\psi(\vec{r}) = f(\vec{r}) = U(\vec{r})\psi(\vec{r}), \quad \text{with } U(\vec{r}) = \frac{2\mu}{\hbar^2}V(\vec{r}). \quad (20)$$

The expansion of ψ in plane waves now involves the integral (continuum sum),

$$\psi(\vec{r}) = \int d\vec{k}' c_{\vec{k}'} \phi_{\vec{k}'}(\vec{r}) \quad (21)$$

with

$$f(\vec{r}) = \int d\vec{k}' a_{\vec{k}'} \phi_{\vec{k}'}(\vec{r}) = \int d\vec{k}' \int d\vec{r}' \phi_{\vec{k}'}^*(\vec{r}') \phi_{\vec{k}'}(\vec{r}) f(\vec{r}'). \quad (22)$$

Now,

$$\psi(\vec{r}) = \int d\vec{k}' \int d\vec{r}' \frac{\phi_{\vec{k}'}^*(\vec{r}') \phi_{\vec{k}'}(\vec{r})}{(k'^2 - k'^2)} U(\vec{r}') \psi(\vec{r}'). \quad (23)$$

We will regain the original wave equation for $\psi(\vec{r})$; the operator $(k^2 + \nabla^2)$ acting on $\psi(\vec{r})$ gives

$$\begin{aligned} (k^2 + \nabla^2)\psi(\vec{r}) &= \int d\vec{k}' \int d\vec{r}' \frac{e^{i\vec{k}'\cdot(\vec{r}-\vec{r}')}}{(2\pi)^3} U(\vec{r}') \psi(\vec{r}') \\ &= \int d\vec{r}' \left(\int d\vec{k}' \frac{e^{i\vec{k}'\cdot(\vec{r}-\vec{r}')}}{(2\pi)^3} \right) U(\vec{r}') \psi(\vec{r}') \\ &= \int d\vec{r}' \delta(\vec{r} - \vec{r}') U(\vec{r}') \psi(\vec{r}') = U(\vec{r})\psi(\vec{r}). \end{aligned} \quad (24)$$

As we can see from this result, the properties of the Dirac delta function are such that the interchange of $\int d\vec{k}'$ and $\int d\vec{r}'$ were permissible. If we attempt a similar interchange in eq. (23), to get a Green's function in a form analogous to that of eq. (13), with the discrete sum replaced by the integral $\int d\vec{k}'$, the additional singularities at the values $k' = \pm k$ will cause the integral to diverge. In order to gain the Green's function, we need to modify the $\int d\vec{k}'$ integral. In addition, because the free wave solution, $\phi_{\vec{k}}(\vec{r})$, will automatically satisfy the homogeneous part of eq. (20), we can add it to the solution, and seek solutions to eq. (20) of the form

$$\psi_{\vec{k}}(\vec{r}) = \phi_{\vec{k}}(\vec{r}) + \int d\vec{r}' G(\vec{r}, \vec{r}') U(\vec{r}') \psi_{\vec{k}}(\vec{r}'), \quad (25)$$

with

$$G(\vec{r}, \vec{r}') = \frac{1}{(2\pi)^3} \int_{\text{mod.}} d\vec{k}' \frac{e^{i\vec{k}' \cdot (\vec{r} - \vec{r}')}}{(k'^2 - k^2)}, \quad (26)$$

where the $\int d\vec{k}'$ must be modified to avoid the troubles caused by the singularities at $k' = \pm k$. To see how these singularity problems can be avoided in a way that leads to a Green's function leading to a solution ψ tailored to the boundary conditions of our problem, let us first set up the k' integral without modification. We shall introduce polar coordinates for the vector, \vec{k}' , choosing the vector $\vec{r} - \vec{r}'$ to be along the z direction, (see Fig. 45.1), so

$$\begin{aligned} G(\vec{r}, \vec{r}') &= -\frac{1}{(2\pi)^3} \int d\vec{k}' \frac{e^{ik'|\vec{r}-\vec{r}'| \cos \theta_{k'}}}{(k'^2 - k^2)} \\ &= -\frac{1}{(2\pi)^3} 2\pi \int_0^\infty dk' k'^2 \int_0^\pi d\theta_{k'} \sin \theta_{k'} \frac{e^{ik'|\vec{r}-\vec{r}'| \cos \theta_{k'}}}{(k'^2 - k^2)} \\ &= -\frac{1}{(2\pi)^2} \int_0^\infty dk' k'^2 \int_{-1}^{+1} d\xi \frac{e^{ik'|\vec{r}-\vec{r}'|\xi}}{(k'^2 - k^2)} \\ &= -\frac{1}{(2\pi)^2} \frac{1}{i|\vec{r} - \vec{r}'|} \int_0^\infty dk' k' \frac{(e^{ik'|\vec{r}-\vec{r}'|} - e^{-ik'|\vec{r}-\vec{r}'|})}{(k'^2 - k^2)}. \end{aligned} \quad (27)$$

Because the last integrand is an even function of k' , we can convert it to more symmetrical form

$$\begin{aligned} G(\vec{r}, \vec{r}') &= \frac{i}{2(2\pi)^2} \frac{1}{|\vec{r} - \vec{r}'|} (I_1 - I_2), \quad \text{with} \\ (I_1 - I_2) &= \left(\int_{-\infty}^{+\infty} \frac{dk' k'}{(k'^2 - k^2)} e^{ik'|\vec{r}-\vec{r}'|} - \int_{-\infty}^{+\infty} \frac{dk' k'}{(k'^2 - k^2)} e^{-ik'|\vec{r}-\vec{r}'|} \right). \end{aligned} \quad (28)$$

Without modification, both integrals diverge because of the singularities at $k' = \pm k$. We shall try to overcome this difficulty by replacing $k \rightarrow k + i\eta$ and taking

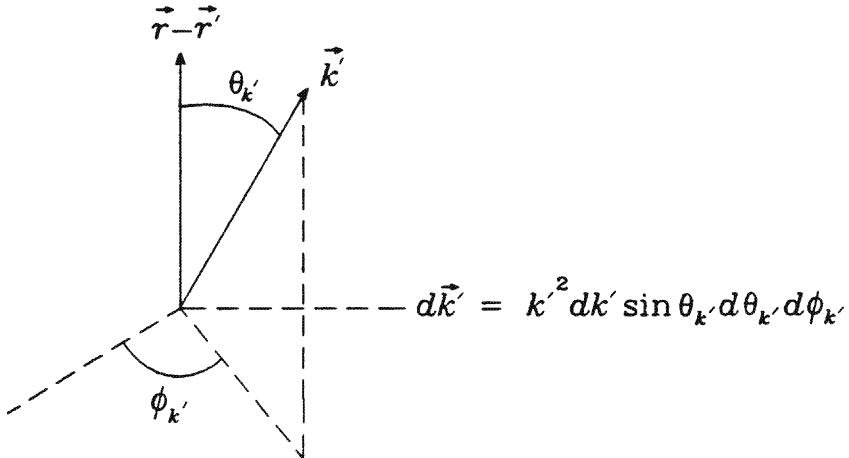


FIGURE 45.1.

the limit $\eta \rightarrow 0$ after doing the integrals by contour integration techniques.

$$I_1 = \lim_{\eta \rightarrow 0} \int_{-\infty}^{+\infty} \frac{dk' k' e^{ik' |\vec{r} - \vec{r}'|}}{(k' - k - i\eta)(k' + k + i\eta)} = \lim_{\eta \rightarrow 0} \oint_{C_1} \frac{dk' k' e^{ik' |\vec{r} - \vec{r}'|}}{(k' - k - i\eta)(k' + k + i\eta)}, \quad (29)$$

where the contour, C_1 (see Fig. 45.2), has been chosen such that the integral over the semicircle in the upper half of the complex k' plane goes to zero as its radius goes to infinity, so the integral is given by the residue theorem

$$\begin{aligned} I_1 &= \lim_{\eta \rightarrow 0} \left(2\pi i \left[\left(\frac{k' e^{ik' |\vec{r} - \vec{r}'|}}{(k' + k + i\eta)} \right) \right]_{k' = k+i\eta} = 2\pi i \frac{1}{2} e^{i(k+i\eta)|\vec{r} - \vec{r}'|} \right) \\ &= i\pi e^{ik|\vec{r} - \vec{r}'|}. \end{aligned} \quad (30)$$

Similarly, the integral I_2 can be converted to a contour integral over the contour, C_2 , in the lower half of the complex k' plane (see Fig. 45.2). The residue theorem at the pole $k' = -k - i\eta$ now gives

$$I_2 = -i\pi e^{ik|\vec{r} - \vec{r}'|}, \quad (31)$$

so with the prescription, $k \rightarrow k + i\eta$, the integrals have been done, and the Green's function becomes

$$G(\vec{r}, \vec{r}') = -\frac{1}{4\pi} \frac{e^{ik|\vec{r} - \vec{r}'|}}{|\vec{r} - \vec{r}'|} \equiv G^{(+)}(\vec{r}, \vec{r}'); \quad (32)$$

i.e., this Green's function has the form proper for an outgoing spherical wave, required by the physical boundary conditions of our scattering solution. With the modification, $k \rightarrow k - i\eta$, however, we would have obtained a solution corresponding to an incoming spherical wave,

$$G^{(-)}(\vec{r}, \vec{r}') = -\frac{1}{4\pi} \frac{e^{-ik|\vec{r} - \vec{r}'|}}{|\vec{r} - \vec{r}'|}. \quad (33)$$

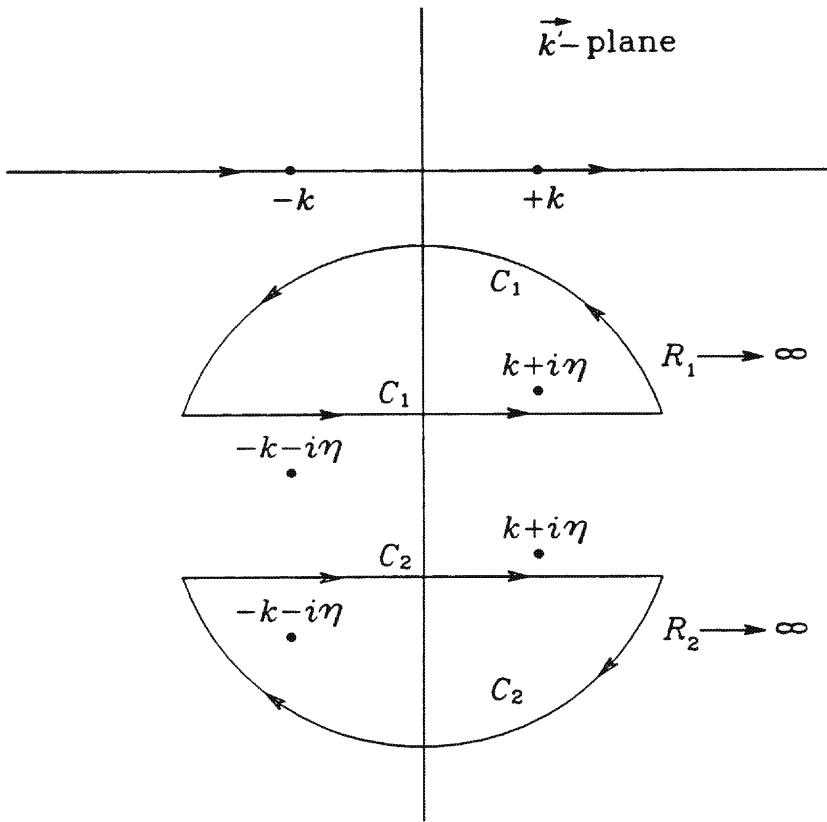


FIGURE 45.2. Green's function contours.

The solution we need is

$$\psi_{\vec{k}}^{(+)}(\vec{r}) = \frac{e^{i\vec{k}\cdot\vec{r}}}{(2\pi)^{\frac{3}{2}}} + \int d\vec{r}' G^{(+)}(\vec{r}, \vec{r}') U(\vec{r}') \psi(\vec{r}'). \quad (34)$$

Because we shall be interested in $\psi^{(+)}$, particularly in the limit $r \rightarrow \infty$, we shall need to expand $|\vec{r} - \vec{r}'|$ in the Green's function. In particular,

$$\begin{aligned} |\vec{r} - \vec{r}'| &= \sqrt{(r^2 + r'^2 - 2rr' \cos \Theta)} = r - r' \cos \Theta + \text{Order}\left(\frac{r'^2}{r}\right) \\ \frac{1}{|\vec{r} - \vec{r}'|} &= \frac{1}{r} + \text{Order}\left(\frac{r'}{r^2}\right). \end{aligned} \quad (35)$$

Therefore, in the needed limit $r \rightarrow \infty$, our $\psi^{(+)}$ has the form

$$\psi_{\vec{k}}^{(+)}(\vec{r}) \longrightarrow \frac{e^{i\vec{k}\cdot\vec{r}}}{(2\pi)^{\frac{3}{2}}} - \frac{e^{ikr}}{4\pi r} \int d\vec{r}' e^{-ikr' \cos \Theta} U(\vec{r}') \psi_{\vec{k}}(\vec{r}'). \quad (36)$$

This equation does not solve our problem, however. We have merely converted our differential equation for ψ into the form of an integral equation that would give us the needed asymptotic form of our solution, if we could do the integral. The integral contains the unknown $\psi_{\vec{k}}$, however. Moreover, we would need to know it in the region where the potential is different from zero, hence, in the region of small \vec{r}' . Nevertheless, the integral equation may be very useful for approximate solutions in the limit of high incoming energy.

Before looking at this case, let us note that we could expand the Green's function in spherical harmonics, by using the expansion

$$\begin{aligned} e^{-ikr' \cos \Theta} &= \sum_l i^l (2l+1) j_l(kr') (-1)^l P_l(\cos \Theta) \\ &= \sum_{l,m} (-i)^l (2l+1) j_l(kr') \frac{4\pi}{(2l+1)} Y_{lm}(\theta, \phi) Y_{lm}^*(\theta', \phi'). \end{aligned} \quad (37)$$

Now, using the asymptotic form for the spherical Hänkel function, $h_l^{(1)}$ [see eq. (26) of math. appendix to Chapter 41], we have, as $r \rightarrow \infty$,

$$h_l^{(1)}(kr) \rightarrow (-i)^{l+1} \frac{e^{ikr}}{r}, \quad \text{or} \quad \frac{e^{ikr}}{r} \rightarrow ik(i)^l h_l^{(1)}(kr), \quad (38)$$

so

$$G^{(+)}(\vec{r}, \vec{r}') = -\frac{1}{4\pi} \frac{e^{ikr}}{r} e^{-ikr' \cos \Theta} = -ik \sum_{l,m} h_l^{(1)}(kr) j_l(kr') Y_{lm}(\theta, \phi) Y_{lm}^*(\theta', \phi'). \quad (39)$$

Moreover, this expression is valid for all values of r with $r > r'$ (not just for $r \gg r'$), because the differential equation for the Green's function

$$(\nabla^2 + k^2) G^{(+)}(\vec{r}, \vec{r}') = \delta(\vec{r} - \vec{r}') \quad (40)$$

has a source term only at the point $\vec{r} = \vec{r}'$, so for any $r > r'$ the solution must be an outgoing free wave.

Now, if we make a partial wave expansion for the $\psi_{\vec{k}}(\vec{r}')$

$$\psi_{\vec{k}}(\vec{r}') = \sum_{l,m} R_l(kr') Y_{lm}(\theta', \phi') \quad (41)$$

in the Green's function integral, this integral can be put in the form

$$\sum_{lm} \int d\vec{r}' G(\vec{r}, \vec{r}') U(\vec{r}') R_l(kr') Y_{lm}(\theta', \phi').$$

This integral will be particularly simple if $U(\vec{r}')$ is independent of θ' and ϕ' , i.e., if $U(\vec{r}') = U(r')$. Then, we can carry out the θ' and ϕ' integrations, if we substitute for the Green's function through eq. (39), to convert this 3-D integral into a sum over purely radial integrals

$$\sum_{lm} Y_{lm}(\theta, \phi) \int_0^\infty dr' r'^2 \left[-ikh_l^{(1)}(kr) j_l(kr') \right] U(r') R_l(kr'),$$

where we can identify $r'^2 \times$ the quantity in square brackets as the 1-D Green's function, $g_l^{(+)}(r, r')$. In addition, if $U(r')$ has the assumed spherical symmetry, the function $\psi_{\vec{k}}$ must have axial symmetry and be independent of ϕ , so the above sum can contain only terms with $m = 0$. Therefore,

$$\psi_{\vec{k}}(\vec{r}) = \phi_{\vec{k}}(\vec{r}) + \sum_l Y_{l0}(\theta) \int_0^\infty dr' g_l^{(+)}(r, r') U(r') R_l(kr'), \quad (42)$$

with

$$\psi_{\vec{k}}(\vec{r}) = \sum_l R_l(kr) Y_{l0}(\theta), \quad (43)$$

and

$$\phi_{\vec{k}}(\vec{r}) = \frac{1}{(2\pi)^{\frac{3}{2}}} \sum_l i^l \sqrt{4\pi(2l+1)} j_l(kr) Y_{l0}(\theta), \quad (44)$$

so we get the integral equation for the radial functions

$$R_l(kr) = \frac{i^l}{\pi} \sqrt{\frac{(2l+1)}{2}} j_l(kr) + \int_0^\infty dr' g_l^{(+)}(r, r') U(r') R_l(kr'). \quad (45)$$

Actually, we have derived only an expression for $g_l^{(+)}(r, r')$, valid for $r > r'$, namely,

$$g_l^{(+)}(r, r') = -ikr'^2 h_l^{(1)}(kr) j_l(kr'), \quad \text{valid for } r > r'. \quad (46)$$

In an appendix to this chapter, we shall show

$$g_l^{(+)}(r, r') = -ikr'^2 j_l(kr) h_l^{(1)}(kr'), \quad \text{valid for } r < r'. \quad (47)$$

C Summary

We have put the scattering problem into integral equation form,

$$\psi_{\vec{k}}(\vec{r}) = \phi_{\vec{k}}(\vec{r}) + \int d\vec{r}' G^{(+)}(\vec{r}, \vec{r}') U(\vec{r}') \psi_{\vec{k}}(\vec{r}'), \quad \text{with } U(\vec{r}') = \frac{2\mu}{\hbar^2} V(\vec{r}'), \quad (48)$$

$$G^{(+)}(\vec{r}, \vec{r}') = -\frac{1}{4\pi} \frac{e^{ik|\vec{r}-\vec{r}'|}}{|\vec{r}-\vec{r}'|}, \quad (49)$$

where

$$(k^2 + \nabla^2) G(\vec{r}, \vec{r}') = \delta(\vec{r} - \vec{r}'), \quad (50)$$

and

$$\phi_{\vec{k}}(\vec{r}) = \frac{1}{(2\pi)^{\frac{3}{2}}} e^{i\vec{k}\cdot\vec{r}}. \quad (51)$$

For a spherically symmetric $U(r)$,

$$\psi_{\vec{k}}(\vec{r}) = \sum_l R_l(kr) Y_{l0}(\theta), \quad (52)$$

where

$$\begin{aligned} R_l(kr) &= \frac{i^l}{\pi} \sqrt{\frac{(2l+1)}{2}} j_l(kr) + \int_0^\infty dr' g_l^{(+)}(r, r') U(r') R_l(kr'), \\ g_l^{(+)}(r, r') &= -ikr'^2 j_l(kr') h_l^{(1)}(kr), \quad \text{for } r > r', \\ g_l^{(+)}(r, r') &= -ikr'^2 h_l^{(1)}(kr') j_l(kr), \quad \text{for } r < r'. \end{aligned} \quad (53)$$

D Closing Remarks

1. We note the symmetry of $G(\vec{r}, \vec{r}')$:

$$G(\vec{r}, \vec{r}') = G(\vec{r}', \vec{r}). \quad (54)$$

2. The integral equation we have derived is not a solution to our scattering problem because the Green's function integral contains the unknown solution, $\psi(\vec{r}')$. If instead of the equations

$$(E - H_0)G(\vec{r}, \vec{r}') = \frac{\hbar^2}{2\mu} \delta(\vec{r} - \vec{r}'), \quad (55)$$

$$(E - H_0)\psi_{\vec{k}}(\vec{r}) = V(\vec{r})\psi_{\vec{k}}(\vec{r}), \quad (56)$$

we had solved the equations

$$(E - H)\bar{G}(\vec{r}, \vec{r}') = \frac{\hbar^2}{2\mu} \delta(\vec{r} - \vec{r}'), \quad (57)$$

$$(E - H)\phi_{\vec{k}}(\vec{r}) = -V(\vec{r})\phi_{\vec{k}}(\vec{r}), \quad (58)$$

we would have arrived at the integral equation

$$\phi_{\vec{k}}(\vec{r}) = \psi_{\vec{k}}(\vec{r}) - \int d\vec{r}' U(\vec{r}') \bar{G}(\vec{r}, \vec{r}') \phi_{\vec{k}}(\vec{r}'). \quad (59)$$

Now, the integral contains only the simple *known* plane wave function, $\phi_{\vec{k}}$, and if we could calculate $\bar{G}(\vec{r}, \vec{r}')$, we could solve this integral equation for the desired $\psi_{\vec{k}}$. Unfortunately, the $\bar{G}(\vec{r}, \vec{r}')$ for the *full* H (rather than the H_0) is of course difficult if not impossible to calculate.

Mathematical Appendix to Chapter 45

One-Dimensional Green's Functions

To evaluate the 1-D Green's function, $g_l(r, r')$ of eq. (53), it will be useful to study 1-D Green's functions in some generality.

The Green's function, $g(t, t')$, for the 1-D second-order differential equation of the form

$$f_0(t) \frac{d^2\psi}{dt^2} + f_1(t) \frac{d\psi}{dt} + f_2(t)\psi(t) = 0 \quad (1)$$

is a solution of the differential equation

$$f_0(t) \frac{d^2g(t, t')}{dt^2} + f_1(t) \frac{dg(t, t')}{dt} + f_2(t)g(t, t') = \delta(t - t'), \quad (2)$$

that is, an inhomogeneous differential equation of the same form with a delta function point source at $t = t'$. We will assume the $f_i(t)$ are "well-behaved" functions (in the language of physicists). We shall be interested in the special case in which $t = r$, $\psi(t) = R_l(r)$, $f_0 = 1$, $f_1 = 2/r$, $f_2 = (k^2 - l(l+1)/r^2)$. We will seek solutions to eq. (2) of the form

$$\begin{aligned} \text{For } t > t' : \quad g(t, t') &= a_1\psi_1(t) + a_2\psi_2(t), \\ \text{for } t < t' : \quad g(t, t') &= b_1\psi_1(t) + b_2\psi_2(t), \end{aligned} \quad (3)$$

where $\psi_1(t)$, $\psi_2(t)$ are two independent solutions of differential equation (1). The constants a_i , b_i are then functions of t' . Also, at $t = t'$, $g(t, t')$ must be continuous. If it were not, $\frac{dg}{dt}$ would contain a delta function and the second derivative of g would contain a derivative of a delta function, but the right-hand side of eq. (2) contains only a delta function, not a derivative of a delta function. Thus,

$$g(t = t' + \epsilon, t') - g(t = t' - \epsilon, t') = 0, \quad (4)$$

but

$$\left[\frac{dg(t, t')}{dt} \right]_{t=t'+\epsilon} - \left[\frac{dg(t, t')}{dt} \right]_{t=t'-\epsilon} \neq 0. \quad (5)$$

To determine its value, integrate eq. (2) over an interval from $t = t' - \epsilon$ to $t = t' + \epsilon$,

$$\int_{t'-\epsilon}^{t'+\epsilon} dt f_0(t) \frac{d^2g(t, t')}{dt^2} + \int_{t'-\epsilon}^{t'+\epsilon} dt f_1(t) \frac{dg(t, t')}{dt} + \int_{t'-\epsilon}^{t'+\epsilon} dt f_2(t)g(t, t') = 1, \quad (6)$$

leading to

$$f_0(t') \left(\left[\frac{dg(t, t')}{dt} \right]_{t=t'+\epsilon} - \left[\frac{dg(t, t')}{dt} \right]_{t=t'-\epsilon} \right) = 1, \quad (7)$$

where we have made use of the continuity of $g(t, t')$, and of course the assumed continuity of the $f_i(t)$ at $t = t'$. The boundary conditions, eqs. (4) and (7), lead to

$$\begin{aligned} a_1\psi_1(t') + a_2\psi_2(t') &= b_1\psi_1(t') + b_2\psi_2(t'), \\ a_1\psi'_1(t') + a_2\psi'_2(t') &= b_1\psi'_1(t') + b_2\psi'_2(t') + \frac{1}{f_0(t')}, \end{aligned} \quad (8)$$

where the primes on the ψ 's stand for derivatives. These equations can be solved for the a_i

$$a_1 = b_1 - \frac{\psi_2(t')}{f_0(t')W(t')},$$

$$a_2 = b_2 + \frac{\psi_1(t')}{f_0(t')W(t')}, \quad (9)$$

where $W(t')$ is the Wronskian

$$W(t') = \psi_1(t') \frac{d\psi_2}{dt'} - \psi_2(t') \frac{d\psi_1}{dt'}, \quad (10)$$

leading to

$$\begin{aligned} \text{For } t < t' : g(t, t') &= b_1 \psi_1(t) + b_2 \psi_2(t), \\ \text{for } t > t' : g(t, t') &= b_1 \psi_1(t) + b_2 \psi_2(t) - \frac{[\psi_1(t)\psi_2(t') - \psi_2(t)\psi_1(t')]}{f_0(t')W(t')}. \end{aligned} \quad (11)$$

The Wronskian follows from the differential equation, in particular, from

$$\begin{aligned} \psi_1 \left(f_0 \frac{d^2\psi_2}{dt^2} + f_1 \frac{d\psi_2}{dt} + f_0 \psi_2 \right) &= 0, \\ -\psi_2 \left(f_0 \frac{d^2\psi_1}{dt^2} + f_1 \frac{d\psi_1}{dt} + f_0 \psi_1 \right) &= 0. \end{aligned} \quad (12)$$

By adding these equations, we get

$$f_0 \frac{d}{dt} \left(\psi_1 \frac{d\psi_2}{dt} - \psi_2 \frac{d\psi_1}{dt} \right) + f_1 \left(\psi_1 \frac{d\psi_2}{dt} - \psi_2 \frac{d\psi_1}{dt} \right) = 0, \quad (13)$$

$$\frac{dW}{dt} = -\frac{f_1}{f_0} W, \quad \text{or} \quad \ln W = - \int dt \frac{f_1(t)}{f_0(t)}. \quad (14)$$

The One-Dimensional Radial Green's Functions, $g_l(r, r')$

For our radial functions, with $\psi = R_l(kr)$, the functions $f_0 = 1$, $f_1 = 2/r$ lead to

$$\frac{dW}{W} = -\frac{2}{r} dr, \quad W(r) = \frac{\text{const.}}{r^2}. \quad (15)$$

For the two solutions, ψ_1 and ψ_2 , we shall choose $\psi_1 = j_l(kr)$; $\psi_2 = n_l(kr)$. To determine the constant in the above expression for the Wronskian, it is sufficient to use the asymptotic form for $j_l(kr)$ and $n_l(kr)$ and let $r \rightarrow \infty$, which leads at once to $W(r) = 1/(kr^2)$.

Now, for $r < r'$, our general result gives

$$g_l(r, r') = b_1(r')j_l(kr) + b_2(r')n_l(kr), \quad (16)$$

but because the differential equation for g_l has a singularity *only* at $r = r'$ through the delta function source term, the solution for $r < r'$ must be regular at $r = 0$, and the coefficient b_2 must be zero. Thus, with our general result for the 1-D g , eq. (9), we have

$$\begin{aligned} \text{For } r < r' : g_l(r, r') &= b_1(r')j_l(kr), \\ \text{for } r > r' : g_l(r, r') &= a_1(r')j_l(kr) + a_2(r')n_l(kr) \\ &= [b_1(r') - kr'^2 n_l(kr')] + j_l(kr) \\ &\quad + kr'^2 j_l(kr')n_l(kr). \end{aligned} \quad (17)$$

From eq. (46) of the main body of Chapter 45, we know, for $r > r'$,

$$\begin{aligned} g_l(r, r') &= -ikr'^2 j_l(kr') h_l^{(1)}(kr) \\ &= -ikr'^2 j_l(kr')(j_l(kr) + in_l(kr)). \end{aligned} \quad (18)$$

Comparing with the above, this gives

$$b_1(r') = -ikr'^2(j_l(kr') + in_l(kr')) = -ikr'^2 h_l^{(1)}(kr'). \quad (19)$$

Thus, we have, for $r < r'$,

$$g_l(r, r') = b_1(r') j_l(kr) = -ikr'^2 h_l(kr') j_l(kr), \quad (20)$$

which is the result given by eq. (47).

The Born Approximation

In the last chapter, we merely reformulated the scattering problem. Instead of solving the scattering problem by finding a solution to a differential equation with the appropriate boundary condition, we will instead try to solve it by finding a solution to an integral equation with the appropriate Green's function.

$$\psi_{\vec{k}}(\vec{r}) = \phi_{\vec{k}}(\vec{r}) + \int d\vec{r}' G^{(+)}(\vec{r}, \vec{r}') \frac{2\mu}{\hbar^2} V(\vec{r}') \psi_{\vec{k}}(\vec{r}'). \quad (1)$$

Because we cannot do the integral containing the *unknown* $\psi_{\vec{k}}(\vec{r}')$, we are far from a solution. If $V(\vec{r})$ is a weak potential, however, so it can be treated by perturbation theory, or if the energy is very large, so the average $V(\vec{r})$ is small compared with this energy, we can solve the integral equation by an iteration technique. If

$$|V(\vec{r}')|_{\text{Average}} \ll \frac{\hbar^2 k^2}{2\mu}, \quad (2)$$

in a first approximation for $\psi_{\vec{k}}(\vec{r})$, we can replace $\psi_{\vec{k}}(\vec{r}')$ in the integral by the zeroth approximation for the problem, $\phi_{\vec{k}}(\vec{r}')$, to yield

$$\psi_{\vec{k}}(\vec{r}) \approx \frac{1}{(2\pi)^{\frac{3}{2}}} \left(e^{i\vec{k}\cdot\vec{r}} - \frac{1}{4\pi} \int d\vec{r}' \frac{e^{i\vec{k}\cdot|\vec{r}-\vec{r}'|}}{|\vec{r}-\vec{r}'|} \frac{2\mu}{\hbar^2} V(\vec{r}') e^{i\vec{k}\cdot\vec{r}'} \right), \quad (3)$$

where this approximate solution is known as the first Born approximation. Even without putting this first approximation back into the integral equation to get the next approximation, and perhaps iterating this process a number of times, the simple first Born approximation may be a useful good approximation. In that case,

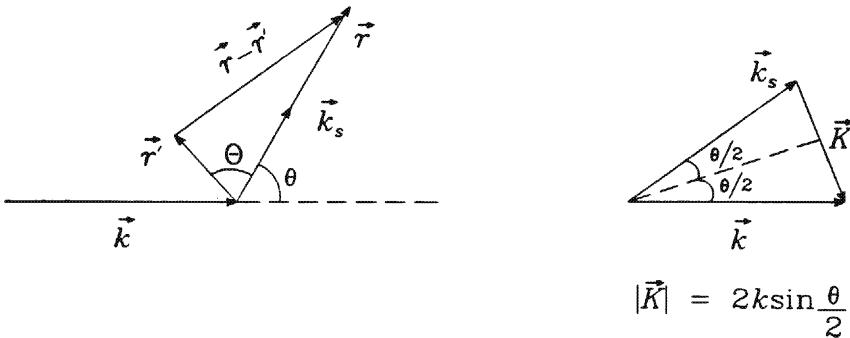


FIGURE 46.1.

if we use the asymptotic form

$$\frac{e^{ik|\vec{r}-\vec{r}'|}}{|\vec{r}-\vec{r}'|} \rightarrow \frac{e^{ikr}}{r} e^{-ikr' \cos \Theta} = \frac{e^{ikr}}{r} e^{-i\vec{k}_s \cdot \vec{r}'}, \quad (4)$$

where \vec{k}_s , the \vec{k} vector in the direction of the scattered wave, is along the direction of the vector \vec{r} from the scattering center to the detector [see Fig. 46.1(a)], we get

$$\psi_{\vec{k}}(\vec{r}) \rightarrow \frac{1}{(2\pi)^{\frac{3}{2}}} \left(e^{i\vec{k} \cdot \vec{r}} - \frac{e^{ikr}}{r} \left[\frac{\mu}{2\pi\hbar^2} \int d\vec{r}' V(\vec{r}') e^{i(\vec{k}-\vec{k}_s) \cdot \vec{r}'} \right] \right), \quad (5)$$

so the first Born approximation for the scattering amplitude is given by

$$f(\theta, \phi)_{1^{\text{st}} \text{Born}} = -\frac{\mu}{2\pi\hbar^2} \int d\vec{r}' V(\vec{r}') e^{i(\vec{k}-\vec{k}_s) \cdot \vec{r}'} . \quad (6)$$

In the special case when the scattering potential is spherically symmetric, so $V(\vec{r}') = V(r')$, it is easy to reduce the 3-D Born integral to a radial integral. For that purpose, it is useful to define the vector $\vec{K} = \vec{k} - \vec{k}_s$ [see Fig. 46.1(b)], with magnitude $K = |\vec{K}| = 2k \sin \frac{\theta}{2}$, and choose it to be along the z direction, so

$$\begin{aligned} \int d\vec{r}' V(\vec{r}') e^{i(\vec{k}-\vec{k}_s) \cdot \vec{r}'} &= \int d\vec{r}' V(r') e^{iKr' \cos \theta'} \\ &= 2\pi \int_0^\infty dr' r'^2 V(r') \int_{-1}^{+1} d\zeta' e^{iKr' \zeta'} = 2\pi \int_0^\infty dr' r'^2 V(r') \frac{2}{Kr'} \sin Kr' \\ &= \frac{4\pi}{K} \int_0^\infty dr' r' V(r') \sin Kr'. \end{aligned} \quad (7)$$

This equation leads to the first Born approximation of the scattering amplitude

$$f(\theta)_{1^{\text{st}} \text{Born}} = -\frac{2\mu}{K\hbar^2} \int_0^\infty dr' r' V(r') \sin Kr', \quad \text{with } K = 2k \sin \frac{\theta}{2}. \quad (8)$$

A Application: The Yukawa Potential

As a simple example, let us choose an attractive potential of Yukawa form

$$V(r) = -g^2 \frac{e^{-\beta r}}{r}, \quad (9)$$

with $\beta = \frac{mc}{\hbar}$, where m is the mass of the exchanged particle. Note: this is the first potential that Yukawa had in mind, where m should be the mass of the meson (the pion) exchanged between nucleons to give rise to the nucleon–nucleon interaction. The real pion-exchange potential, however, is more complicated and has strong spin-dependence, but retains the basic exponential factor, $e^{-\frac{m_\pi c r}{\hbar}}/r$. For this potential, the first Born approximation gives

$$f(\theta) = \frac{2\mu g^2}{\hbar^2 K} \int_0^\infty dr' e^{-\beta r'} \sin Kr' = \frac{2\mu g^2}{\hbar^2 K} \frac{K}{[\beta^2 + K^2]}, \quad (10)$$

leading to

$$\frac{d\sigma}{d\Omega} = |f(\theta)|^2 = \frac{4\mu^2 g^4}{\hbar^4} \frac{1}{[\beta^2 + 4k^2 \sin^2 \frac{\theta}{2}]^2}. \quad (11)$$

B The Screened Coulomb Potential

First, the first Born approximation leads to an undetermined integral for a pure Coulomb potential. With

$$V(r) = \frac{Z_1 Z_2 e^2}{r}, \quad (12)$$

the first Born approximation would lead to

$$f(\theta)_{\text{1st Born}} = -\frac{\mu Z_1 Z_2 e^2}{\hbar^2 k \sin \frac{\theta}{2}} \int_0^\infty dr' \sin Kr', \quad (13)$$

leading to the undetermined radial integral. The Coulomb potential has such a far reach the plane wave is not a good enough zeroth approximation. (See the mathematical appendix for Chapter 42). For a screened Coulomb potential, however, with

$$V(r) = \frac{Z_1 Z_2 e^2}{r} e^{-\beta r}, \quad (14)$$

and with a very small value for the screening constant β , we might get a reasonable approximation for the Coulomb potential. If we consider α particle scattering from a Helium atom, the above might be a very good approximation for the needed potential if β is of the order of an inverse atomic dimension. Yet, this potential would give us the effects of α - α scattering when the α particle is near the He nucleus of the atom. Because the form of this screened Coulomb potential is the

same as that of the Yukawa potential, the differential scattering cross section is given by

$$\frac{d\sigma}{d\Omega} = \frac{4\mu^2 Z_1^2 Z_2^2 e^4}{\hbar^4} \frac{1}{[\beta^2 + 4k^2 \sin^2 \frac{\theta}{2}]^2}. \quad (15)$$

In the limit $\beta \rightarrow 0$, this equation yields

$$\frac{d\sigma}{d\Omega} = \frac{\mu^2 Z_1^2 Z_2^2 e^4}{4\hbar^4 k^4 \sin^4 \frac{\theta}{2}} = \frac{Z_1^2 Z_2^2 e^4}{16E^2 \sin^4 \frac{\theta}{2}} = \left(\frac{d\sigma}{d\Omega} \right)_{\text{Rutherford}}. \quad (16)$$

That is, this limiting value of the Born approximation for the screened Coulomb potential gives us the classical Rutherford result. This is also the correct quantum-mechanical result for α nucleus scattering. The exact quantum-mechanical result for the scattering amplitude for Coulomb scattering is given by (see the appendix to this chapter),

$$f(\theta)_{\text{exact Coul.}} = -\frac{\mu Z_1 Z_2 e^2}{2\hbar^2 k^2 \sin^2 \frac{\theta}{2}} e^{[-i\gamma \ln \sin^2 \frac{\theta}{2} + 2i\sigma_0]}, \quad \text{where } \gamma = \frac{\mu Z_1 Z_2 e^2}{\hbar^2 k}, \quad (17)$$

and σ_0 is the argument of the Gamma function $\Gamma(1 + i\gamma)$. Because the differential cross section is given by $|f(\theta)|^2$, the logarithmic dependence on $\sin^2 \frac{\theta}{2}$ of the exponential does not come into play! The classical and quantum-mechanical results, however, are different for the scattering of identical particles from identical particles, say, α - α scattering.

C Identical Particle Coulomb Scattering

Even the classical Rutherford formula must be modified if we scatter identical particles from identical particles. For α - α scattering, e.g., the detector at the position θ in the center of mass system will give a count both if the incoming projectile is scattered into the direction θ [see Fig. 46.2(a)], and if the incoming projectile is scattered into direction $(\pi - \theta)$, so the α particle that was the original “target” particle is scattered into direction θ [see Fig. 46.2(b)], because the detector can not distinguish “projectile” α particles from “target” α particles. Thus,

$$\left(\frac{d\sigma}{d\Omega} \right)_{\text{classical}} = \frac{\gamma^2}{4k^2} \left(\frac{1}{\sin^4 \frac{\theta}{2}} + \frac{1}{\cos^4 \frac{\theta}{2}} \right). \quad (18)$$

For the quantum-mechanical result, we must remember that the α particle has spin $s = 0$. Thus, α particles are bosons. The two-particle functions must be orbitally symmetric under the exchange of particle indices 1 and 2. Thus, solutions must be of the form,

$$\psi(\vec{r}_1, \vec{r}_2) + \psi(\vec{r}_2, \vec{r}_1),$$

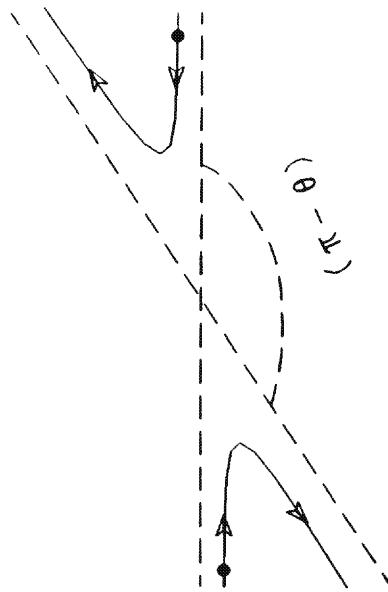
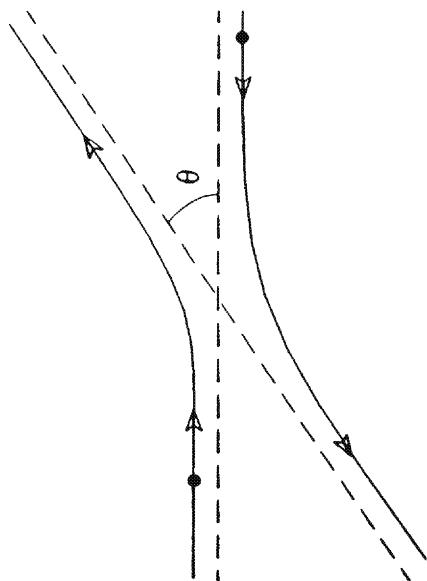


FIGURE 46.2.



or, with the relative position vector $\vec{r} = \vec{r}_1 - \vec{r}_2$, the relative motion function must have the form,

$$\psi(\vec{r}) + \psi(-\vec{r}),$$

so, in the limit $r \rightarrow \infty$,

$$\psi_{\vec{k}} \rightarrow \left(\left(e^{i\vec{k}\cdot\vec{r}} + e^{-i\vec{k}\cdot\vec{r}} \right)_{\text{Coul. mod.}} + [f(\theta) + f(\pi - \theta)] \left(\frac{e^{ikr}}{r} \right)_{\text{Coul. mod.}} \right), \quad (19)$$

where the Coulomb modified plane waves and outgoing spherical waves are (see mathematical appendix to this chapter),

$$\left(e^{i\vec{k}\cdot\vec{r}} \right)_{\text{Coul. mod.}} = e^{i(\vec{k}\cdot\vec{r} + \gamma \ln(kr(1 - \cos \theta)))}, \quad \left(\frac{e^{ikr}}{r} \right)_{\text{Coul. mod.}} = \frac{e^{i(kr - \gamma \ln 2kr)}}{r}, \quad (20)$$

with

$$f(\theta) = -\gamma \frac{e^{-i\gamma \ln \sin^2 \frac{\theta}{2}} e^{2i\sigma_0}}{2k \sin^2 \frac{\theta}{2}}, \quad (21)$$

where σ_0 is the argument of the complex number, $\Gamma(1 + i\gamma)$ (see mathematical appendix to Chapter 42). In the center of mass system, the differential cross section is now

$$\begin{aligned} \left(\frac{d\sigma}{d\Omega} \right)_{\text{C.M.}} &= |f(\theta) + f(\pi - \theta)|^2 \\ &= \frac{\gamma^2}{4k^2} \left| \frac{e^{-i\gamma \ln \sin^2 \frac{\theta}{2}}}{\sin^2 \frac{\theta}{2}} + \frac{e^{-i\gamma \ln \cos^2 \frac{\theta}{2}}}{\cos^2 \frac{\theta}{2}} \right|^2 \\ &= \frac{\gamma^2}{4k^2} \left(\frac{1}{\sin^4 \frac{\theta}{2}} + \frac{1}{\cos^4 \frac{\theta}{2}} + 2 \frac{\cos[\gamma \ln(\tan^2 \frac{\theta}{2})]}{\sin^2 \frac{\theta}{2} \cos^2 \frac{\theta}{2}} \right). \end{aligned} \quad (22)$$

Finally, for identical particle scattering, the transformation from the center of mass to the laboratory system is very simple (see Chapter 41),

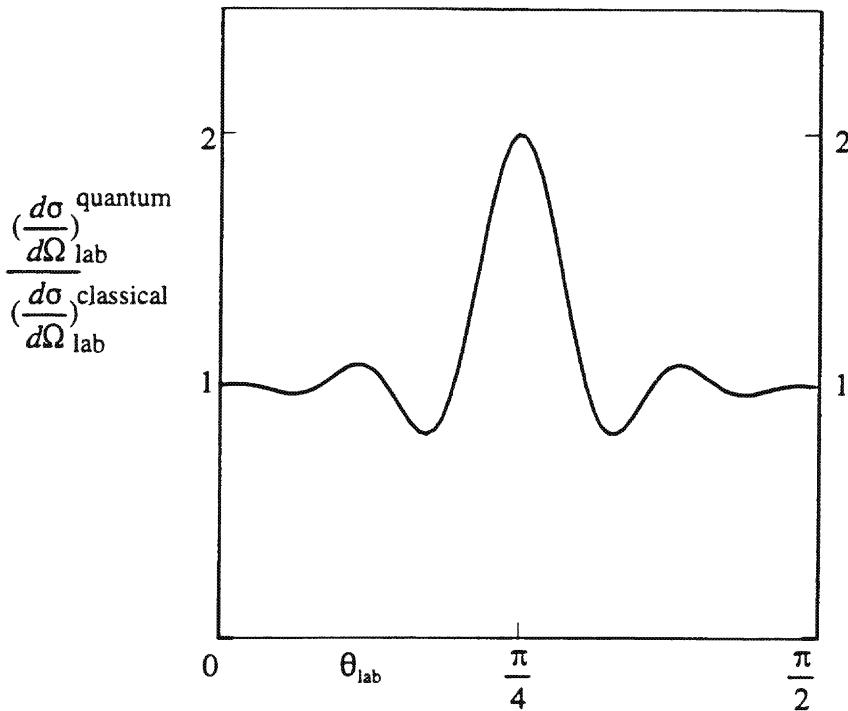
$$\theta_{\text{lab}} = \frac{\theta}{2}, \quad \left(\frac{d\sigma}{d\Omega} \right)_{\text{lab}} = 4 \cos \theta_{\text{lab}} \left(\frac{d\sigma}{d\Omega} \right)_{\text{C.M.}}, \quad (23)$$

so

$$\left(\frac{d\sigma}{d\Omega} \right)_{\text{lab}} = \frac{\gamma^2 \cos \theta_{\text{lab}}}{k^2} \left(\frac{1}{\sin^4 \theta_{\text{lab}}} + \frac{1}{\cos^4 \theta_{\text{lab}}} + 2 \frac{\cos[\gamma \ln(\tan^2 \theta_{\text{lab}})]}{\sin^2 \theta_{\text{lab}} \cos^2 \theta_{\text{lab}}} \right). \quad (24)$$

The cross term is very important. Fig. 46.3 shows the ratio of the quantum-mechanical differential cross section to the classical cross section for this case of the scattering of spin $s = 0$ bosons from identical spin $s = 0$ bosons.

Finally, for proton-proton Coulomb scattering, the situation is a little more complicated. Protons are $s = \frac{1}{2}$ particles and, hence, fermions. If both projectile and target protons are unpolarized, the two-proton system will be in the spin-antisymmetric state, with two-particle spin $S = 0, \frac{1}{4}$ of the time and in the spin-symmetric state, with two-particle spin $S = 1, \frac{3}{4}$ of the time. Hence, the orbital

FIGURE 46.3. Differential scattering cross sections for $\alpha-\alpha$ scattering.

functions will be in an orbitally symmetric state $\frac{1}{4}$ of the time and in an orbitally antisymmetric state $\frac{3}{4}$ of the time. Thus, for proton–proton Coulomb scattering

$$\left(\frac{d\sigma}{d\Omega}\right)_{C.M.} = \frac{1}{4}|f(\theta) + f(\pi - \theta)|^2 + \frac{3}{4}|f(\theta) - f(\pi - \theta)|^2, \quad (25)$$

leading to a formula like that of eq. (24) in which the coefficient of 2 in the cross term is replaced by $(\frac{1}{4} - \frac{3}{4}) \times 2 = -1$, leading to quite a different angular distribution.

Mathematical Appendix to Chapter 46

Exact Solution for the Pure Coulomb Scattering Problem

In the appendix to Chapter 42, we solved the problem for Coulomb scattering in a partial wave expansion, where the relative motion function was expanded in radial functions, $R_l(kr)$, and in spherical harmonics, $\psi(r, \theta, \phi) = \sum_l R_l(kr) Y_{l0}(\theta, \phi)$. Our main aim there was to get the asymptotic form in the limit of large r of the incoming and outgoing Coulomb spherical waves. These results are particularly useful if the long-range part of the potential is dominated by the Coulomb potential,

but if, in addition, a short-range potential exists, such as a nuclear potential. As in any partial wave expansion, this approach leads to differential and total scattering cross sections in terms of infinite series in the l 's of the partial waves. For the case of pure Coulomb scattering, however, we can find an exact solution that gives us the scattering amplitude exactly, (without need of an infinite series). This amplitude would apply, e.g., for proton–nucleus, or α -nucleus scattering, or α – α scattering, at energies low enough, so the proton or α particle has a very low probability of tunneling through the repulsive Coulomb barrier into the small r region, where the nuclear force would become effective.

We want to solve the Schrödinger equation for the relative motion ψ

$$\begin{aligned}\nabla^2\psi + \left(\frac{2\mu E}{\hbar^2} - \frac{2\mu Z_1 Z_2 e^2}{\hbar^2} \frac{1}{r}\right)\psi &= 0, \\ \nabla^2\psi + \left(k^2 - \frac{2\gamma k}{r}\right)\psi &= 0,\end{aligned}\quad (1)$$

where γ is the Coulomb parameter

$$\gamma = \frac{\mu Z_1 Z_2 e^2}{\hbar^2 k} = \frac{c}{v} \alpha Z_1 Z_2. \quad (2)$$

We want to solve this problem with the appropriate boundary conditions; i.e., we seek a solution in the form of a Coulomb-corrected incoming plane wave + a Coulomb-corrected outgoing spherical wave. This boundary condition motivates us to first make the substitution

$$\psi(\vec{r}) = e^{i\vec{k}\cdot\vec{r}} \chi(\vec{r}). \quad (3)$$

With

$$\begin{aligned}\vec{\nabla}\psi &= e^{i\vec{k}\cdot\vec{r}} (\vec{\nabla}\chi + i\vec{k}\chi), \\ \nabla^2\psi &= e^{i\vec{k}\cdot\vec{r}} (\nabla^2\chi + 2i\vec{k}\cdot\vec{\nabla}\chi - k^2\chi),\end{aligned}\quad (4)$$

this leads to the equation

$$\nabla^2\chi + 2i\vec{k}\cdot\vec{\nabla}\chi - \frac{2\gamma k}{r}\chi = 0. \quad (5)$$

If we choose the z axis along the direction of \vec{k} , $\chi(\vec{r})$ will be a function of r and θ only. It will be particularly useful to transform from r, θ , to parabolic coordinates, ξ, η , where

$$\begin{aligned}\xi &= r - z = r(1 - \cos\theta), \\ \eta &= r + z = r(1 + \cos\theta).\end{aligned}\quad (6)$$

It will be sufficient to seek solutions of the form $e^{i\vec{k}\cdot\vec{r}}\chi(\xi)$, i.e., solutions independent of the variable η . It will be shown, a posteriori, that these have the desired asymptotic form of a Coulomb-corrected plane wave + a Coulomb-corrected spherical outgoing wave. (Solutions of the form $e^{i\vec{k}\cdot\vec{r}}\chi(\eta)$ would have given us solutions with the asymptotic form of a Coulomb-corrected plane wave + a Coulomb-corrected spherical incoming wave.)

With $\chi = \chi(\xi, \text{only})$, $\xi = r - z = r(1 - \cos \theta)$,

$$\vec{\nabla} \chi = \frac{d\chi}{d\xi} \left(\frac{x}{r} \vec{e}_1 + \frac{y}{r} \vec{e}_2 + \left(\frac{z}{r} - 1 \right) \vec{e}_3 \right) = \frac{d\chi}{d\xi} \left(\frac{\vec{r}}{r} - \frac{\vec{k}}{k} \right), \quad (7)$$

so

$$2ik \cdot \vec{\nabla} \chi = \frac{2ik}{r} (\cos \theta - 1) r \frac{d\chi}{d\xi} = -\frac{2}{r} ik\xi \frac{d\chi}{d\xi}, \quad (8)$$

and

$$\begin{aligned} \nabla^2 \chi &= \frac{d\chi}{d\xi} \vec{\nabla} \cdot \left(\frac{\vec{r}}{r} - \frac{\vec{k}}{k} \right) + \left(\vec{\nabla} \frac{d\chi}{d\xi} \right) \cdot \left(\frac{\vec{r}}{r} - \frac{\vec{k}}{k} \right) \\ &= \frac{d\chi}{d\xi} \left(\frac{3}{r} - \frac{\vec{r} \cdot \vec{r}}{r^3} \right) + \frac{d^2\chi}{d\xi^2} \left(\frac{\vec{r}}{r} - \frac{\vec{k}}{k} \right) \cdot \left(\frac{\vec{r}}{r} - \frac{\vec{k}}{k} \right) \\ &= \frac{2}{r} \frac{d\chi}{d\xi} + 2 \frac{d^2\chi}{d\xi^2} \left(1 - \frac{\vec{k} \cdot \vec{r}}{kr} \right) = \frac{2}{r} \left(\frac{d\chi}{d\xi} + \xi \frac{d^2\chi}{d\xi^2} \right), \end{aligned} \quad (9)$$

leading to the new equation

$$\frac{2}{r} \left(\xi \frac{d^2\chi}{d\xi^2} + (1 - ik\xi) \frac{d\chi}{d\xi} - \gamma k \chi \right) = 0. \quad (10)$$

Introducing the new variable,

$$t = ik\xi, \quad (11)$$

$$\begin{aligned} t \frac{d^2\chi}{dt^2} + (1 - t) \frac{d\chi}{dt} + i\gamma \chi(t) &= 0, \\ t \frac{d^2\chi}{dt^2} + (c - t) \frac{d\chi}{dt} - a \chi(t) &= 0, \end{aligned} \quad (12)$$

so

$$\chi(ik\xi) = {}_1F_1(-i\gamma; 1; ik\xi). \quad (13)$$

The solutions are confluent hypergeometric functions and

$$\psi = e^{ikr} {}_1F_1(-i\gamma; 1; ikr(1 - \cos \theta)). \quad (14)$$

Now recall (see mathematical appendix to Chapter 42)

$${}_1F_1(a; c; t) = \frac{\Gamma(c)}{2\pi i} \oint_C \frac{dz e^z}{z^c (1 - \frac{t}{z})^a}, \quad (15)$$

where $a = -i\gamma$, $c = 1$, $t = ikr(1 - \cos \theta)$, so (with $\Gamma(1) = 1$)

$${}_1F_1(-i\gamma; 1; ikr(1 - \cos \theta)) = \frac{1}{2\pi i} \oint_C \frac{dz e^z (z - t)^{i\gamma}}{z^{1+i\gamma}}. \quad (16)$$

The contour, C , can again be deformed as shown in Fig. 46.4 into the two loops, C_1 and C_2 . In the limit $r \rightarrow \infty$, only the small circular parts of the contours, C_1

and C_2 , make a nonnegligible contribution to these integrals. Thus,

$$\begin{aligned} & \lim_{r \rightarrow \infty} \frac{1}{2\pi i} \oint_{C_1} \frac{dze^z [z - ikr(1 - \cos \theta)]^{i\gamma}}{z^{1+i\gamma}} \\ &= \lim_{r \rightarrow \infty} \frac{[-ikr(1 - \cos \theta)]^{i\gamma}}{2\pi i} \oint_{C_1} \frac{dze^z}{z^{1+i\gamma}} \left[1 - \frac{z}{ikr(1 - \cos \theta)} \right]^{i\gamma} \\ &= \frac{[-ikr(1 - \cos \theta)]^{i\gamma}}{2\pi i} \oint_{C_1} \frac{dze^z}{z^{1+i\gamma}} = \frac{[-ikr(1 - \cos \theta)]^{i\gamma}}{\Gamma(1 + i\gamma)}, \end{aligned} \quad (17)$$

where we have used

$$\frac{1}{2\pi i} \oint \frac{dze^z}{z^\alpha} = \frac{1}{\Gamma(\alpha)}, \quad (18)$$

where the contour is now a circle about the origin. Similarly, for the contour integral for the contour, C_2 , where we use $t = ikr(1 - \cos \theta)$,

$$\begin{aligned} & \lim_{t \rightarrow \infty} \frac{1}{2\pi i} \oint_{C_2} \frac{dze^z (z - t)^{i\gamma}}{z^{1+i\gamma}} = \lim_{t \rightarrow \infty} \frac{1}{2\pi i} \frac{e^t}{t^{1+i\gamma}} \oint_{C_2} \frac{d(z - t)e^{(z-t)}(z - t)^{i\gamma}}{(1 + \frac{(z-t)}{t})^{1+i\gamma}} \\ &= \lim_{t \rightarrow \infty} \frac{e^t}{t^{1+i\gamma}} \frac{1}{2\pi i} \oint_{C_2} \frac{dze^z z^{i\gamma}}{(1 + \frac{z}{t})^{1+i\gamma}} \rightarrow \frac{e^t}{t^{1+i\gamma}} \frac{1}{2\pi i} \oint_{C_2} dze^z z^{i\gamma} \\ &= \frac{e^t}{t^{1+i\gamma}} \frac{1}{\Gamma(-i\gamma)} = \frac{e^{ikr(1-\cos\theta)}}{[ikr(1-\cos\theta)]^{1+i\gamma} \Gamma(-i\gamma)}, \end{aligned} \quad (19)$$

where the contour integral about the singularity at $z = t = ikr(1 - \cos \theta)$ of the first line has been transformed to a contour integral about the point $z = 0$ in the next line.

Combining the two contour integrals, we have

$$\begin{aligned} & \lim_{r \rightarrow \infty} {}_1F_1(-i\gamma; 1; ikr(1 - \cos \theta)) \\ &= \left(\frac{[-ikr(1 - \cos \theta)]^{i\gamma}}{\Gamma(1 + i\gamma)} + \frac{e^{ikr(1-\cos\theta)}}{[ikr(1-\cos\theta)]^{1+i\gamma} \Gamma(-i\gamma)} \right), \end{aligned} \quad (20)$$

so, with

$$\psi(\vec{r}) = e^{ikr \cos \theta} {}_1F_1(-i\gamma; 1; ikr(1 - \cos \theta)), \quad (21)$$

$$\begin{aligned} \psi &\rightarrow \frac{e^{ikr \cos \theta} [-ikr(1 - \cos \theta)]^{i\gamma}}{\Gamma(1 + i\gamma)} \\ &+ \frac{e^{ikr}}{[ikr(1 - \cos \theta)]} \frac{1}{[ikr(1 - \cos \theta)]^{i\gamma} \Gamma(-i\gamma)}. \end{aligned} \quad (22)$$

Now, we shall use the Γ function properties

$$\Gamma(1 + i\gamma) = i\gamma \Gamma(i\gamma) = e^{i\frac{\pi}{2}\gamma} |\Gamma(i\gamma)| e^{i\arg \Gamma(i\gamma)} = |\Gamma(1 + i\gamma)| e^{i\sigma_0}, \quad (23)$$

so

$$\arg \Gamma(i\gamma) = (\sigma_0 - \frac{\pi}{2}). \quad (24)$$

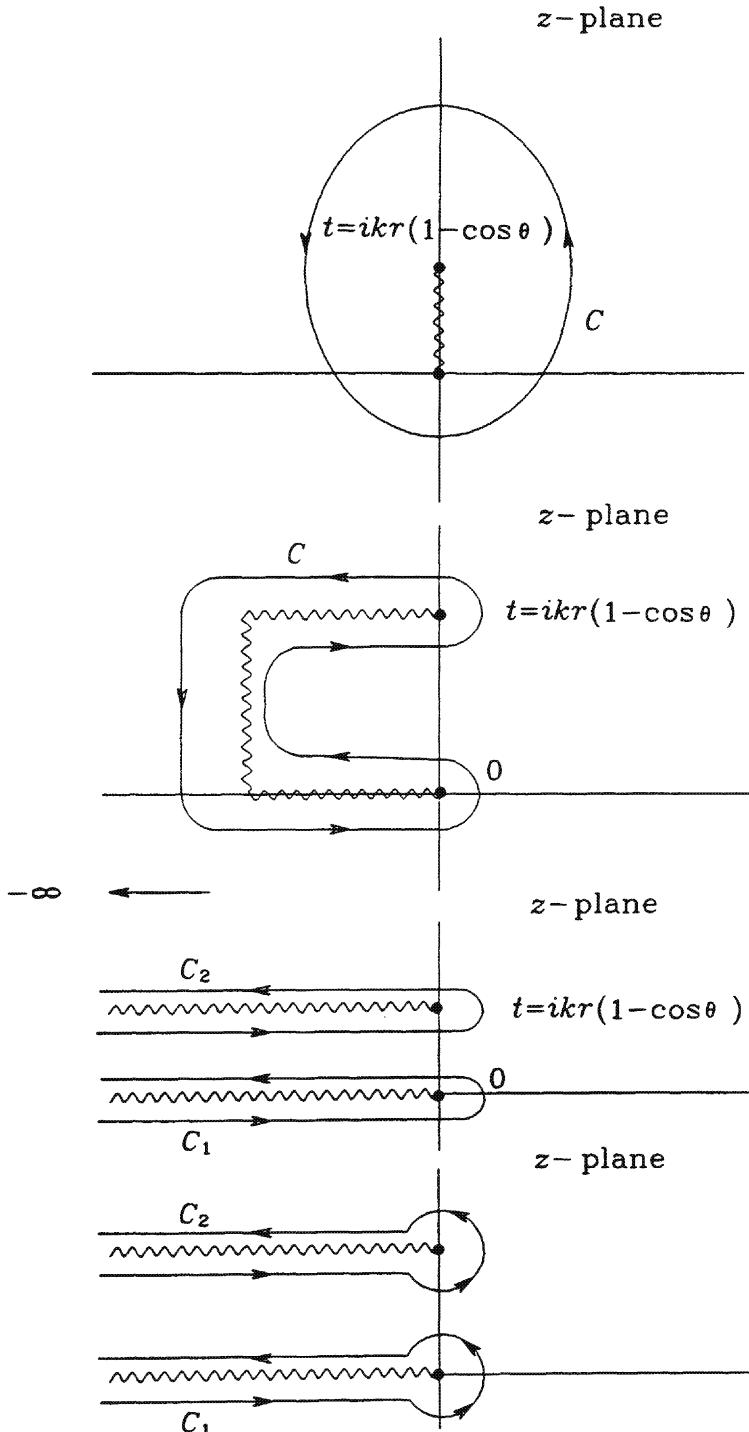


FIGURE 46.4. Contours for eqs. (16), (17), and (19).

We shall also use

$$(\mp i)^{i\gamma} = e^{\pm\gamma\frac{\pi}{2}}, \quad (kr(1 - \cos\theta))^{i\gamma} = e^{i\gamma\ln[kr(1 - \cos\theta)]}, \quad (25)$$

to rewrite

$$\begin{aligned} \psi(\vec{r}) \rightarrow & \frac{e^{i\gamma\frac{\pi}{2}}}{i\gamma\Gamma(i\gamma)} \left(e^{i(kr\cos\theta + \gamma\ln[kr(1 - \cos\theta)])} \right. \\ & \left. + \frac{\gamma}{k(1 - \cos\theta)} \frac{\Gamma(i\gamma)}{\Gamma(-i\gamma)} \frac{e^{i(kr - \gamma\ln[kr(1 - \cos\theta)])}}{r} \right), \end{aligned} \quad (26)$$

or

$$\psi(\vec{r}) \rightarrow \text{const} \left(e^{i(\vec{k}\cdot\vec{r} + \gamma\ln[kr(1 - \cos\theta)])} + \frac{\gamma e^{2i(\sigma_0 - \frac{\pi}{2})}}{k(1 - \cos\theta)} \frac{e^{i(kr - \gamma\ln[kr(1 - \cos\theta)])}}{r} \right), \quad (27)$$

or

$$\psi(\vec{r}) \rightarrow \text{const} \left(e^{i(\vec{k}\cdot\vec{r} + \gamma\ln[kr(1 - \cos\theta)])} + \frac{(-\gamma)e^{2i\sigma_0}e^{-i\gamma\ln\sin^2\frac{\theta}{2}}}{2k\sin^2\frac{\theta}{2}} \frac{e^{i(kr - \gamma\ln 2kr)}}{r} \right). \quad (28)$$

This relation has the form of a Coulomb modified incoming plane wave + a Coulomb modified outgoing spherical scattered wave,

$$\psi(\vec{r}) \rightarrow \text{const} \left(e^{i(\vec{k}\cdot\vec{r} - \gamma\ln[kr(1 - \cos\theta)])} + f(\theta) \frac{e^{i(kr - \gamma\ln 2kr)}}{r} \right), \quad (29)$$

with

$$f(\theta) = \frac{-\gamma e^{2i\sigma_0} e^{-i\gamma\ln\sin^2\frac{\theta}{2}}}{2k\sin^2\frac{\theta}{2}}, \quad \text{with} \quad \gamma = \frac{\mu e^2 Z_1 Z_2}{\hbar^2 k}. \quad (30)$$

Because, still,

$$|\vec{S}_{\text{inc.}}| = \frac{\hbar k}{\mu} |\text{const}|^2 + \text{Order}\left(\frac{1}{r}\right), \quad (31)$$

and

$$\left(\vec{S}_{\text{scatt.}} \cdot \frac{\vec{r}}{r} \right) = \frac{\hbar k}{\mu} \frac{|f(\theta)|^2}{r^2} |\text{const}|^2 + \text{Order}\left(\frac{1}{r^3}\right), \quad (32)$$

we still have

$$\frac{d\sigma}{d\Omega} = |f(\theta)|^2 = \frac{\gamma^2}{4k^2 \sin^4\frac{\theta}{2}} = \frac{Z_1^2 Z_2^2 e^4}{16E^2 \sin^4\frac{\theta}{2}}, \quad (33)$$

so that the quantum-mechanical result for the differential cross section agrees with the classical Rutherford result. The exponential factor,

$$e^{-i\gamma\ln\sin^2\frac{\theta}{2}},$$

however, does play an important role in the Coulomb scattering of identical charged particles.

Problems

4. Find the differential scattering cross section for neutron nucleus scattering in first Born approximation under the assumption the neutron nucleus interaction can be approximated by a square well, $V = -|V_0|$, for $r \leq a$, $V = 0$ for $r > a$. Show in particular, the differential cross section is strongly forward-peaked and the angular range of the forward peak can be used to determine the size of the nucleus. Calculate the value of θ for the first zero of the differential cross section for a beam with $E = 100$ MeV, assuming $a = 5$ fm (medium-heavy nucleus). Would you expect the first Born approximation to be good under these conditions?

5. For purely electromagnetic probes, the spherical drop model of the nucleus with a uniform charge distribution of radius a , total charge Ze , is a good model for the nucleus. Show the differential scattering cross section for μ^- nucleus scattering is given in first Born approximation by

$$\frac{d\sigma}{d\Omega} = \left(\frac{d\sigma}{d\Omega} \right)_{\text{Rutherford}} \left[\frac{3}{qa} j_1(qa) \right]^2, \quad \text{with } q = 2k \sin \frac{\theta}{2}.$$

Make a plot of this differential cross section as a function of θ and show how it can be used to determine a , the radius of the nucleus. If you want to place the first zero in the differential cross section at $\theta = 60^\circ$ for a nucleus with $a = 10$ fm, what energy is required for the μ^- beam? (Convince yourself the corresponding problem for e^- nucleus scattering requires relativistic quantum theory. Most of our detailed knowledge about the electromagnetic structure of the nucleus comes from high-energy e^- nucleus scattering experiments).

The μ^- nucleus potential is the simple Coulomb potential, with

$$V(r) = -\frac{Ze^2}{r} \quad \text{for } r \geq a, \quad V(r) = -\frac{Ze^2}{a} \left(\frac{3}{2} - \frac{r^2}{2a^2} \right) \quad \text{for } r \leq a.$$

Note: the long-range $r \rightarrow \infty$ contribution to the integral can be handled by screening as for the simple point charge; i.e., we can replace

$$-\frac{Ze^2}{r} \rightarrow -\frac{Ze^2}{r} e^{-br}$$

and take the limit $b \rightarrow 0$.

6. For the 1-D radial function, $u_l(r)$, for a spherically symmetric potential, $V(r)$, which remains finite as $r \rightarrow 0$ and goes to zero as $r \rightarrow \infty$, show

$$\left[u_l \frac{du_l^{(0)}}{dr} - u_l^{(0)} \frac{du_l}{dr} \right]_{r=\infty} = -\frac{2\mu}{\hbar^2} \int_0^\infty dr V(r) u_l(r) u_l^{(0)}(r),$$

where $u_l^{(0)}(r)$ is the corresponding radial function for the case, $V(r) = 0$. Use this result to derive the Born approximation for the phase shifts:

$$\sin \delta_l^{\text{Born}} = -\frac{2\mu k}{\hbar^2} \int_0^\infty dr r^2 V(r) [j_l(kr)]^2.$$

Use the Born approximation result for $f(\theta)$ to “derive” the “well-known” expansion

$$\frac{\sin\left(2kr \sin \frac{\theta}{2}\right)}{\left(2kr \sin \frac{\theta}{2}\right)} = \sum_l (2l+1) P_l(\cos \theta) [j_l(kr)]^2.$$

7. Use the general Born series to derive the second-order term for $f(\theta)$ in the Born approximation from the coordinate space integrations. For a spherically symmetric $V(r)$, perform all angular integrations and show the resultant expression can be reduced to a single l sum:

$$(f(\theta))^{Born(2)} = \sum_l (2l+1) P_l(\cos \theta) I_l,$$

where the I_l can be expressed in terms of double radial integrals involving V and spherical Bessel and Hänkel functions. Note: With both \vec{r}' and \vec{r}'' finite, $G^{(+)}(\vec{r}', \vec{r}'')$ is best expressed in terms of:

$$G^{(+)}(\vec{r}', \vec{r}'') = \sum_l g_l(r', r'') \sum_{m=-l}^{+l} Y_{lm}(\theta', \phi') Y_{lm}^*(\theta'', \phi'').$$

8. The most common isotope of Lithium ($Z = 3$) is ${}^7_3\text{Li}_4$, a nucleus with a spin of $\frac{3}{2}$. If an unpolarized beam of ${}^7\text{Li}$ nuclei is incident on an identical ${}^7\text{Li}$ target nucleus with random spin orientations at a center of mass energy, $p^2/(2\mu) = 2\text{MeV}$, show the scattering is dominated by the pure Coulomb repulsion potential. (Effectively, the nuclear force does not come into play. Tunneling through the Coulomb barrier is negligible. A reasonable estimate for the ${}^7\text{Li}$ nuclear radius is 2.3 fm.) Show, however, at this energy, the exact scattering amplitude for the Coulomb potential must be taken into account for this scattering of identical particles from identical (indistinguishable) particles. Find the fraction of spin-symmetric and spin-antisymmetric states, and calculate $\frac{d\sigma}{d\Omega}$ as a function of θ in the center of mass system. In particular, calculate the ratio

$$\frac{\left(\left(\frac{d\sigma}{d\Omega}\right)_{\text{quantum mech.}}\right)}{\left(\left(\frac{d\sigma}{d\Omega}\right)_{\text{classical}}\right)}.$$

Also, calculate the differential cross section in the laboratory system as a function of θ_{lab} .

9. A low energy beam of spin $s = 1$ particles is scattered from a target of identical (indistinguishable) spin $s = 1$ target particles. Assume the scattering process is governed by a spin-independent potential leading to the following phase shifts:

$$\delta_0 = \frac{3}{2}\pi, \quad \delta_1 = \frac{1}{3}\pi, \quad \delta_2 = \frac{1}{2}\pi, \quad \delta_l = 0, \quad \text{for } l \geq 3.$$

Find the differential scattering cross section as a function of θ (center of mass system), assuming (a) the incident beam is unpolarized and the target spins have

random orientations. (b) Repeat, assuming the incident beam is perfectly longitudinally polarized, with a pure $m_s = +1$, and the target spins still have random orientations. Assume the detector is insensitive to the spin orientation.

Operator Form of Scattering Green's Function and the Integral Equation for the Scattering Problem

So far, we have worked strictly in coordinate representation for the very limited problem of the scattering of a structureless point particle from another structureless point particle. To generalize to more complicated situations involving composite projectile and target particles, with the possibility of inelastic collision processes or rearrangement collisions, or even to iterate the Born approximation for the case of structureless point particles, it will be advantageous to recast both the scattering Green's function and the scattering integral equation into operator form.

In coordinate representation, we solved the scattering problem,

$$\begin{aligned}(E - H)\psi_k^{(+)}(\vec{r}) &= 0 \\ (E - H_0)\psi_k^{(+)}(\vec{r}) &= (E - H_0)\phi_{\vec{k}}(\vec{r}) + V(\vec{r})\psi_{\vec{k}}^{(+)}(\vec{r}),\end{aligned}\quad (1)$$

by introducing the Green's function, $G^{(+)}(\vec{r}, \vec{r}')$, where

$$(E - H_0)G^{(+)}(\vec{r}, \vec{r}') = \delta(\vec{r} - \vec{r}'), \quad (2)$$

and converting eq. (1) into the form of an integral equation. [In Chapters 45 and 46, we found it convenient to multiply the operators $(E - H_0)$ and $(E - H)$ in these equations through by the factor $\frac{2\mu}{\hbar^2}$ to carry out the integrations in k space. We will find it more convenient now to go back to the original Schrödinger normalization. In this normalization, the Green's function of Chapter 45 would have been $-\frac{2\mu}{\hbar^2} e^{ik|\vec{r}-\vec{r}'|}/4\pi|\vec{r}-\vec{r}'|$.]

Just as we can take the state vector $|\psi\rangle$ and expand it in terms of a set of (1) base vectors $|n\rangle$, the eigenstates of a complete set of commuting operators with a discrete spectrum, e.g., the eigenstates $|n_1 n_2 n_3\rangle$ of H_0 in the box normalization; or (2) base vectors $|k'\rangle$, the eigenvectors of k_x, k_y, k_z for the continuum plane

wave states; or (3) base vectors $|\vec{r}'\rangle$ in the coordinate representation that are the eigenvectors of the operators x, y, z ,

$$\begin{aligned} |\psi\rangle &= \sum_n |n\rangle \langle n| \psi\rangle, \\ |\psi\rangle &= \int d\vec{k}' |\vec{k}'\rangle, \langle \vec{k}'| \psi\rangle \\ |\psi\rangle &= \int d\vec{r}' |\vec{r}'\rangle, \langle \vec{r}'| \psi\rangle \end{aligned} \quad (3)$$

so, we can think of the Green's function not only in coordinate representation, but also in any representation, expressed in terms of any convenient basis. In fact, we will introduce an operator form of the Green's function and then express the Green's operator in any convenient basis. In coordinate representation, we have

$$G^{(+)}(\vec{r}, \vec{r}') = \lim_{\epsilon \rightarrow 0} \int d\vec{k}' \frac{\phi_{\vec{k}'}(\vec{r}) \phi_{\vec{k}'}^*(\vec{r}')}{(E(k) - E(k') + i\epsilon)}. \quad (4)$$

Again, we have changed from $(k^2 - k'^2)$ to $E(k) - E(k')$ in this Green's function, and therefore from $k + i\eta$ to $E(k) + i\epsilon$, with $E(k) + i\epsilon = \frac{\hbar^2}{2\mu}(k^2 + 2ik\eta + \dots)$, so $\epsilon = (\frac{\hbar^2 k}{\mu})\eta$. We will now think of this coordinate representation of the Green's function as the coordinate representation matrix element of an operator, the Green's operator, $G_{\text{op.}}^{(+)}$,

$$G^{(+)}(\vec{r}, \vec{r}') = \langle \vec{r}| G_{\text{op.}}^{(+)} | \vec{r}' \rangle = \lim_{\epsilon \rightarrow 0} \int d\vec{k}' \langle \vec{r} | \vec{k}' \rangle \frac{1}{E(k) - E(k') + i\epsilon} \langle \vec{k}' | \vec{r}' \rangle, \quad (5)$$

with

$$\langle \vec{r} | \vec{k}' \rangle = \frac{1}{(2\pi)^{\frac{3}{2}}} e^{i\vec{k}' \cdot \vec{r}}, \quad \langle \vec{k}' | \vec{r}' \rangle = \langle \vec{r}' | \vec{k}' \rangle^* = \frac{1}{(2\pi)^{\frac{3}{2}}} e^{-i\vec{k}' \cdot \vec{r}'}, \quad (6)$$

so

$$G_{\text{op.}}^{(+)} = \lim_{\epsilon \rightarrow 0} \int d\vec{k}' |\vec{k}'\rangle \langle \vec{k}'| \frac{1}{E(k) - E(k') + i\epsilon} |\vec{k}'\rangle \langle \vec{k}'|. \quad (7)$$

Henceforth, the limit, $\lim_{\epsilon \rightarrow 0}$, will be quietly understood whenever an ϵ appears in an expression. Also, we could have written the Green's operator in the basis-independent form

$$G_{\text{op.}}^{(+)} = \frac{1}{E - H_0 + i\epsilon}. \quad (8)$$

If this is left-multiplied by the unit operator in the form, $\int d\vec{k}'' |\vec{k}''\rangle \langle \vec{k}''|$ and right-multiplied by a unit operator in the form, $\int d\vec{k}' |\vec{k}'\rangle \langle \vec{k}'|$, we get

$$\begin{aligned} G_{\text{op.}}^{(+)} &= \int d\vec{k}'' \int d\vec{k}' |\vec{k}''\rangle \langle \vec{k}''| \frac{1}{E(k) - H_0 + i\epsilon} |\vec{k}'\rangle \langle \vec{k}'| \\ &= \int d\vec{k}' |\vec{k}'\rangle \frac{1}{E(k) - E(k') + i\epsilon} \langle \vec{k}'|. \end{aligned} \quad (9)$$

where we have used $H_0|\vec{k}'\rangle = E(k')|\vec{k}'\rangle$, and $\langle \vec{k}''|\vec{k}'\rangle = \delta(\vec{k}'' - \vec{k}')$, to regain the form of the Green operator first given in eq. (7). We could have used other forms of the unit operator, such as $\sum_n |n\rangle\langle n|$, to gain different realizations of this operator.

A The Lippmann–Schwinger Equation

The operator form of the Green's function will be particularly convenient if we want to generalize our scattering problem to one involving composite target or projectile particles, or if we want to iterate the Born approximation to get the higher order Born approximation terms. With the operator form of the Green's function, it is not necessary to write the integral equation form of the scattering problem

$$\psi^{(+)}(\vec{r}) = \phi(\vec{r}) + \int d\vec{r}' G^{(+)}(\vec{r}, \vec{r}') V(\vec{r}') \psi^{(+)}(\vec{r}') \quad (10)$$

in coordinate representation. In representation-independent state vector form, this equation becomes

$$|\psi_{\vec{k}}^{(+)}\rangle = |\phi_{\vec{k}}\rangle + \frac{1}{E - H_0 + i\epsilon} V |\psi_{\vec{k}}^{(+)}\rangle, \quad (11)$$

where the state vector $|\psi_{\vec{k}}^{(+)}\rangle$ is the state vector for an incoming plane wave in the α channel, with relative momentum, $\hbar\vec{k}$, and spherical outgoing waves in *all* energetically possible outgoing channels. This operator form of the scattering problem integral equation is known as the Lippmann–Schwinger equation. In this form, it is easy to iterate to get the Born solution to the equation in an infinite series, the Born expansion. Substituting for $|\psi_{\vec{k}}^{(+)}\rangle$ in the right-hand side, we get

$$|\psi_{\vec{k}}^{(+)}\rangle = |\phi_{\vec{k}}\rangle + \frac{1}{E - H_0 + i\epsilon} V \left(|\phi_{\vec{k}}\rangle + \frac{1}{E - H_0 + i\epsilon} V |\psi_{\vec{k}}^{(+)}\rangle \right). \quad (12)$$

Substituting for $|\psi_{\vec{k}}^{(+)}\rangle$ again (and again) in the right-hand side, we get the Born series

$$\begin{aligned} |\psi_{\vec{k}}^{(+)}\rangle &= |\phi_{\vec{k}}\rangle + \frac{1}{E - H_0 + i\epsilon} V |\phi_{\vec{k}}\rangle \\ &\quad + \frac{1}{E - H_0 + i\epsilon} V \frac{1}{E - H_0 + i\epsilon} V |\phi_{\vec{k}}\rangle \\ &\quad + \frac{1}{E - H_0 + i\epsilon} V \frac{1}{E - H_0 + i\epsilon} V \frac{1}{E - H_0 + i\epsilon} V |\phi_{\vec{k}}\rangle \\ &\quad + \dots, \end{aligned} \quad (13)$$

with solution

$$|\psi_{\vec{k}}^{(+)}\rangle = |\phi_{\vec{k}}\rangle + |\psi_{\vec{k}}^{(1)}\rangle + |\psi_{\vec{k}}^{(2)}\rangle + \dots \quad (14)$$

To get the second-order term in coordinate representation, we now introduce unit operators of type $\int d\vec{r}' |\vec{r}'\rangle\langle\vec{r}'|$ to get

$$\begin{aligned}\psi_{\vec{k}}^{(2)}(\vec{r}) &= \int d\vec{r}'' \int d\vec{r}''' \int d\vec{r}'''' \int d\vec{r}' \langle \vec{r}' | \frac{1}{E - H_0 + i\epsilon} |\vec{r}''' \rangle \langle \vec{r}'' | V | \vec{r}'''' \rangle \\ &\quad \times \langle \vec{r}''' | \frac{1}{E - H_0 + i\epsilon} |\vec{r}'''' \rangle \langle \vec{r}'''' | V | \vec{r}' \rangle \langle \vec{r}' | \phi_{\vec{k}} \rangle \\ &= \int d\vec{r}'' \int d\vec{r}' G^{(+)}(\vec{r}, \vec{r}'') V(\vec{r}'') G^{(+)}(\vec{r}'', \vec{r}') V(\vec{r}') \phi_{\vec{k}}(\vec{r}'),\end{aligned}\quad (15)$$

where we have used

$$\langle \vec{r}'' | V | \vec{r}'''' \rangle = V(\vec{r}'') \delta(\vec{r}'' - \vec{r}''') \text{ and } \langle \vec{r}' | \frac{1}{E - H_0 + i\epsilon} |\vec{r}'' \rangle = G^{(+)}(\vec{r}, \vec{r}'') \quad (16)$$

to reduce the expression to the form of a double 3-D integral involving two Green's functions. The Green's function, $G(\vec{r}, \vec{r}'')$ is needed only in its asymptotic form, as $r \rightarrow \infty$,

$$-\frac{2\mu}{\hbar^2} \frac{e^{ikr}}{4\pi r} e^{-i\vec{k}_s \cdot \vec{r}''},$$

but the Green's function, $G^{(+)}(\vec{r}'', \vec{r}')$, is needed for all values of \vec{r}' and \vec{r}'' in the form

$$-\frac{2\mu}{\hbar^2} \frac{e^{ik|\vec{r}'' - \vec{r}'|}}{4\pi |\vec{r}'' - \vec{r}'|}.$$

For spherically symmetric potentials this is best expanded in spherical harmonics [see eqs. (39) and (53) of Chapter 45] to actually carry out the integrals.

$$G^{(+)}(\vec{r}'', \vec{r}') = \sum_{lm} \frac{2\mu}{\hbar^2} \frac{1}{r'^2} g_l(r'', r') Y_{lm}(\theta'', \phi'') Y_{lm}^*(\theta', \phi'). \quad (17)$$

Inelastic Scattering Processes and Rearrangement Collisions

So far, we have seen the usefulness of the operator form of the Green's function and the integral equation for the scattering problem in iterating the Born approximation for the scattering of structureless point particles from structureless point particles. The method becomes equally useful in discussing the scattering of composite particles from composite particles, where inelastic processes and rearrangement collisions come into play.

A Inelastic Scattering Processes

Consider the case in which we might have a scattering of a projectile from a composite target particle (e.g., μ^- -atom scattering or μ^- -nucleus scattering; we choose a μ^- as our projectile to avoid having identical particles as the components of our composite target particle). Now, it will be useful to decompose

$$H = H_0 + V, \quad (1)$$

where H_0 will include, besides the kinetic energy operator for the relative motion, the Hamiltonian for the internal degrees of freedom of the composite particle.

$$H_0 = -\frac{\hbar^2}{2\mu} \nabla_{\text{rel.}}^2 + H_{\text{int.}}(\vec{\xi}), \quad (2)$$

with state vectors, $|\vec{k}, n\rangle$, such that

$$H_0 |\vec{k}, n\rangle = \left(\frac{\hbar^2 k^2}{2\mu} + E_n^{\text{int.}} \right) |\vec{k}, n\rangle, \quad \langle \vec{r}, \vec{\xi} | \vec{k}, n \rangle = \frac{1}{(2\pi)^{\frac{3}{2}}} e^{i\vec{k}\cdot\vec{r}} \chi_n(\vec{\xi}), \quad (3)$$

with

$$H_{\text{int.}}(\vec{\xi})\chi_n(\vec{\xi}) = E_n^{\text{int.}}\chi_n(\vec{\xi}), \quad (4)$$

where $\vec{\xi}$ are the internal variables of the composite particle. [Note: If both projectile and target particles are composite particles, $\chi_n(\vec{\xi}) \equiv \chi_{n_a}(\xi_a)\chi_{n_A}(\xi_A)$, and $E_n^{\text{int.}} = E_{n_a}^{\text{int.}} + E_{n_A}^{\text{int.}}$.] Now, the analogue of eq. (7) of Chapter 47 can be written as

$$G_{\text{op.}}^{(+)} = \sum_{n'} \int d\vec{k}' |\vec{k}', n'\rangle \frac{1}{\frac{\hbar^2}{2\mu}k^2 + E_{n=0}^{\text{int.}} - \frac{\hbar^2}{2\mu}k'^2 - E_{n'}^{\text{int.}} + i\epsilon} \langle \vec{k}', n'|, \quad (5)$$

where conservation of energy now requires the scattered k vector, \vec{k}_s (see Fig. 48.1), have magnitude given by

$$\frac{\hbar^2}{2\mu}k_s^2 = \frac{\hbar^2}{2\mu}k^2 + E_{n=0}^{\text{int.}} - E_{n'}^{\text{int.}}, \quad (6)$$

so the coordinate representation for the Green's function becomes

$$\langle \vec{r}, \vec{\xi} | G_{\text{op.}}^{(+)} | \vec{r}', \vec{\xi}' \rangle = \sum_{n'} \chi_{n'}(\vec{\xi}) \left(\int d\vec{k}' \frac{\phi_{\vec{k}'}(\vec{r})\phi_{\vec{k}'}^*(\vec{r}')}{{\hbar^2}/{2\mu}(k_s^2 - k'^2) + i\epsilon} \right) \chi_{n'}^*(\vec{\xi}'). \quad (7)$$

If we perform the \vec{k}' integration as before, we get

$$G^{(+)}(\vec{r}, \vec{\xi}; \vec{r}', \vec{\xi}') = -\frac{1}{4\pi} \frac{2\mu}{\hbar^2} \sum_{n'} \chi_{n'}(\vec{\xi}) \chi_{n'}^*(\vec{\xi}') \frac{e^{ik_s|\vec{r}-\vec{r}'|}}{|\vec{r}-\vec{r}'|}. \quad (8)$$

The magnitude k_s is now dependent on n' . The integral equation becomes

$$\psi_{\vec{k}}^{(+)}(\vec{r}, \vec{\xi}) = \phi_{\vec{k}}(\vec{r})\chi_{n=0}(\vec{\xi}) + \int d\vec{r}' \int d\vec{\xi}' G^{(+)}(\vec{r}, \vec{\xi}; \vec{r}', \vec{\xi}') V(\vec{r}', \vec{\xi}') \psi_{\vec{k}}^{(+)}(\vec{r}', \vec{\xi}'). \quad (9)$$

In first Born approximation, in the limit $r \rightarrow \infty$, in which

$$\frac{e^{ik_s|\vec{r}-\vec{r}'|}}{|\vec{r}-\vec{r}'|} \rightarrow \frac{e^{ik_s r}}{r} e^{-i\vec{k}_s \cdot \vec{r}'},$$

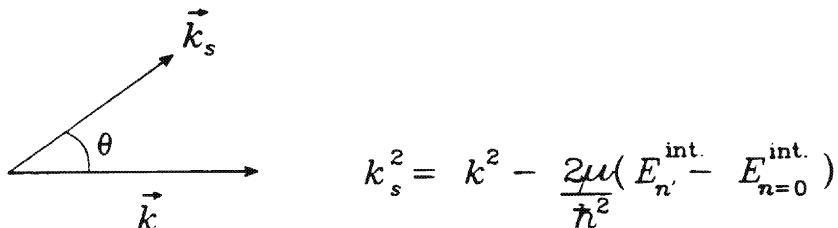


FIGURE 48.1.

we get the result

$$\begin{aligned}\psi_k^{(+)}(\vec{r}, \vec{\xi}) \rightarrow & \frac{1}{(2\pi)^{\frac{3}{2}}} \left(e^{i\vec{k} \cdot \vec{r}} \chi_{n=0}(\vec{\xi}) - \frac{1}{4\pi} \frac{2\mu}{\hbar^2} \sum_{n'} \chi_{n'}(\vec{\xi}) \frac{e^{ik_s r}}{r} \right. \\ & \times \int d\vec{r}' \int d\vec{\xi}' V(\vec{r}', \vec{\xi}') e^{i(\vec{k}-\vec{k}_s) \cdot \vec{r}'} \chi_n^*(\vec{\xi}') \chi_{n=0}(\vec{\xi}') \left. \right),\end{aligned}\quad (10)$$

with

$$k_s^2 = k^2 - \frac{2\mu}{\hbar^2} (E_{n'}^{\text{int.}} - E_{n=0}^{\text{int.}}), \quad (11)$$

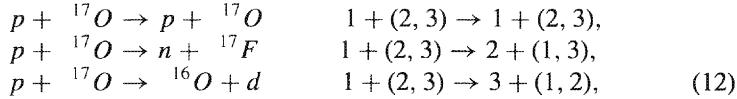
where the coefficient of $\frac{e^{ik_s r}}{r} \chi_{n'}(\vec{\xi})$, with $n' = 0$ and, hence, $k_s = |\vec{k}_s| = k$, gives the scattering amplitude for elastic scattering, and the coefficients of terms with $n' = 1, 2, \dots$ and, hence, $k_s < k$ give the scattering amplitudes for the inelastic processes, where the composite target particle ends in the excited state with internal energy, $E_{n'}^{\text{int.}}$.

B Rearrangement Collisions

Consider, e.g., the scattering of a μ^- from a hydrogen atom. In this case, we can have, besides the elastic scattering process, not only the inelastic scattering processes in which the hydrogen atom ends in an excited state, but also we could have a rearrangement collision, in which the μ^- is captured by the proton to make a muonic atom while the atomic electron is scattered. (Because the ground-state energy of the hydrogen atom is -13.61 eV, whereas the ground-state energy of the muonic atom is ≈ -2.5 KeV, the scattered electron would have an energy greater than 2.5 KeV. An electron in the 2.5 to 3 KeV range would have a $v/c \approx 0.1$, which is small enough for a treatment by nonrelativistic quantum mechanics and the Born approximation should be good.) If we label the μ^- particle 1, the e^- particle 2, and the p^+ particle 3, the rearrangement collision, $1 + (2, 3) \rightarrow 2 + (1, 3)$, is possible.

An even more complex three-particle system could be illustrated by the scattering of a proton from the nucleus ^{17}O , which can be modelled by a neutron orbiting the doubly magic nucleus, ^{16}O , with a $n-^{16}O$ binding energy of -4.146 MeV. Because the first excited state of the tightly bound ^{16}O nucleus is at 6.06 MeV, we could approximate this nucleus as an inert particle if the incident proton energy is not too large. Thus, we could think of the proton as particle 1, the neutron as particle 2, and the ^{16}O -nucleus as particle 3. Now, we could have all three arrangements of the particles labeled 1, 2, 3 (see Fig. 48.2). The proton could scatter elastically or inelastically from ^{17}O . (The first excited state of ^{17}O is at only 0.871 MeV.) The proton could also be captured, however, by the ^{16}O nucleus to make ^{17}F , with a $p-^{16}O$ binding energy of -0.601 MeV, the neutron being knocked out in the reaction and being scattered. Finally, the proton could capture the loosely bound neutron from ^{16}O to make a deuteron, with binding energy of -2.226 MeV,

which is scattered relative to the ^{16}O nucleus. Thus, the rearrangement collisions,



are all possible. In addition, if sufficient incident kinetic energy exists, we could have a final state with three outgoing particles, proton, neutron, and ${}^{16}O$. These three-particle states would be excited states of all three final rearrangements, involving breakup of the two-particle aggregates. If insufficient energy for such a breakup exists, we may have to consider only the above three rearrangement processes. Now, it will be convenient to split the full Hamiltonian, H , into an H_0 and an interaction term, V , in three different ways.

$$\begin{aligned} H = H_0 + V &= -\frac{\hbar^2}{2\mu_{1,23}} \nabla_{1,23}^2 + H_{\text{int.}}(2, 3) + V_{12} + V_{13} \\ &= H'_0 + V' = -\frac{\hbar^2}{2\mu_{2,13}} \nabla_{2,13}^2 + H_{\text{int.}}(1, 3) + V_{12} + V_{23} \\ &= H''_0 + V'' = -\frac{\hbar^2}{2\mu_{3,12}} \nabla_{3,12}^2 + H_{\text{int.}}(1, 2) + V_{13} + V_{23}. \end{aligned} \quad (13)$$

It will now be useful to rewrite the integral equation for the scattering process in three different ways. For this purpose, we will first rewrite the Lippmann-Schwinger equation in terms of the *full* Green's operator

$$\overline{G}_{\text{op.}}^{(+)} = \frac{1}{E - H + i\epsilon}, \quad (14)$$

$$|\psi_{\vec{k}}^{(+)}\rangle = \left(1 + \frac{1}{E - H + i\epsilon} V\right) |\phi_{\vec{k}}\rangle. \quad (15)$$

To derive this equation, which is the operator form of eq. (59) of Chapter 45, act on the operator, $E - H + i\epsilon = E - H_0 + i\epsilon - V$, with $\overline{G}_{\text{op.}}^{(+)}$ from the left and with $G_{\text{op.}}^{(+)} V$ from the right to yield

$$\begin{aligned} \frac{1}{E - H + i\epsilon} \left(E - H + i\epsilon = E - H_0 + i\epsilon - V \right) \frac{1}{E - H_0 + i\epsilon} V \\ \frac{1}{E - H_0 + i\epsilon} V = \frac{1}{E - H + i\epsilon} V \left(1 - \frac{1}{E - H_0 + i\epsilon} V \right). \end{aligned} \quad (16)$$

Now, let this act on $|\psi_{\vec{k}}^{(+)}\rangle$, and use the Lippmann-Schwinger equation

$$\frac{1}{E - H_0 + i\epsilon} V |\psi_{\vec{k}}^{(+)}\rangle = |\psi_{\vec{k}}^{(+)}\rangle - |\phi_{\vec{k}}\rangle \quad (17)$$

to yield

$$|\psi_{\vec{k}}^{(+)}\rangle - |\phi_{\vec{k}}\rangle = \frac{1}{E - H + i\epsilon} V |\phi_{\vec{k}}\rangle, \quad (18)$$

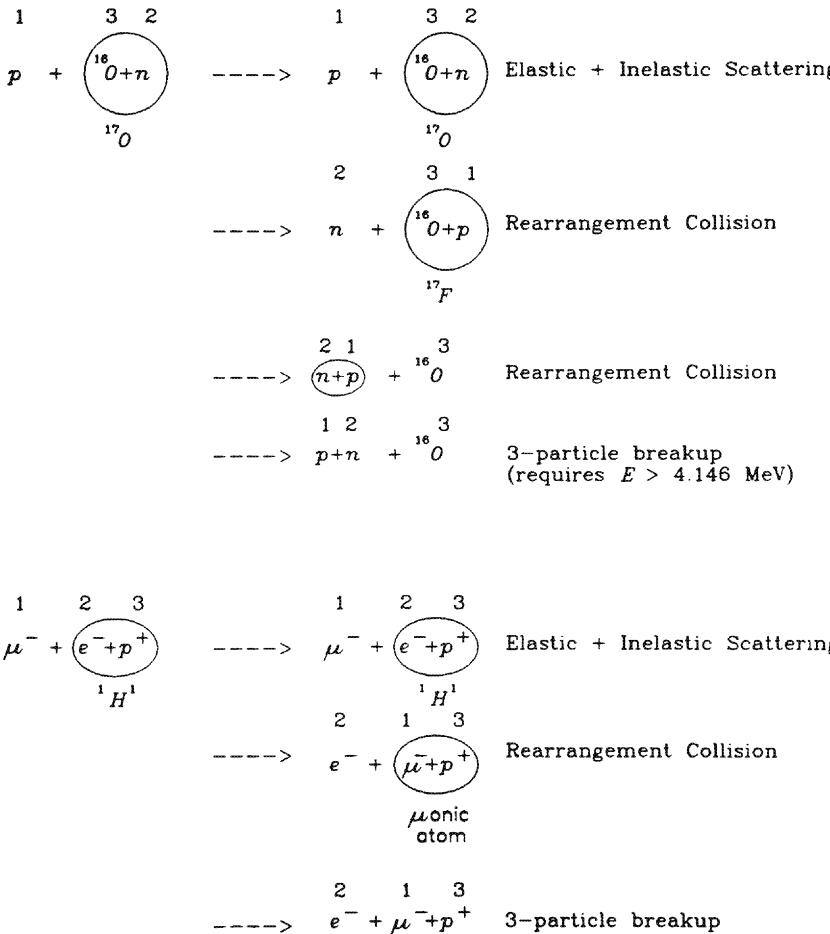


FIGURE 48.2. Rearrangement collisions for three-particle systems.

which is eq. (15). Now, our purpose is not to find a coordinate or other representation of the *full* Green operator, but to rearrange this relation to write the Lippmann–Schwinger equation in terms of the primed and double-primed operators, which are needed for the rearrangement collisions. For this purpose, we shall rewrite

$$(E - H + i\epsilon)|\psi_k^{(+)}\rangle = (E - H + i\epsilon)\left(1 + \frac{1}{E - H + i\epsilon} V\right)|\phi_k\rangle \\ = (E - H_0 + i\epsilon)|\phi_k\rangle = i\epsilon|\phi_k\rangle. \quad (19)$$

Because we are to take the limit $\epsilon \rightarrow 0$, the right-hand side is zero. Let us be careful about this limit, however. Acting on the left-hand side with a Green's operator of

the type

$$\frac{1}{E - H'_0 + i\epsilon},$$

we get

$$\begin{aligned} \frac{1}{E - H'_0 + i\epsilon} (E - H + i\epsilon) |\psi_{\vec{k}}^{(+)}\rangle &= \frac{1}{E - H'_0 + i\epsilon} (E - H'_0 - V' + i\epsilon) |\psi_{\vec{k}}^{(+)}\rangle \\ &= \left(1 - \frac{1}{E - H'_0 + i\epsilon} V'\right) |\psi_{\vec{k}}^{(+)}\rangle \\ &= \frac{i\epsilon}{E - H'_0 + i\epsilon} |\phi_{\vec{k}}\rangle = \frac{i\epsilon}{E - H_0 + V' - V + i\epsilon} |\phi_{\vec{k}}\rangle \\ &= \frac{i\epsilon}{V' - V + i\epsilon} |\phi_{\vec{k}}\rangle = 0, \end{aligned} \quad (20)$$

where we have used $H_0 - H'_0 = V' - V$ and the fact that $V' - V$ cannot give a zero when acting on $|\phi_{\vec{k}}\rangle$, so

$$\lim_{\epsilon \rightarrow 0} \frac{i\epsilon}{V' - V + i\epsilon} |\phi_{\vec{k}}\rangle = 0,$$

unlike the limit

$$\lim_{\epsilon \rightarrow 0} \frac{i\epsilon}{E - H_0 + i\epsilon} |\phi_{\vec{k}}\rangle = \lim_{\epsilon \rightarrow 0} \frac{i\epsilon}{i\epsilon} |\phi_{\vec{k}}\rangle = |\phi_{\vec{k}}\rangle.$$

Thus, we have

$$\left(1 - \frac{1}{E - H'_0 + i\epsilon} V'\right) |\psi_{\vec{k}}^{(+)}\rangle = 0, \quad (21)$$

or we get an equation for $|\psi_{\vec{k}}^{(+)}\rangle$ in the form

$$|\psi_{\vec{k}}^{(+)}\rangle = \frac{1}{E - H'_0 + i\epsilon} V' |\psi_{\vec{k}}^{(+)}\rangle. \quad (22)$$

In exactly the same way, we could have gotten still a third form for $|\psi_{\vec{k}}^{(+)}\rangle$ by replacing H'_0 and V' in this equation by H''_0 and V'' . Thus, we have three different ways of writing the Lippmann–Schwinger equation, leading to three different forms for the integral equations of this scattering problem for our system of three particles.

$$\begin{aligned} |\psi_{\vec{k}}^{(+)}\rangle &= |\phi_{\vec{k}}\rangle + \frac{1}{E - H_0 + i\epsilon} V |\psi_{\vec{k}}^{(+)}\rangle, \\ |\psi_{\vec{k}}^{(+)}\rangle &= \frac{1}{E - H'_0 + i\epsilon} V' |\psi_{\vec{k}}^{(+)}\rangle, \\ |\psi_{\vec{k}}^{(+)}\rangle &= \frac{1}{E - H''_0 + i\epsilon} V'' |\psi_{\vec{k}}^{(+)}\rangle. \end{aligned} \quad (23)$$

In all three forms of this scattering equation, the vector, $|\psi_{\vec{k}}^{(+)}\rangle$, contains besides the incoming plane wave for the motion of particle 1 relative to the bound system

of particles (2, 3) the spherical outgoing waves corresponding to both elastic and inelastic scattering of particle 1 from the system (2, 3), as well as the spherical outgoing waves for particle 2 moving away from the system (1, 3), as well as the spherical outgoing waves for particle 3 moving away from the system (1, 2). When converted to integral equation form, none of the three integral equations is easy to solve. In Born approximation, however, when the incident energy is large enough compared with the potentials, V_{12} , V_{13} , and V_{23} , we may get a reasonably good approximate solution. For this purpose, however, the first form is best for the elastic and inelastic scattering of particle 1, whereas the second form would be best for getting an approximate value for the cross section for the rearrangement, $1 + (2, 3) \rightarrow 2 + (1, 3)$, and the last form would be best for the rearrangement collision of type $1 + (2, 3) \rightarrow 3 + (1, 2)$.

Differential Scattering Cross Sections for Rearrangement Collisions: Born Approximation

Let us calculate in some detail the differential scattering cross section for a rearrangement collision of the type $1 + (2, 3) \rightarrow 2 + (1, 3)$, where the incident channel, particle 1 incident on the composite particle made of (2, 3), will be designated by the channel index, α , and the outgoing channel, with particle 2 leaving the composite system (1, 3), will be designated by channel index, β . We will assume the spins of particles 1, 2, 3 (if any) need not be considered. The relative position vector and internal coordinate in channel α are then

$$\vec{r}_\alpha = \vec{r}_1 - \frac{(m_2 \vec{r}_2 + m_3 \vec{r}_3)}{(m_2 + m_3)}, \quad \vec{\xi}_\alpha = \vec{r}_2 - \vec{r}_3, \quad (1)$$

and the reduced mass in channel α is $\mu_\alpha = m_1 m_{23} / (m_1 + m_{23})$ and the incident $\vec{k}_\alpha \equiv \vec{k}$. Similarly,

$$\vec{r}_\beta = \vec{r}_2 - \frac{(m_1 \vec{r}_1 + m_3 \vec{r}_3)}{(m_1 + m_3)}, \quad \vec{\xi}_\beta = \vec{r}_1 - \vec{r}_3, \quad (2)$$

with reduced mass in the β channel given by $\mu_\beta = m_2 m_{13} / (m_2 + m_{13})$. To find the necessary scattering amplitude, we shall use the coordinate representation $\langle \vec{r}_\beta, \vec{\xi}_\beta | \psi_{\vec{k}}^{(+)} \rangle$ and calculate this through the second (or primed) form of eq. (23) of Chapter 48, which is appropriate for the β channel.

$$\begin{aligned} \langle \vec{r}_\beta, \vec{\xi}_\beta | \psi_{\vec{k}}^{(+)} \rangle &= \langle \vec{r}_\beta, \vec{\xi}_\beta | \frac{1}{E - H'_0 + i\epsilon} V' | \psi_{\vec{k}}^{(+)} \rangle \\ &= \sum_{n'} \int d\vec{k}' \langle \vec{r}_\beta, \vec{\xi}_\beta | \vec{k}', n' \rangle \langle \vec{k}', n' | \frac{1}{E - H'_0 + i\epsilon} | \vec{k}', n' \rangle \\ &\quad \times \langle \vec{k}', n' | V' | \psi_{\vec{k}}^{(+)} \rangle, \end{aligned} \quad (3)$$

where $|\vec{k}', n'\rangle$ is an eigenvector of H'_0 , with

$$H'_0 |\vec{k}', n'\rangle = E(k', n') |\vec{k}', n'\rangle = \left(\frac{\hbar^2}{2\mu_\beta} k'^2 + E_{\beta, n'}^{\text{int.}} \right) |\vec{k}', n'\rangle. \quad (4)$$

We shall now insert a unit operator in the form of

$$\int \int d\vec{r}'_\beta d\vec{\xi}'_\beta |\vec{r}'_\beta, \vec{\xi}'_\beta\rangle \langle \vec{r}'_\beta, \vec{\xi}'_\beta|$$

between the bra $\langle \vec{k}', n'|$ and V' to obtain

$$\begin{aligned} \langle \vec{r}_\beta \vec{\xi}_\beta | \psi_k^{(+)} \rangle &= \sum_{n'} \int d\vec{k}' \int d\vec{r}'_\beta \int d\vec{\xi}'_\beta \langle \vec{r}_\beta \vec{\xi}_\beta | \vec{k}', n' \rangle \frac{1}{E - E(k', n') + i\epsilon} \\ &\times \langle \vec{k}', n' | \vec{r}'_\beta \vec{\xi}'_\beta \rangle \langle \vec{r}'_\beta \vec{\xi}'_\beta | V' | \psi_k^{(+)} \rangle \\ &= \sum_{n'} \int d\vec{k}' \int d\vec{r}'_\beta \int d\vec{\xi}'_\beta \frac{1}{(2\pi)^{\frac{3}{2}}} e^{i\vec{k}' \cdot \vec{r}_\beta} \chi_{n'}(\vec{\xi}_\beta) \\ &\times \frac{1}{E - \frac{\hbar^2}{2\mu_\beta} k'^2 - E_{\beta, n'}^{\text{int.}} + i\epsilon} \frac{1}{(2\pi)^{\frac{3}{2}}} e^{-i\vec{k}' \cdot \vec{r}'_\beta} \chi_{n'}^*(\vec{\xi}'_\beta) \langle \vec{r}'_\beta, \vec{\xi}'_\beta | V' | \psi_k^{(+)} \rangle. \end{aligned} \quad (5)$$

In addition, we shall use energy conservation to rename

$$E = \frac{\hbar^2}{2\mu_\alpha} k^2 + E_{\alpha, 0}^{\text{int.}} = \frac{\hbar^2}{2\mu_\beta} k_{\beta, n'}^2 + E_{\beta, n'}^{\text{int.}} \quad (6)$$

and evaluate the Green's function

$$\begin{aligned} G^{(+)}(\vec{r}_\beta, \vec{\xi}_\beta; \vec{r}'_\beta, \vec{\xi}'_\beta) &= \frac{1}{(2\pi)^3} \sum_{n'} \int d\vec{k}' \frac{e^{i\vec{k}' \cdot (\vec{r}_\beta - \vec{r}'_\beta)}}{\frac{\hbar^2}{2\mu_\beta} (k_{\beta, n'}^2 - k'^2) + i\epsilon} \chi_{n'}(\vec{\xi}_\beta) \chi_{n'}^*(\vec{\xi}'_\beta) \\ &= -\frac{1}{4\pi} \frac{2\mu_\beta}{\hbar^2} \sum_{n'} \frac{e^{ik_{\beta, n'} |\vec{r}_\beta - \vec{r}'_\beta|}}{|\vec{r}_\beta - \vec{r}'_\beta|} \chi_{n'}(\vec{\xi}_\beta) \chi_{n'}^*(\vec{\xi}'_\beta). \end{aligned} \quad (7)$$

With this Green's function

$$\langle \vec{r}_\beta \vec{\xi}_\beta | \psi_k^{(+)} \rangle = \int d\vec{r}'_\beta \int d\vec{\xi}'_\beta G^{(+)}(\vec{r}_\beta, \vec{\xi}_\beta; \vec{r}'_\beta, \vec{\xi}'_\beta) V'(\vec{r}'_\beta, \vec{\xi}'_\beta) \langle \vec{r}'_\beta, \vec{\xi}'_\beta | \psi_k^{(+)} \rangle. \quad (8)$$

Now, as usual, we will take the limit, $r_\beta \rightarrow \infty$, so

$$\frac{e^{ik_{\beta, n'} |\vec{r}_\beta - \vec{r}'_\beta|}}{|\vec{r}_\beta - \vec{r}'_\beta|} \rightarrow \frac{e^{ik_{\beta, n'} r_\beta}}{r_\beta} e^{-ik_{\beta, n'} \vec{r}'_\beta} \quad (9)$$

and, therefore,

$$\langle \vec{r}_\beta \vec{\xi}_\beta | \psi_k^{(+)} \rangle \rightarrow \sum_{n'} \frac{e^{ik_{\beta, n'} r_\beta}}{r_\beta} \chi_{n'}(\vec{\xi}_\beta) \frac{f_{n'}(\theta_\beta, \phi_\beta)}{(2\pi)^{\frac{3}{2}}}, \quad (10)$$

with

$$f_{n'}(\theta_\beta, \phi_\beta) =$$

$$\begin{aligned} & -\frac{\mu_\beta}{2\pi\hbar^2}(2\pi)^{\frac{3}{2}} \int d\vec{r}'_\beta \int d\vec{\xi}'_\beta e^{-i\vec{k}_{\beta,n'} \cdot \vec{r}'_\beta} \chi_{n'}^*(\vec{\xi}'_\beta) V'(\vec{r}'_\beta, \vec{\xi}'_\beta) \psi_k^{(+)}(\vec{r}'_\beta, \vec{\xi}'_\beta) \\ & = -\frac{\mu_\beta}{2\pi\hbar^2}(2\pi)^3 \langle \phi_{\vec{k}_{\beta,n'}} | V' | \psi_k^{(+)} \rangle, \end{aligned} \quad (11)$$

where

$$\langle \phi_{\vec{k}_{\beta,n'}} | \vec{r}'_\beta \vec{\xi}'_\beta \rangle = \frac{1}{(2\pi)^{\frac{3}{2}}} e^{-i\vec{k}_{\beta,n'} \cdot \vec{r}'_\beta} \chi_{n'}^*(\vec{\xi}'_\beta). \quad (12)$$

The inverse factor $(2\pi)^{\frac{3}{2}}$ is needed in the spherical outgoing wave factor, because our plane wave has this same inverse normalization. Now, in first Born approximation, we can replace $|\psi_k^{(+)}\rangle$ by $|\phi_{\vec{k}}\rangle$, where now

$$\langle \vec{r}'_\beta \vec{\xi}'_\beta | \phi_{\vec{k}} \rangle = \frac{e^{i\vec{k} \cdot \vec{r}'_\alpha}}{(2\pi)^{\frac{3}{2}}} \chi_0(\vec{\xi}'_\alpha), \quad (13)$$

where \vec{r}'_α and $\vec{\xi}'_\alpha$ must be expressed in terms of \vec{r}'_β and $\vec{\xi}'_\beta$ via

$$\begin{aligned} \vec{r}'_\alpha &= -\frac{m_2}{(m_2 + m_3)} \vec{r}'_\beta + \frac{m_3(m_1 + m_2 + m_3)}{(m_1 + m_3)(m_2 + m_3)} \vec{\xi}'_\beta \\ \vec{\xi}'_\alpha &= \vec{r}'_\beta + \frac{m_1}{(m_1 + m_3)} \vec{\xi}'_\beta. \end{aligned} \quad (14)$$

The first Born approximation value for the scattering amplitude for this rearrangement process is then

$$\begin{aligned} f_{n'}(\theta_\beta, \phi_\beta) &= -\frac{\mu_\beta}{2\pi\hbar^2} \times \\ & \int d\vec{r}'_\beta \int d\vec{\xi}'_\beta e^{i\vec{k} \cdot \vec{r}'_\alpha} e^{-i\vec{k}_{\beta,n'} \cdot \vec{r}'_\beta} \chi_{n'}^*(\vec{\xi}'_\beta) \chi_0(\vec{\xi}'_\alpha) V'(\vec{r}'_\beta, \vec{\xi}'_\beta). \end{aligned} \quad (15)$$

To get the rearrangement collision cross section, we need to remember the flux in the incident plane wave is

$$\vec{S} = \frac{1}{(2\pi)^3} \frac{\hbar\vec{k}}{\mu_\alpha} = \frac{1}{(2\pi)^3} \vec{v}_\alpha. \quad (16)$$

Note: In a box normalization where the factor $(2\pi)^3$ would have been replaced by the factor L^3 , this \vec{S} would have had the proper dimension of (v/L^3) or $(1/\text{length}^2 \text{time})$, one of the advantages of a box normalization. Also, $\vec{k} \equiv \vec{k}_{\alpha,0}$.

The radial flux in the outgoing spherical wave is (in our present normalization)

$$S_r = \frac{1}{(2\pi)^3} \frac{\hbar k_{\beta,n'}}{\mu_\beta} \frac{1}{r_\beta^2} |f_{n'}(\theta_\beta, \phi_\beta)|^2, \quad (17)$$

leading to the differential cross section for the rearrangement collision

$$\begin{aligned} \left(\frac{d\sigma}{d\Omega} \right)_{\beta,n'} &= \frac{\mu_\alpha k_{\beta,n'}}{\mu_\beta k} |f_{n'}(\theta_\beta, \phi_\beta)|^2 = \frac{v_\beta}{v_\alpha} |f_{n'}(\theta_\beta, \phi_\beta)|^2 \\ &= \frac{\mu_\beta \mu_\alpha}{(2\pi\hbar^2)^2} \frac{k_{\beta,n'}}{k} (2\pi)^6 |\langle \phi_{\vec{k}_{\beta,n'}} | V' | \phi_{\vec{k}} \rangle|^2. \end{aligned} \quad (18)$$

Problems

10. Show the Born approximation differential cross section for the elastic scattering of a μ^- from a hydrogen atom in its ground state is

$$\left(\frac{d\sigma}{d\Omega}\right)^{\text{elastic}} = \left[\frac{2\mu}{m_e} a_0 \frac{8 + (a_0 q)^2}{[4 + (a_0 q)^2]^2} \right]^2, \quad a_0 = \frac{\hbar^2}{m_e e^2}, \quad q = 2k \sin \frac{\theta}{2}.$$

Make the approximation $(m_e/m_{\text{proton}}) = 0$, so the center of mass of the hydrogen atom is at the proton. All spin dependences can be neglected: The interaction potential is

$$V = -\frac{e^2}{r_1} + \frac{e^2}{|\vec{r}_1 - \vec{r}_2|}.$$

11. Find the Born approximation differential cross section for the inelastic scattering cross section of a μ^- from a hydrogen atom, where the hydrogen atom is excited from the $n = 1$ state to the $n = 2$ state

$$\left(\frac{d\sigma}{d\Omega}\right)_{1s \rightarrow 2s} = \left(\frac{d\sigma}{d\Omega}\right)_{1s \rightarrow 2s} + \left(\frac{d\sigma}{d\Omega}\right)_{1s \rightarrow 2p}.$$

Show, in particular, $f(\theta)_{1s \rightarrow 2p}$ has the form

$$f(\theta)_{1s \rightarrow 2p} = -i \frac{\sqrt{2}}{3} \frac{\mu}{m_e} a_0 \int_0^\infty d\xi j_1(qa_0\xi) F(\xi),$$

with

$$F(\xi) = \left(\frac{2^8}{3^4} - \left[\frac{4}{3} \xi^3 + \frac{32}{9} \xi^2 + \frac{2^7}{3^3} \xi + \frac{2^8}{3^4} \right] e^{-\frac{3}{2}\xi} \right),$$

and use the identity

$$\frac{dj_0(\rho)}{d\rho} = -j_1(\rho)$$

to do the integral. Show

$$\left(\frac{d\sigma}{d\Omega}\right)_{1s \rightarrow 2p} = \left(\frac{\mu}{m_e}\right)^2 \frac{k_s}{k} \frac{1}{q^2} \frac{288}{\left[\frac{9}{4} + (qa_0)^2\right]^6}.$$

Now,

$$q = \sqrt{k^2 + k_s^2 - 2kk_s \cos \theta}, \quad \text{with } k_s^2 = k^2 - \frac{3}{4} \frac{\mu m_e e^4}{\hbar^4}.$$

For problems 10 and 11, note:

for $r_2 < r_1$:

$$\left(-\frac{1}{r_1} + \frac{1}{|\vec{r}_1 - \vec{r}_2|} \right) = \sum_{l=1}^{\infty} \frac{r_2^l}{r_1^{l+1}} \frac{4\pi}{(2l+1)} \sum_{m=-l}^{+l} Y_{lm}^*(\theta_1, \phi_1) Y_{lm}(\theta_2, \phi_2),$$

and

for $r_2 > r_1$:

$$\left(-\frac{1}{r_1} + \frac{1}{|\vec{r}_1 - \vec{r}_2|}\right) = \left(-\frac{1}{r_1} + \frac{1}{r_2}\right) + \sum_{l=1}^{\infty} \frac{r_1^l}{r_2^{l+1}} \frac{4\pi}{(2l+1)} \sum_{m=-l}^{+l} Y_{lm}^*(\theta_1, \phi_1) Y_{lm}(\theta_2, \phi_2)$$

12. Find the Born approximation differential cross section for the μ^- hydrogen atom scattering for the rearrangement process in which the electron is scattered into the direction θ and the μ^- is captured by the proton to make a muonic atom in its 1s ground state. For a μ^- beam of 10 keV incident energy, make a rough numerical estimate of this cross section relative to the elastic cross section of problem 10 to show it is very small. (In making your calculation, show $k_\beta \ll k_\alpha$, so $\vec{k}_\alpha + \frac{m_\mu}{m_\mu + m_p} \vec{k}_\beta \approx \vec{k}_\alpha$ for this case and make this approximation). Show the scattering amplitude, $f(\theta)$, can be written in the form

$$\sum_l f_l P_l(\cos \theta),$$

and use $f_{l=0}$ to make your rough order of magnitude estimate. (Note: The needed Born integral can actually be done in closed form, but the resultant expression is rather complicated.)

13. For the elastic scattering of an e^- from a hydrogen atom in its ground state, both a direct and an exchange contribution exists. If the e^- in the incident beam is labeled “1” and the e^- in the hydrogen atom is labeled “2,” the direct contribution comes from the scattering of “1,” and the exchange contribution comes from the rearrangement collision, where “2” is the scattered particle and “1” is captured by the proton. In Born approximation, with $(ka_0)^2 \gg 1$, the scattering amplitude, $f(\theta)_{\text{direct}}$, can be read from problem 10. (Again, make the approximation $m_e/m_{\text{proton}} \approx 0$.) Evaluate the exchange contribution to the scattering amplitude, $f(\theta)_{\text{exchange}}$, and show

$$\left(\frac{d\sigma}{d\Omega}\right)_{\text{elastic}} = \frac{1}{4} |f(\theta)_{\text{direct}} + f(\theta)_{\text{exchange}}|^2 + \frac{3}{4} |f(\theta)_{\text{direct}} - f(\theta)_{\text{exchange}}|^2$$

if the incident electron beam is unpolarized and no spin alignment of the hydrogen target exists.

The exchange integral can be carried out in closed form (see T. Y. Wu, Can. J. Phys. 38 (1960) 1654). Because the expression is rather complicated, evaluate the exchange contribution in series form

$$f(\theta)_{\text{exchange}} = \sum_l (f_l)_{\text{exchange}} P_l(\cos \theta)$$

and convince yourself this series converges rapidly for $(ka_0)^2 \gg 1$. Estimate roughly the importance of the exchange contribution for $\theta = 60^\circ$, and $(ka_0)^2 = 20$, by making the approximation, $f(\theta)_{\text{exchange}} \approx (f_{l=0})_{\text{exchange}}$.

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A Specific Example of a Rearrangement Collision: The (*d*, *p*) Reaction on Nucleus A

To show in detail how the rearrangement collision integrals are calculated, we shall study the (*d*, *p*) reaction on nucleus A, e.g., ^{16}O , to make nucleus B, e.g., ^{17}O , that is, a nucleus in which the extra neutron captured by nucleus A orbits this nucleus in a particular shell model orbit with orbital angular momentum, *L*.

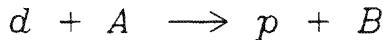
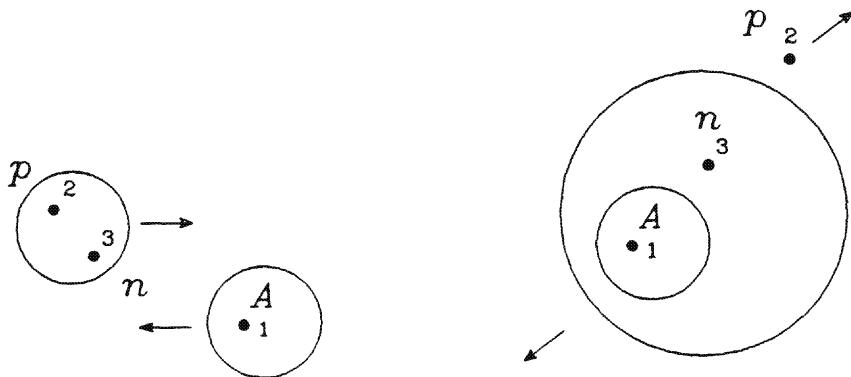


This equation fits the case of Chapter 48, if we label nucleus A by particle label 1, the proton by particle label 2, and the neutron by particle label 3. In the center of mass system the composite particle (2,3) is then incident on particle 1 (see Fig. 50.1). We have

$$\begin{aligned}\vec{r}_\alpha &= \frac{(m_n \vec{r}_3 + m_p \vec{r}_2)}{(m_n + m_p)} - \vec{r}_1, \\ \vec{\xi}_\alpha &= \vec{r}_2 - \vec{r}_3, \\ \vec{r}_\beta &= \vec{r}_2 - \frac{(m_n \vec{r}_3 + m_A \vec{r}_1)}{(m_n + m_A)}, \\ \vec{\xi}_\beta &= \vec{r}_3 - \vec{r}_1.\end{aligned}\tag{1}$$

(Note: We have changed some signs from Chapter 49, because we think of the deuteron as the projectile and nucleus A as the target. All results of Chapter 49, however, apply.) Energy conservation now gives us

$$\frac{\hbar^2}{2\mu_\beta} k_{\beta,n'}^2 + E_{\beta,n'}^{\text{int.}} = \frac{\hbar^2}{2\mu_\alpha} k^2 + E_{\alpha,0}^{\text{int.}}\tag{2}$$

FIGURE 50.1. Rearrangement for a (*d*, *p*) reaction.

For the case in which $A = {}^{16}O$, and if we choose the ground state of ${}^{17}O$, with $n' = 0$, this process would give

$$k_\beta^2 = \frac{m_p m_B}{(m_p + m_B)} \left[\frac{(m_d + m_A)}{m_d m_A} k^2 + \frac{2}{\hbar^2} (E_{\alpha,0}^{\text{int.}} - E_{\beta,0}^{\text{int.}}) \right]. \quad (3)$$

With $E_{\alpha,0} = -\epsilon_\alpha = -2.226 \text{ MeV}$, and with $E_{\beta,0}^{\text{int.}} = -\epsilon_B = -4.146 \text{ MeV}$ for the ground state of ${}^{17}O = B$, we would have

$$k_\beta^2 = .5319 k^2 + .0874 \text{ fm}^{-2}. \quad (4)$$

We shall do the calculation for the ground state of nucleus *B*, so we can dispense with the subscript, $n' = 0$, for economy of notation. All of our results, however, would hold for $n' \neq 0$. To get the differential cross section for this rearrangement collision process in first Born approximation, we need to calculate the Born plane wave matrix element

$$(2\pi)^3 \langle \phi_{\vec{k}_\beta} | V' | \phi_{\vec{k}} \rangle = I_{pn} + I_{pA} = \int d\vec{r}'_\beta \int d\vec{\xi}'_\beta e^{-i\vec{k}_\beta \cdot \vec{r}'_\beta} \chi_{n=0}^*(\vec{\xi}'_\beta) (V_{pn}(\vec{r}'_{23}) + V_{pA}(\vec{r}'_{21})) \chi_{n=0}(\vec{\xi}'_\alpha) e^{i\vec{k} \cdot \vec{r}'_\alpha}. \quad (5)$$

To actually do the integrals, it will be convenient to switch from the integration variables, \vec{r}'_β , $\vec{\xi}'_\beta$, to new integration variables, \vec{r}'_{23} and \vec{r}'_{31} , where these are the internal variables for channels α and β , respectively. Also, now that we have reduced the calculation to a calculation of a (multiple) integral, so all variables are dummy integration variables, we can dispense with the primes on all of these variables for economy of notation. We therefore change to the new integration variables, \vec{r}_{23} and \vec{r}_{31} , where

$$\vec{r}_{23} = \vec{r}_2 - \vec{r}_3 = \vec{\xi}_\alpha,$$

$$\begin{aligned}\vec{r}_{31} &= \vec{r}_3 - \vec{r}_1 = \vec{\xi}_\beta, \\ \vec{r}_\alpha &= \vec{r}_{31} + \frac{m_p}{m_d} \vec{r}_{23}, \\ \vec{r}_\beta &= \vec{r}_{23} + \frac{m_A}{m_B} \vec{r}_{31}.\end{aligned}\quad (6)$$

Also, the Jacobian of the transformation has the value unity

$$d\vec{r}_\beta d\vec{\xi}_\beta = \begin{vmatrix} 1 & \frac{m_A}{m_B} \\ 0 & 1 \end{vmatrix}^3 d\vec{r}_{23} d\vec{r}_{31}, \quad (7)$$

so

$$\begin{aligned}I_{pn} + I_{pA} &= \int d\vec{r}_{23} \int d\vec{r}_{31} e^{-i\vec{r}_{23} \cdot (\vec{k}_\beta - \frac{m_p}{m_d} \vec{k})} \chi_0^{\text{deut.}}(\vec{r}_{23}) \\ &\times \left(V_{pn}(\vec{r}_{23}) + V_{pA}(\vec{r}_{23}) \right) e^{i\vec{r}_{31} \cdot (\vec{k} - \frac{m_A}{m_B} \vec{k}_\beta)} \chi_{n'=0}^{*B}(\vec{r}_{31}).\end{aligned}\quad (8)$$

It would be useful to define vectors, \vec{v} , and $\vec{\kappa}$ (see Fig. 50.2),

$$\begin{aligned}\vec{v} &= \vec{k}_\beta - \frac{m_p}{m_d} \vec{k}, \\ \vec{\kappa} &= \vec{k} - \frac{m_A}{m_B} \vec{k}_\beta.\end{aligned}\quad (9)$$

The vectors \vec{v} and $\vec{\kappa}$ lie in the scattering plane defined by the incident \vec{k} and the scattered \vec{k}_β , so the azimuth angles ϕ for all four vectors can be chosen as $\phi = 0$. The directions and the magnitudes of the vectors \vec{v} and $\vec{\kappa}$ are therefore functions of the scattering angle, θ , given by

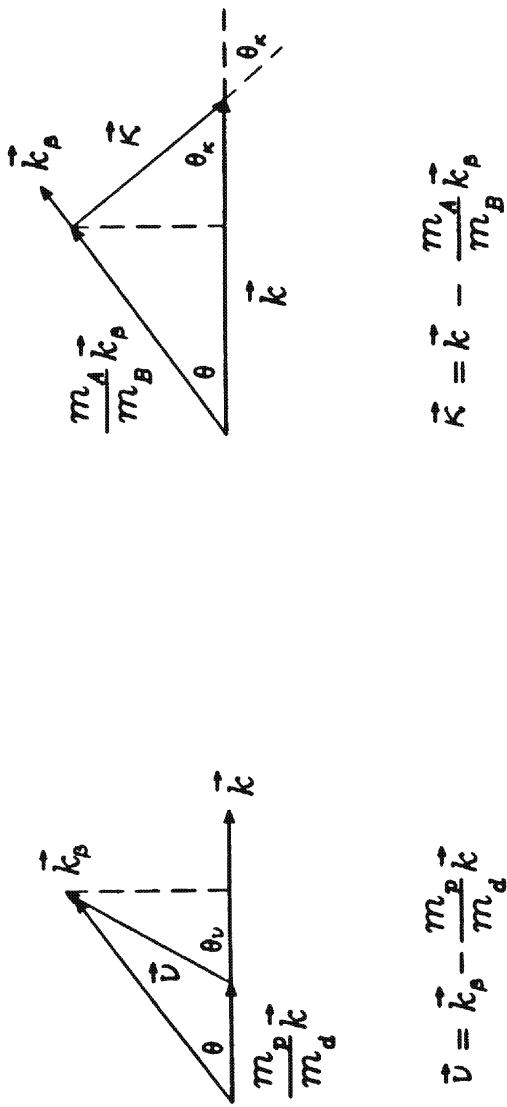
$$\begin{aligned}v &= \sqrt{k_\beta^2 + \left(\frac{m_p}{m_d}\right)^2 k^2 - 2 \frac{m_p}{m_d} k k_\beta \cos \theta}, \\ \kappa &= \sqrt{k^2 + \left(\frac{m_A}{m_B}\right)^2 k_\beta^2 - 2 \frac{m_A}{m_B} k k_\beta \cos \theta},\end{aligned}\quad (10)$$

$$\begin{aligned}\tan \theta_v &= \frac{\frac{k_\beta}{v} \sin \theta}{\left(\frac{k_\beta}{v} \cos \theta - \frac{m_p}{m_d} \frac{k}{v}\right)} = \frac{\sin \theta}{\left(\cos \theta - \frac{m_p}{m_d} \frac{k}{k_\beta}\right)}, \\ \tan \theta_\kappa &= \frac{\frac{k_\beta}{\kappa} \frac{m_A}{m_B} \sin \theta}{\left(\frac{k}{\kappa} - \frac{k_\beta}{\kappa} \frac{m_A}{m_B} \cos \theta\right)} = \frac{\sin \theta}{\left(\frac{k}{k_\beta} \frac{m_B}{m_A} - \cos \theta\right)}.\end{aligned}\quad (11)$$

The integral involving the *p*-*n* interaction, V_{pn} , is then

$$I_{pn} = \int d\vec{r}_{31} e^{i\vec{\kappa} \cdot \vec{r}_{31}} \chi_0^{*B}(\vec{r}_{31}) \int d\vec{r}_{23} e^{-i\vec{v} \cdot \vec{r}_{23}} V_{pn}(\vec{r}_{23}) \chi_0^{\text{deut.}}(\vec{r}_{23}). \quad (12)$$

We could now take some reasonable approximation for the *p*-*n* potential, perhaps even a square well of the appropriate width and depth. We can avoid, however, choosing a specific V_{pn} (realizing the full proton-neutron interaction is very complicated on a fundamental level, involving exchanges not only of pions, but also of ρ and ω vector mesons, hard-core terms caused by quark-quark interactions

FIGURE 50.2. The vectors, \vec{v} and \vec{k}' of eq. (9).

at extremely short range). Instead, we can use the Schrödinger equation for the bound state of the deuteron

$$\left(-\frac{\hbar^2}{2\mu_{pn}}\nabla_{23}^2 + V_{pn}(\vec{r}_{23})\right)\chi^{\text{deut.}}(\vec{r}_{23}) = E_d^{\text{int.}}\chi^{\text{deut.}}(\vec{r}_{23}) = -|\epsilon_d|\chi^{\text{deut.}}(\vec{r}_{23}) \quad (13)$$

to convert

$$V_{pn}(\vec{r}_{23})\chi^{\text{deut.}}(\vec{r}_{23}) = \left(\frac{\hbar^2}{2\mu_{pn}}\nabla_{23}^2 - |\epsilon_d|\right)\chi^{\text{deut.}}(\vec{r}_{23}), \quad (14)$$

where $|\epsilon_d| = 2.226$ MeV is the (positive) binding energy of the deuteron. The 3-D integral

$$\int d\vec{r}_{23}\phi_{\vec{v}}\nabla_{23}^2\chi^{\text{deut.}},$$

with $\phi_{\vec{v}} = e^{-i\vec{v}\cdot\vec{r}_{23}}$ can now be evaluated by use of Green's theorem II, a special case of Gauss' theorem

$$\int d\vec{r}_{23}(\phi_{\vec{v}}\nabla_{23}^2\chi^{\text{deut.}} - \chi^{\text{deut.}}\nabla_{23}^2\phi_{\vec{v}}) = (\text{surface integral at } \infty), \quad (15)$$

where the surface integral at ∞ goes to zero as a result of the exponential fall-off of χ and $\nabla\chi$ as $r_{23} \rightarrow \infty$. Thus, we can evaluate the needed integral via

$$\begin{aligned} \int d\vec{r}_{23}e^{-i\vec{v}\cdot\vec{r}_{23}}\nabla_{23}^2\chi^{\text{deut.}}(\vec{r}_{23}) &= \int d\vec{r}_{23}\chi^{\text{deut.}}(\vec{r}_{23})\nabla_{23}^2e^{-i\vec{v}\cdot\vec{r}_{23}} \\ &= -v^2 \int d\vec{r}_{23}e^{-i\vec{v}\cdot\vec{r}_{23}}\chi^{\text{deut.}}(\vec{r}_{23}). \end{aligned} \quad (16)$$

This equation gives us

$$\int d\vec{r}_{23}e^{-i\vec{v}\cdot\vec{r}_{23}}V_{pn}(\vec{r}_{23})\chi^{\text{deut.}}(\vec{r}_{23}) = -\left(\frac{\hbar^2 v^2}{2\mu_{pn}} + |\epsilon_d|\right) \int d\vec{r}_{23}e^{-i\vec{v}\cdot\vec{r}_{23}}\chi^{\text{deut.}}(\vec{r}_{23}). \quad (17)$$

For purposes of doing our integral, a two-parameter deuteron wave function that fits both the experimental binding energy and the triplet scattering length is sufficient. Such a wave function was constructed by Hulthén with two exponentials

$$\chi^{\text{deut.}}(\vec{r}_{23}) = R^{\text{deut.}}(r_{23})Y_{00}(\theta_{23}, \phi_{23}) = \mathcal{N} \frac{(e^{-\frac{r_{23}}{r_0}} - e^{-\eta \frac{r_{23}}{r_0}})}{r_{23}} \frac{1}{\sqrt{4\pi}}, \quad (18)$$

with parameters and normalization factor, \mathcal{N} , given by

$$r_0 = 4.26\text{fm}, \quad \eta = 6.2, \quad \mathcal{N} = \left[\frac{2\eta(1+\eta)}{r_0(\eta-1)^2} \right]^{\frac{1}{2}}.$$

We can now evaluate our *p-n* interaction integral

$$\begin{aligned} I_{pn} &= -\left(\frac{\hbar^2}{2\mu_{pn}}v^2 + |\epsilon_d|\right) \int d\vec{r}_{23}e^{-i\vec{v}\cdot\vec{r}_{23}}R^{\text{deut.}}(r_{23})Y_{00}(\theta_{23}, \phi_{23}) \\ &\times \int d\vec{r}_{31}e^{i\vec{k}\cdot\vec{r}_{31}}R_{NL}(r_{31})Y_{LM}^*(\theta_{31}, \phi_{31}), \end{aligned} \quad (19)$$

where we have taken the internal wave function, $\chi_{n=0}^B(\vec{r}_{31})$, as a single-particle shell model wave function describing the orbital motion of the neutron around the nucleus *A* in an orbit given by quantum numbers, *NLM*, by

$$\chi_{n=0}^B(\vec{r}_{31}) = R_{NL}(r_{31})Y_{LM}(\theta_{31}, \phi_{31}),$$

where this might be approximated by a 3-D harmonic oscillator function, if the effective potential felt by the odd neutron caused by its interaction with the *A* nucleons of nucleus *A* can be approximated by a parabolic potential for this bound ground state of nucleus *B*.

For purposes of doing the triple \vec{r}_{23} integral, we can choose our *z* axis along the direction of the \vec{v} vector, and expand the exponential via

$$e^{-i\vec{v}\cdot\vec{r}_{23}} = \sum_{l'} (-i)^{l'} \sqrt{4\pi(2l'+1)} j_{l'}(vr_{23}) Y_{l'0}(\theta_{23}). \quad (20)$$

The orthogonality of the spherical harmonics permits us to do the θ_{23} and ϕ_{23} integrals, where only the term with $l' = 0$ will survive. Similarly, for purposes of doing the triple \vec{r}_{31} integral, we can choose our *z* axis along the direction of the $\vec{\kappa}$ vector, and expand the exponential via

$$e^{i\vec{\kappa}\cdot\vec{r}_{31}} = \sum_{l''} (i)^{l''} \sqrt{4\pi(2l''+1)} j_{l''}(kr_{31}) Y_{l''0}(\theta_{31}). \quad (21)$$

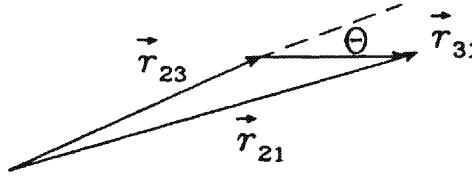
The orthogonality of the spherical harmonics picks out the single term with $l'' = L$ and $M = 0$ and permits us to do the trivial θ_{31} and ϕ_{31} integrals. Our final result for I_{pn} is

$$\begin{aligned} I_{pn} &= -4\pi i^L \sqrt{(2L+1)} \left(\frac{\hbar^2}{2\mu_{pn}} v^2 + |\epsilon_d| \right) F_{\text{deut.}}(v) F_{B,\text{NL}}(\kappa), \\ F_{\text{deut.}}(v) &= \int_0^\infty r^2 dr j_0(vr) R^{\text{deut.}}(r), \\ F_{B,\text{NL}}(\kappa) &= \int_0^\infty r^2 dr j_L(\kappa r) R_{NL}(r), \end{aligned} \quad (22)$$

where $R^{\text{deut.}}(r)$ can be taken as the radial part of the Hulthén wave function and $R_{NL}(r)$ is the radial part of a single-particle shell model wave function, which could be approximated by a 3-D harmonic oscillator wave function. Recall v and κ are θ -dependent [see eq. (10)].

The integral, I_{pA} , is somewhat more complicated than the integral, I_{pn} , because the interaction, V_{pA} , depends on both of our integration variables. If $V_{pA}(\vec{r}_{21})$ depends only on the magnitude of $\vec{r}_{21} = \vec{r}_{23} + \vec{r}_{31}$, however, we can expand V_{pA} in terms of Legendre polynomials, $P_l(\cos \Theta)$, where Θ is the angle between the vectors \vec{r}_{31} and \vec{r}_{23} (see Fig. 50.3).

$$\begin{aligned} V_{pA}(|\vec{r}_{23} + \vec{r}_{31}|) &= \sum_{l'} v_{l'}(r_{23}, r_{31}) P_{l'}(\cos \Theta) \\ &= \sum_{l'} v_{l'}(r_{23}, r_{31}) \frac{4\pi}{(2l'+1)} \sum_{m'} Y_{l'm'}(\theta_{23}, \phi_{23}) Y_{l'm'}^*(\theta_{31}, \phi_{31}). \end{aligned} \quad (23)$$



$$|\vec{r}_{21}| = \sqrt{r_{23}^2 + r_{31}^2 + 2r_{23}r_{31}\cos\Theta}$$

FIGURE 50.3.

The interaction V_{pA} is the interaction of the proton labeled particle 2, with all nucleons of nucleus *A*, averaged over the positions of these nucleons, as given by the ground-state wave function of nucleus *A*. We do not attempt to calculate it from a fundamental nucleon–nucleon interaction, but instead replace it with an effective interaction with a few parameters adjusted to fit the elastic scattering cross sections for the scattering of protons from nucleus *A*. An example of a form that has been used is a simple Gaussian interaction, with parameters V_0 and r_0 adjusted to fit the elastic proton–(nucleus *A*) scattering cross sections, i.e.,

$$V_{pA} = -V_0 e^{-|\vec{r}_{23} + \vec{r}_{31}|^2/r_0^2} = -V_0 e^{-(r_{23}^2 + r_{31}^2 + 2r_{23}r_{31}\cos\Theta)/r_0^2}, \quad (24)$$

with

$$v_{l'}(r_{23}, r_{31}) = -V_0 e^{-(r_{23}^2 + r_{31}^2)/r_0^2} \frac{(2l' + 1)}{2} \int_0^\pi d\Theta \sin\Theta e^{-2(r_{23}r_{31}\cos\Theta)/r_0^2} P_{l'}(\cos\Theta). \quad (25)$$

In this case, $v_{l'}(r_{23}, r_{31})$ is of the form

$$v_{l'}(r_{23}, r_{31}) = e^{-(r_{23}^2/r_0^2)} e^{-(r_{31}^2/r_0^2)} f_{l'}(r_{23}r_{31}/r_0^2), \quad (26)$$

which can facilitate the calculation of the integral. With this type of V_{pA} , we get

$$I_{pA} = \sum_{l', m'} \frac{4\pi}{(2l' + 1)} \int d\vec{r}_{31} e^{i\vec{k}\cdot\vec{r}_{31}} Y_{l'm'}^*(\theta_{31}\phi_{31}) R_{NL}(r_{31}) Y_{LM}^*(\theta_{31}, \phi_{31}) \\ \times \int d\vec{r}_{23} v_{l'}(r_{23}, r_{31}) e^{-i\vec{v}\cdot\vec{r}_{23}} Y_{l'm'}(\theta_{23}, \phi_{23}) R^{\text{deut.}}(r_{23}) \frac{1}{\sqrt{4\pi}}. \quad (27)$$

We now expand the exponentials in terms of spherical Bessel functions and spherical harmonics

$$e^{-i\vec{v}\cdot\vec{r}_{23}} = \sum_{\bar{l}} (-i)^{\bar{l}} j_{\bar{l}}(vr_{23}) \sum_m 4\pi Y_{\bar{l}m}^*(\theta_{23}, \phi_{23}) Y_{\bar{l}m}(\theta_v, \phi_v), \\ e^{i\vec{k}\cdot\vec{r}_{31}} = \sum_{l''} i^{l''} j_{l''}(\kappa r_{31}) \sum_{m''} 4\pi Y_{l''m''}(\theta_{31}, \phi_{31}) Y_{l''m''}^*(\theta_{31}, \phi_{31}), \quad (28)$$

to obtain

$$\begin{aligned}
I_{pA} = & (4\pi)^3 \sum_{l'm'} \sum_{\bar{l}\bar{m}} \sum_{l''m''} t^{l''-\bar{l}} \int_0^\infty dr_{31} r_{31}^2 j_{l''}(\kappa r_{31}) R_{NL}(r_{31}) \\
& \times \int_0^\infty dr_{23} r_{23}^2 j_{l'}(\nu r_{23}) \left(R^{\text{deut.}}(r_{23}) \frac{1}{\sqrt{4\pi}} \right) \frac{v_{l'}(r_{23}, r_{31})}{(2l'+1)} \\
& \times \left[\int d\Omega_{23} Y_{l'm'}(\theta_{23}, \phi_{23}) Y_{\bar{l}\bar{m}}^*(\theta_{23}, \phi_{23}) \right] \\
& \times \left[\int d\Omega_{31} Y_{l''m''}(\theta_{31}, \phi_{31}) Y_{l'm'}^*(\theta_{31}, \phi_{31}) Y_{LM}^*(\theta_{31}, \phi_{31}) \right] \\
& \times Y_{\bar{l}\bar{m}}(\theta_v, \phi_v) Y_{l''m''}^*(\theta_\kappa, \phi_\kappa). \tag{29}
\end{aligned}$$

Now, we use the orthogonality of the spherical harmonics

$$\int d\Omega_{23} Y_{l'm'}(\theta_{23}, \phi_{23}) Y_{\bar{l}\bar{m}}^*(\theta_{23}, \phi_{23}) = \delta_{l'\bar{l}} \delta_{m'\bar{m}} \tag{30}$$

and the well-known integral

$$\begin{aligned}
& \int d\Omega_{31} Y_{l''m''}(\theta_{31}, \phi_{31}) Y_{l'm'}^*(\theta_{31}, \phi_{31}) Y_{LM}^*(\theta_{31}, \phi_{31}) \\
& = \sqrt{\frac{(2l'+1)(2L+1)}{4\pi(2l''+1)}} \langle L0l'0 | l''0 \rangle \langle LMl'm' | l''m'' \rangle \tag{31}
\end{aligned}$$

to reduce I_{pA} to radial integrals.

$$\begin{aligned}
I_{pA} = & (4\pi)^2 \sum_{l'm'l''m''} (i)^{l''-l'} \sqrt{\frac{(2L+1)}{(2l'+1)(2l''+1)}} \langle L0l'0 | l''0 \rangle \langle LMl'm' | l''m'' \rangle \\
& \times Y_{l'm'}(\theta_v, \phi_v) Y_{l''m''}^*(\theta_\kappa, \phi_\kappa) \int_0^\infty dr_{31} r_{31}^2 j_{l''}(\kappa r_{31}) R_{NL}(r_{31}) \\
& \times \int_0^\infty dr_{23} r_{23}^2 j_{l'}(\nu r_{23}) R^{\text{deut.}}(r_{23}) v_{l'}(r_{23}, r_{31}). \tag{32}
\end{aligned}$$

The dependence on the scattering angle, θ , now sits both in the factors v and κ of the spherical Bessel functions, [see eq. (10)] and the angles θ_v and θ_κ of the spherical harmonics [see eq. (11)]. In addition, we recall the vectors \vec{v} and $\vec{\kappa}$ lie in the scattering plane, formed by the vectors \vec{k} and \vec{k}_β , for which we have chosen $\phi = 0$. Thus, we only need the spherical harmonics for $\phi_v = 0$, $\phi_\kappa = 0$.

Eqs. (22) and (32) permit us to calculate the scattering amplitude for the (*d*, *p*) reaction. The contribution from V_{pn} is the most important. In particular, the L dependence of I_{pn} comes from the so-called form factor, $F_{B,NL}(\kappa) = \int_0^\infty r^2 dr j_L(\kappa r) R_{NL}(r)$ of eq. (22). For $L = 0$, the spherical Bessel function peaks at $\kappa r = 0$, and therefore makes its largest contribution to the integral for angles θ near $\theta = 0$. For ever larger values of L , the spherical Bessel functions peak at larger values of the argument κr and therefore make larger contributions to the integral at larger values of κ and, hence, at larger values of θ . Hence, the differential cross sections for the (*d*, *p*) reaction are strongly L -dependent, peaking at $\theta = 0$ for $L = 0$ and at larger angles, the larger the L value. Fig. 50.4 shows angular

dependences for such differential cross sections. Historically, this L selectivity of $\frac{d\sigma}{d\Omega}$ for this reaction was used to establish the L values of shell model orbits.

Final Remarks: We have ignored the spins of both proton and neutron. It is well known the energy positions of shell model orbits are strongly j -dependent. Thus, the $d_{\frac{3}{2}}$ level in ^{17}O lies much higher in energy than the $d_{\frac{5}{2}}$ level, which makes the ground state of ^{17}O . Despite this strong spin-orbit coupling effect of the shell model single-particle energies, this spin-orbit term does not play a strong role in the (d , p) reaction. The differential cross sections for transitions to the $d_{\frac{5}{2}}$ ground state and the excited $d_{\frac{3}{2}}$ state have an almost identical θ -dependence, characteristic of the orbital angular momentum, $L = 2$.

The first Born approximation we have used here uses zeroth-order wave functions that are plane waves, eigenfunctions of our simple H_0 , which included only the kinetic energy part of the relative motion Hamiltonian. A more sophisticated Born approximation, the so-called distorted wave Born approximation, includes within H_0 not only the kinetic energy term of the relative motion, but also an average potential for the incoming projectile, fitted to the elastic scattering cross sections for the projectile (deuteron- ^{16}O elastic scattering in our example), and a similar average potential for the outgoing particle, the proton in our case, where this potential is fitted to the elastic proton- ^{17}O scattering cross sections. Although this more sophisticated distorted wave Born approximation gives much better quantitative results, qualitatively the plane wave Born approximation gives similar results. Historically, therefore, it was an important tool in determining the L values of shell model orbits.

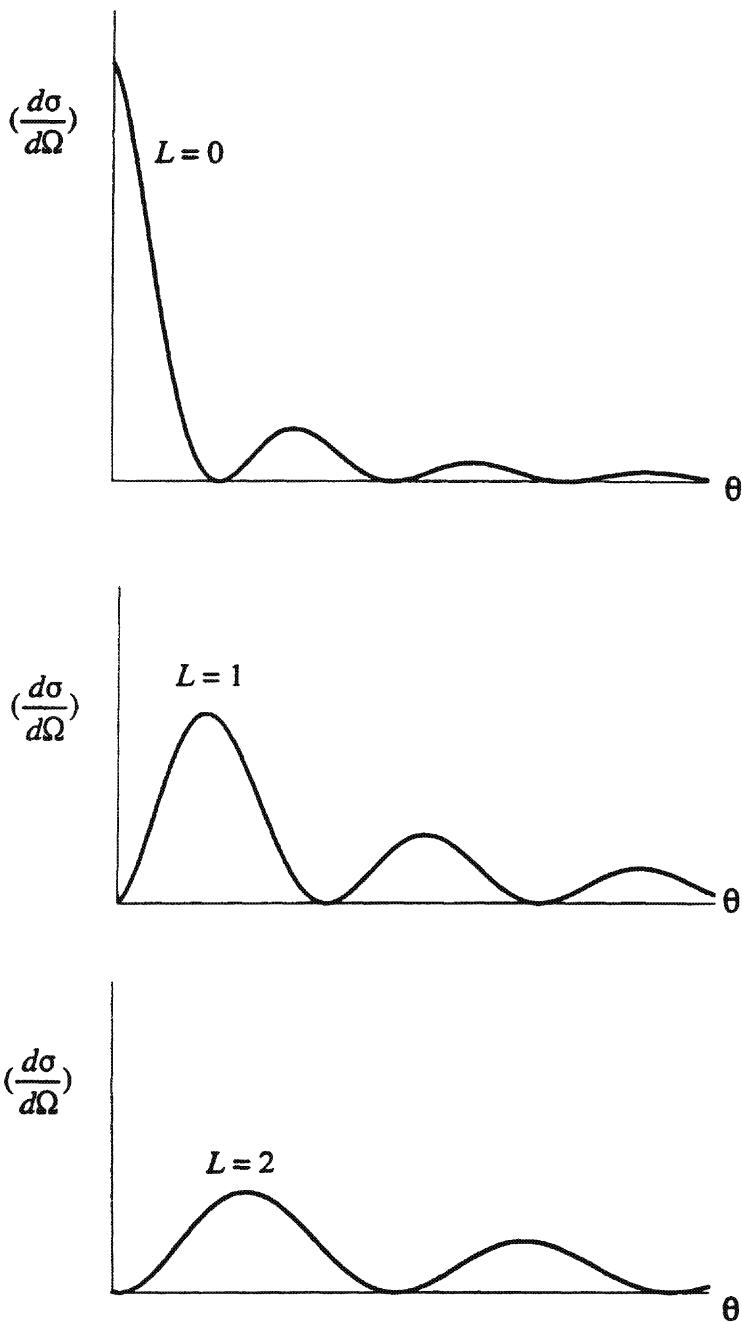


FIGURE 50.4. Plane-wave Born approximation differential cross sections for a $d + A \rightarrow p + B$ reaction. Here L is the orbital angular momentum of the captured neutron shell model orbit.

51

The S Matrix

In what we have done so far, we have essentially calculated matrix elements, or approximate expressions for matrix elements of the so-called S matrix. We have also assumed conservation of energy. Let us now show our approximations come from the S matrix formalism. We will also show the energy conservation follows automatically from this formalism.

The S matrix is defined through

$$S_{fi} = \langle \psi_f^{(-)} | \psi_i^{(+)} \rangle, \quad (1)$$

where i is shorthand for all the quantum numbers, \vec{k}_i , n_{ai} , n_{Ai} , for the initial channel, similarly for f for the final quantum

numbers of the final channel. Also, $|\psi_f^{(-)}\rangle$ is defined through the Green's function, $G^{(-)}$, with incoming spherical waves

$$\begin{aligned} |\psi_f^{(-)}\rangle &= |\phi_f\rangle + \frac{1}{E_f - H_0 - i\epsilon} V |\psi_f^{(-)}\rangle \\ &= |\phi_f\rangle + \frac{1}{E_f - H - i\epsilon} V |\phi_f\rangle. \end{aligned} \quad (2)$$

Using, the second form and assuming H and V are hermitian, $H^\dagger = H$, $V^\dagger = V$, this relation yields

$$\langle \psi_f^{(-)} | = \langle \phi_f | + \langle \phi_f | V \frac{1}{E_f - H + i\epsilon}. \quad (3)$$

Using this form for the bra of the matrix element S_{fi} , we get

$$\begin{aligned} S_{fi} &= \langle \phi_f | \psi_i^{(+)} \rangle + \langle \phi_f | V \frac{1}{E_f - H + i\epsilon} | \psi_i^{(+)} \rangle \\ &= \langle \phi_f | \psi_i^{(+)} \rangle + \langle \phi_f | V \frac{1}{E_f - E_i + i\epsilon} | \psi_i^{(+)} \rangle, \end{aligned} \quad (4)$$

where we have used $H|\psi_i^{(+)}\rangle = E_i|\psi^{(+)}\rangle$. Now, we write $|\psi_i^{(+)}\rangle$ in the first term as

$$|\psi_i^{(+)}\rangle = |\phi_i\rangle + \frac{1}{E_i - H_0 + i\epsilon} V |\psi_i^{(+)}\rangle \quad (5)$$

to get

$$\begin{aligned} \langle \phi_f | \psi_i^{(+)} \rangle &= \langle \phi_f | \phi_i \rangle + \langle \phi_f | \frac{1}{E_i - H_0 + i\epsilon} V |\psi_i^{(+)}\rangle \\ &= \langle \phi_f | \phi_i \rangle + \langle \phi_f | \frac{1}{E_i - E_f + i\epsilon} V |\psi_i^{(+)}\rangle, \end{aligned} \quad (6)$$

where we have used the left action of H_0 on $\langle \phi_f |$ in the second line. Combining eqs. (4) and (6), we get

$$\begin{aligned} S_{fi} &= \langle \phi_f | \phi_i \rangle + \langle \phi_f | \left(V \frac{1}{E_f - E_i + i\epsilon} + \frac{1}{E_i - E_f + i\epsilon} V \right) |\psi_i^{(+)}\rangle \\ &= \langle \phi_f | \phi_i \rangle + \lim_{\epsilon \rightarrow 0} \frac{(-2i\epsilon)}{(E_f - E_i)^2 + \epsilon^2} \langle \phi_f | V |\psi_i^{(+)}\rangle \\ &= \langle \phi_f | \phi_i \rangle - 2i\pi\delta(E_f - E_i) \langle \phi_f | V |\psi_i^{(+)}\rangle \\ &= \delta(\vec{k}_f - \vec{k}_i) \delta_{n_{a,f} n_{a,i}} \delta_{n_{A,f} n_{A,i}} - 2i\pi\delta(E_f - E_i) \langle \phi_f | V |\psi_i^{(+)}\rangle, \end{aligned} \quad (7)$$

where we have used

$$\frac{1}{\pi} \lim_{\epsilon \rightarrow 0} \frac{\epsilon}{(\omega^2 + \epsilon^2)} = \delta(\omega), \quad (8)$$

which follows from

$$\begin{aligned} &\lim_{\epsilon \rightarrow 0} \frac{1}{2\pi} \int_{-\infty}^{\infty} dt e^{-\epsilon|t|} e^{i\omega t} = \delta(\omega) \\ &= \lim_{\epsilon \rightarrow 0} \frac{1}{2\pi} \left(\int_{-\infty}^0 dt e^{(\epsilon+i\omega)t} + \int_0^{\infty} dt e^{-(\epsilon-i\omega)t} \right) \\ &= \lim_{\epsilon \rightarrow 0} \frac{1}{2\pi} \left(\frac{1}{\epsilon + i\omega} + \frac{1}{\epsilon - i\omega} \right) = \lim_{\epsilon \rightarrow 0} \frac{1}{\pi} \frac{\epsilon}{(\omega^2 + \epsilon^2)}. \end{aligned} \quad (9)$$

Eq. (7) gives the initial channel form of S_{fi} ; that is, it is assumed that the final state is in the same channel as the initial state, so S_{fi} is an elastic or an inelastic scattering matrix element. For rearrangement collisions, we need a scattering matrix element of the form, $S_{f'i} = \langle \psi_{f'}^{(-)} | \psi_i^{(+)} \rangle$, where the state $|\phi_{f'}\rangle$ is assumed to be an eigenstate of H'_0 belonging to a different channel. We would now express $\langle \psi_{f'}^{(-)} |$ by

$$\langle \psi_{f'}^{(-)} | = \langle \phi_{f'} | + \langle \phi_{f'} | V' \frac{1}{E_{f'} - H + i\epsilon}, \quad (10)$$

and

$$\langle \phi_{f'} | \psi_i^{(+)} \rangle = \langle \phi_{f'} | \frac{1}{E_i - H'_0 + i\epsilon} V' | \psi_i^{(+)} \rangle, \quad (11)$$

so

$$\begin{aligned} S_{f'i} &= \langle \psi_{f'}^{(-)} | \psi_i^{(+)} \rangle = \langle \phi_{f'} | \left(\frac{1}{E_i - H'_0 + i\epsilon} V' + V' \frac{1}{E_{f'} - H + i\epsilon} \right) | \psi_i^{(+)} \rangle \\ &= \lim_{\epsilon \rightarrow 0} \left(\frac{1}{E_i - E_{f'} + i\epsilon} + \frac{1}{E_{f'} - E_i + i\epsilon} \right) \langle \phi_{f'} | V' | \psi_i^{(+)} \rangle \\ &= -2\pi i \delta(E_{f'} - E_i) \langle \phi_{f'} | V' | \psi_i^{(+)} \rangle. \end{aligned} \quad (12)$$

A The T Matrix

Because the S matrix is often related to the so-called T matrix, let us introduce this T matrix now, through the defining equations

$$\begin{aligned} S_{fi} &= \langle \phi_f | \phi_i \rangle - 2\pi i \delta(E_f - E_i) T_{fi}, \quad \text{with } T_{fi} = \langle \phi_f | V | \psi_i^{(+)} \rangle, \\ S_{f'i} &= -2\pi i \delta(E_{f'} - E_i) T_{f'i}, \quad \text{with } T_{f'i} = \langle \phi_{f'} | V' | \psi_i^{(+)} \rangle. \end{aligned} \quad (13)$$

The T matrix element for a rearrangement collision could be given in two forms

$$T_{f'i} = \langle \phi_{f'} | V' | \psi_i^{(+)} \rangle, \quad \text{also } = \langle \phi_{f'} | V | \psi_i^{(+)} \rangle. \quad (14)$$

In principle, both the last ‘‘preform’’ and the first ‘‘postform’’ for the T matrix element of a rearrangement collision are equally valid, but in first Born approximation, the postform may be the better approximation. Finally, to express $|\psi_i^{(+)}\rangle$ in terms of $|\phi_i\rangle$ through a Born series iteration, it is also useful to introduce the Møller operator, $\Omega^{(+)}$,

$$|\psi_i^{(+)}\rangle = \Omega^{(+)} |\phi_i\rangle, \quad (15)$$

where

$$\begin{aligned} \Omega^{(+)} &= 1 + \frac{1}{E - H + i\epsilon} V \\ &= 1 + \frac{1}{E - H_0 + i\epsilon} V \Omega^{(+)} \\ &= 1 + \frac{1}{E - H_0 + i\epsilon} V + \frac{1}{E - H_0 + i\epsilon} V \frac{1}{E - H_0 + i\epsilon} V + \dots. \end{aligned} \quad (16)$$

Thus,

$$\begin{aligned} T_{fi} &= \langle \phi_f | V | \phi_i \rangle + \langle \phi_f | V \frac{1}{E_i - H_0 + i\epsilon} V | \phi_i \rangle \\ &\quad + \langle \phi_f | V \frac{1}{E_i - H_0 + i\epsilon} V \frac{1}{E_i - H_0 + i\epsilon} V | \phi_i \rangle + \dots \end{aligned} \quad (17)$$

For rearrangement collisions, we could use either the postform or the preform, so

$$T_{f'i} = \langle \phi_{f'} | V' | \phi_i \rangle + \langle \phi_{f'} | V' \frac{1}{E_i - H_0 + i\epsilon} V | \phi_i \rangle + \dots$$

$$= \langle \phi_{f'} | V | \phi_i \rangle + \langle \phi_{f'} | V \frac{1}{E_i - H_0 + i\epsilon} V | \phi_i \rangle + \dots \quad (18)$$

Because the approximations involved in the postforms and preforms are different, but hopefully converge to the same result if a sufficient number of iterations are taken, one sometimes also takes an average of the postform and preform in the hope it will improve the accuracy of the expansion after only a small number of iterations. Thus, also,

$$T_{f'i} = \frac{1}{2} \left(\langle \phi_{f'} | (V' + V) | \phi_i \rangle + \langle \phi_{f'} | (V' + V) \frac{1}{E_i - H_0 + i\epsilon} V | \phi_i \rangle + \dots \right). \quad (19)$$

Finally, recall

$$\frac{d\sigma}{d\Omega} = \frac{\mu_f \mu_i}{(2\pi\hbar^2)^2} \frac{k_{f'}}{k_i} (2\pi)^6 |\langle \phi_{f'} | V' | \psi_i^{(+)} \rangle|^2, \quad (20)$$

[cf., eq. (18) of Chapter 49], so we get

$$\frac{d\sigma}{d\Omega} = \left(\frac{2\pi}{\hbar} \right)^4 \mu_f \mu_i \frac{k_{f'}}{k_i} |T_{f'i}|^2. \quad (21)$$

Final remark:

The Møller operator $\Omega^{(+)}$ could be written in the form

$$\sum_i \int | \psi_i^{(+)} \rangle \langle \phi_i |, \quad (22)$$

where the $\sum_i \int$ symbol is shorthand for the triple integral over all \vec{k}_i and a sum over all n_{a_i} and n_{A_i} , which enumerate the ground and excited states of composite projectile and composite target systems. In particular, the operator, $\Omega^{(+)}$, is not unitary. We have

$$(\Omega^{(+)})^\dagger (\Omega^{(+)}) = \sum_i \int \sum_j \int | \phi_j \rangle \langle \psi_j^{(+)} | \psi_i^{(+)} \rangle \langle \phi_i | = \sum_i \int | \phi_i \rangle \langle \phi_i | = 1, \quad (23)$$

because the $|\phi_i\rangle$ form a complete set. However,

$$\begin{aligned} (\Omega^{(+)}) (\Omega^{(+)})^\dagger &= \sum_i \int | \psi_i^{(+)} \rangle \langle \psi_i^{(+)} | \neq 1 \\ &= 1 - \sum_{\text{bound}} | \psi_b \rangle \langle \psi_b |, \end{aligned} \quad (24)$$

where the right-hand side is no longer unity if the combined system of particles ($a + A$) has some bound states $|\psi_b\rangle$.

Problems

- 14.** A neutron beam is scattered elastically from an odd-mass nucleus made of a very stable core nucleus of mass, m_C , and a loosely bound extra neutron.

(a) Assume the neutron–neutron interaction is much stronger than the interaction of the neutron with the core, so V_{nC} can be neglected compared with V_{nn} .

(b) Assume further the short-range V_{nn} can be approximated by a spin-independent delta function interaction

$$V_{nn} = -V_0 b^3 \delta(\vec{r}_{n1} - \vec{r}_{n2}),$$

where V_0 and b are constants (with dimensions of energy and length, respectively).

(c) Assume the loosely bound neutron is in an s state with internal wave function given by

$$\chi(\vec{r}_{nC}) = \frac{2}{\sqrt{a^3 \sqrt{\pi}}} e^{-(r_{nC}^2/2a^2)} Y_{00}(\theta_{nC}, \phi_{nC}).$$

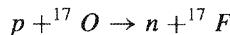
(d) Assume the incident energy is such that the cross section can be calculated in Born approximation.

(e) Assume the incident beam is unpolarized and that there is no spin alignment of the target nucleus.

(f) Assume exchange processes between the incoming neutron and the neutrons in the core nucleus, C , can be neglected.

Show, however, exchange processes between the incoming neutron and the loosely bound extra neutron are important, and calculate the differential cross section in Born approximation. Remember neutrons are $s = \frac{1}{2}$ particles.

15. Calculate the differential cross section for the (p, n) rearrangement collision:



in plane-wave Born approximation.

(a) Assume the ground state of ${}^{17}O$ is approximated well by a bound d state ($l = 2$) shell model wave function describing the motion of the neutron with respect to an inert ${}^{16}O$ closed shell nucleus, C :

$$\chi_{n=2,l=2,m}(\vec{r}_{nC}) = \sqrt{\frac{2}{a^3 \Gamma(\frac{7}{2})}} \left(\frac{r_{nC}}{a}\right)^2 e^{-\frac{1}{2}(r_{nC}^2/a^2)} Y_{l=2,m}(\theta_{nC}, \phi_{nC})$$

with length parameter, $a = 3.5$ fm.

(b) The final wave function in ${}^{17}F$ is approximated by a similar d state shell model wave function, $\chi_{n=2,l=2,m}(\vec{r}_{pC})$, with the same length parameter, a . We assume the final ${}^{17}F$ nucleus is in its ground state. In this case, $E^{\text{int.}}({}^{17}F) - E^{\text{int.}}({}^{17}O) = 2.76$ MeV.

(c) All interactions are assumed to be spin-independent so the spins of the particles play no role in the Born integrals, although both the ${}^{17}O$ and ${}^{17}F$ ground states have total angular momentum, $J = \frac{5}{2}$.

(d) The interaction between the neutron and the ${}^{16}O$ core, C , in the outgoing channel is negligible compared with the neutron proton interaction, V_{np} , i.e., $V_{nC} \ll V_{np}$, similarly, $V_{pC} \ll V_{np}$ in the incident channel.

(e) The short-range neutron–proton interaction can be approximated by a delta function interaction, $V_{np} = -V_0 b^3 \delta(\vec{r}_n - \vec{r}_p)$, with length parameter, $b = 1$ fm, $V_0 = 100$ MeV. Also, let the mass of ${}^{16}O$ be M , and $m_{\text{neutron}} = m_{\text{proton}} = m$.

16. Calculate the differential cross section for the elastic scattering of a proton from the deuteron under the following simplifying assumptions.

(a) The incident energy is such that the differential cross section can be calculated in first Born approximation.

(b) Assume the interaction of the proton with the constituents of the deuteron is spin-independent, short range, and can be approximated by delta function interactions

$$V_{pp} = -V_0 b^3 \delta(\vec{r}_{p_1} - \vec{r}_{p_2}), \quad V_{pn} = -V_0 b^3 \delta(\vec{r}_p - \vec{r}_n).$$

(c) Take $m_p = m_n \approx \frac{1}{2}m_d$.

(d) The bound-state wave function of the deuteron is given by the Hulthen wave function

$$\chi_d^{\text{int.}} = \frac{\mathcal{N}}{r_{pn}} \left(e^{-\frac{r_{pn}}{r_0}} - e^{-\eta \frac{r_{pn}}{r_0}} \right) Y_{00}(\theta_{pn}, \phi_{pn}) \chi_{S=1, M_S}^{\text{spin}},$$

with

$$r_0 = 4.26 \text{ fm}, \quad \eta = 6.2, \quad \mathcal{N} = \left[\frac{2\eta(1+\eta)}{r_0(\eta-1)^2} \right]^{\frac{1}{2}}.$$

Calculate the differential cross section assuming the proton beam is unpolarized and the deuteron target (with $S = 1$) is unaligned; i.e., it has arbitrary spin orientations. In making your calculation, remember the detector cannot distinguish “projectile” protons from “target” protons, so exchange terms have to be considered.

How will the differential cross section change if the incident proton beam is longitudinally polarized, with proton spin projection, $m_s = +\frac{1}{2}$, along the direction of the incident \vec{p}_0 , but the deuteron target is still unaligned?

52

Scattering Theory for Particles with Spin

A Scattering of a Point Particle with Spin from a Spinless Target Particle

For a point particle with spin, our plane wave solutions are of the form $|\phi_{\vec{k}}\rangle = |\vec{k}, sm_s\rangle$ with coordinate representation,

$$\langle \vec{r}_{\text{rel.}}, \vec{\xi}_{\text{int.}} | \vec{k}, sm_s \rangle = \frac{1}{(2\pi)^{\frac{3}{2}}} e^{i\vec{k} \cdot \vec{r}} \chi_{sm_s}(\vec{\xi}_{\text{int.}}).$$

Now, for a true point particle, like the electron or the muon, the nature of the internal variables is unknown. In that case, we merely replace $\vec{\xi}_{\text{int.}}$ with the spin operator \vec{s} itself (or for $s = \frac{1}{2}$ -particles with the Pauli $\vec{\sigma}$ vector). We know how to take matrix elements between such spin states of operators such as the \vec{s} components without having to specify a $\vec{\xi}_{\text{int.}}$. (Nevertheless, when we are in coordinate representation, it may be useful to use an imagined $\vec{\xi}$ and write an integral over $\vec{\xi}$ to designate the process of taking a spin-space matrix element.) To specify the state $|\vec{k}, sm_s\rangle$, we also need to specify the quantization axis for the quantum number m_s . We shall usually take the direction of the incident \vec{k} as the quantization axis, so an $s = \frac{1}{2}$ -particle with $m_s = +\frac{1}{2}$ is polarized longitudinally along the direction of the incident momentum vector, whereas a particle in the state with $m_s = -\frac{1}{2}$ is polarized longitudinally in a direction opposite to the incident momentum direction. If we have incident particles with specific polarization along some z' direction defined through Euler angles, α, β, γ with respect to the incident x, y, z direction,

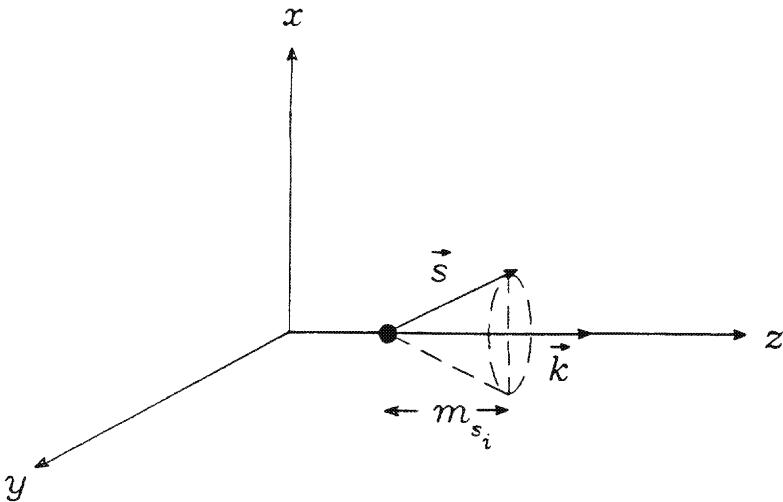


FIGURE 52.1.

however,

$$\chi_{sm'_s}(\vec{s}) = \sum_{m_s} \chi_{sm_s}(\vec{s}) D_{m_s m'_s}^{s*}(\alpha, \beta, \gamma). \quad (1)$$

For an incoming beam with a perpendicular polarization, say, with fixed m'_s along the x axis (see Fig. 52.1), the required rotation is one from the original z axis to the new axis of quantization, the old x axis. The rotation is therefore a simple rotation about the y axis through an angle of $\beta = \frac{\pi}{2}$, with $\alpha = 0$, $\gamma = 0$. In that case,

$$\chi_{sm'_s} = \sum_{m_s} \chi_{sm_s} d_{m_s m'_s}^{\frac{1}{2}}(\beta). \quad (2)$$

Recall: The $d_{mm'}^j(\beta)$ are real, and for $s = \frac{1}{2}$,

$$d_{m_s m'_s}^{\frac{1}{2}}(\beta) = \begin{pmatrix} \cos \frac{\beta}{2} & -\sin \frac{\beta}{2} \\ \sin \frac{\beta}{2} & \cos \frac{\beta}{2} \end{pmatrix}, \quad (3)$$

so for spin $s = \frac{1}{2}$ -particles with incident perpendicular (\perp) polarization along the x axis

$$\chi_{\frac{1}{2}, m'_s = \pm \frac{1}{2}}^{(\perp)} = \pm \frac{1}{\sqrt{2}} \chi_{\frac{1}{2}, +\frac{1}{2}} + \frac{1}{\sqrt{2}} \chi_{\frac{1}{2}, -\frac{1}{2}}, \quad (4)$$

where the spin functions, χ_{sm_s} , without superscript will stand for spin states with longitudinal polarizations specified by m_s .

We shall deal with incoming plane wave states of the type

$$e^{i\vec{k} \cdot \vec{r}} \chi_{sm_s}(\vec{s}) = \sum_l i^l \sqrt{4\pi(2l+1)} j_l(kr) Y_{l0}(\theta) \chi_{sm_s}(\vec{s}), \quad (5)$$

where θ is the angle between the \vec{r} and \vec{k} vectors. When taking matrix elements of scalar (rotationally invariant) interactions between such incoming (plane wave)-spin states and similar outgoing (plane wave)-spin states, it will be very useful to couple the orbital and spin functions to orbital-spin functions of total angular momentum j , with $\vec{l} + \vec{s} = \vec{j}$. This process will facilitate use of the Wigner–Eckart theorem. Thus, we define

$$\mathcal{Y}_{[ls]jm_j}(\theta, \phi, \vec{s}) \equiv \sum_{m_s(m_l)} \langle lm_l sm_s | jm_j \rangle i^l Y_{lm_l}(\theta, \phi) \chi_{sm_s}(\vec{s}). \quad (6)$$

(The factor i^l has been included with the Y_{lm} as a matter of convenience.) Note also the orthonormality of these functions

$$\int \int d\Omega_{\theta, \phi} \int d\vec{\xi} \mathcal{Y}_{[l's]j'm'_j}^*(\theta, \phi, \vec{\xi}) \mathcal{Y}_{[ls]jm_j}(\theta, \phi, \vec{\xi}) = \delta_{l'l} \delta_{j'j} \delta_{m'_j m_j}, \quad (7)$$

which follows from the orthonormality of the spherical harmonics, the orthonormality of the spin functions, and the orthonormality of the Clebsch–Gordan coefficients.

In terms of these vector-coupled orbital-spin functions, eq. (5) can be rewritten as

$$e^{i\vec{k}\cdot\vec{r}} \chi_{sm_s} = \sum_{l,j} \sqrt{4\pi(2l+1)} j_l(kr) \langle l0sm_s | jm_s \rangle \mathcal{Y}_{[ls]jm_s}(\theta, \phi, \vec{s}), \quad (8)$$

where we have used

$$i^l Y_{l0}(\theta, \phi) \chi_{sm_s}(\vec{s}) = \sum_j \langle l0sm_s | jm_s \rangle \mathcal{Y}_{[ls]jm_s}(\theta, \phi, \vec{s}). \quad (9)$$

For the special case of $s = \frac{1}{2}$, the needed Clebsch–Gordan coefficients are

$$\begin{aligned} \langle l0\frac{1}{2} \pm \frac{1}{2} | j = (l + \frac{1}{2}) \pm \frac{1}{2} \rangle &= \sqrt{\frac{(l+1)}{(2l+1)}} \\ \langle l0\frac{1}{2} \pm \frac{1}{2} | j = (l - \frac{1}{2}) \pm \frac{1}{2} \rangle &= \mp \sqrt{\frac{l}{(2l+1)}}. \end{aligned} \quad (10)$$

With these coefficients, we have

$$e^{i\vec{k}\cdot\vec{r}} \chi_{\frac{1}{2}\pm\frac{1}{2}} = \sum_l \sqrt{4\pi} j_l(kr) \left(\sqrt{(l+1)} \mathcal{Y}_{[l\frac{1}{2}]j=(l+\frac{1}{2}), \pm\frac{1}{2}} \mp \sqrt{l} \mathcal{Y}_{[l\frac{1}{2}]j=(l-\frac{1}{2}), \pm\frac{1}{2}} \right). \quad (11)$$

The scattering amplitude now depends on both the angles θ and ϕ and the spin directions and can be written as a $(2s+1) \times (2s+1)$ matrix

$$f(\vec{k}_f, m_{s_f}; \vec{k}, m_{s_i}) \equiv f(\theta, \phi)_{m_{s_f} m_{s_i}} = -\frac{2\mu}{4\pi\hbar^2} (2\pi)^3 \langle \phi_f | V | \psi_i^{(+)} \rangle. \quad (12)$$

m_{s_i} and m_{s_f} are *both* defined with respect to the incident \vec{k} vector chosen along the z axis, and \vec{k}_f makes an angle θ with respect to \vec{k} .

B First Born Approximation

In first Born approximation,

$$f_{m_{sf} m_{s_i}}(\theta, \phi) = -\frac{\mu}{2\pi\hbar^2} \int d\vec{r}' \int d\vec{\xi}' e^{-i\vec{k}_f \cdot \vec{r}'} \chi_{sm_{s_i}}^*(\vec{\xi}') V(\vec{r}', \vec{\xi}') e^{i\vec{k} \cdot \vec{r}'} \chi_{sm_{s_i}}(\vec{\xi}'),$$

where we use

$$e^{i\vec{k}_f \cdot \vec{r}'} \chi_{sm_{s_i}}(\vec{\xi}') = \sum_{l,j} j_l(kr') \sqrt{4\pi(2l+1)} \langle l0sm_{s_i} | jm_{s_i} \rangle \mathcal{Y}_{[ls]jm_{s_i}}(\theta', \phi', \vec{\xi}'), \quad (13)$$

$$\begin{aligned} & e^{-i\vec{k}_f \cdot \vec{r}'} \chi_{sm_{s_i}} * (\vec{\xi}') = \\ & \sum_{l_f} (-i)^{l_f} j_{l_f}(k_f r') 4\pi \sum_{m_f} Y_{l_f m_f}(\theta, \phi) Y_{l_f m_f}^*(\theta', \phi') \chi_{sm_{s_i}}^*(\vec{\xi}') = \\ & \sum_{l_f m_f} \sum_{j_f} 4\pi j_{l_f}(k_f r') \langle l_f m_f sm_{s_i} | jm_{j_f} \rangle \mathcal{Y}_{[l_f s] j_f m_{l_f}}^*(\theta', \phi', \vec{\xi}') Y_{l_f m_f}(\theta, \phi). \end{aligned} \quad (14)$$

In first Born approximation, therefore,

$$\begin{aligned} f(\theta, \phi)_{m_{sf} m_{s_i}} &= -\frac{2\mu}{\hbar^2} \sqrt{4\pi} \\ &\times \sum_{l,j} \sum_{l_f, m_f, j_f} \sqrt{(2l+1)} \langle l0sm_{s_i} | jm_{s_i} \rangle \langle l_f m_f sm_{s_i} | j_f m_{j_f} \rangle Y_{l_f m_f}(\theta, \phi) \\ &\times \int d\vec{r}' \int d\vec{\xi}' j_{l_f}^*(k_f r') \mathcal{Y}_{[l_f s] j_f m_{l_f}}^*(\theta', \phi', \vec{\xi}') \\ &\times V(\vec{r}', \vec{\xi}') \mathcal{Y}_{[ls]jm_{s_i}}(\theta', \phi', \vec{\xi}') j_l(kr'). \end{aligned} \quad (15)$$

For a rotationally invariant $V(\vec{r}, \vec{\xi}) = V(\vec{r}, \vec{s})$, i.e., for a V that is a spherical tensor of rank 0, the Wigner–Eckart theorem tells us the matrix element of such a V is diagonal in j and m_j and independent of m_j . Thus,

$$\int \int d\Omega' \int d\vec{\xi}' \mathcal{Y}_{[l_f s] j_f m_{l_f}} V(\vec{r}', \vec{s}) \mathcal{Y}_{[ls]jm_{s_i}} = \mathcal{V}_{l_f, l}^{s, j}(r') \delta_{j_f j} \delta_{m_{l_f} m_{s_i}}, \quad (16)$$

and

$$\begin{aligned} f(\vec{k}_f, m_{s_i}; \vec{k}, m_{s_i}) &= f(\theta, \phi)_{m_{sf} m_{s_i}} = -\frac{2\mu}{\hbar^2} \sqrt{4\pi} \sum_{l, l_f} \sum_j \sqrt{(2l+1)} \\ &\times \langle l0sm_{s_i} | jm_{s_i} \rangle \langle l_f(m_{s_i} - m_{s_f}) sm_{s_f} | jm_{s_i} \rangle Y_{l_f(m_{s_i} - m_{s_f})}(\theta, \phi) \\ &\times \int_0^\infty dr' r'^2 j_{l_f}^*(k_f r') \mathcal{V}_{l_f, l}^{s, j}(r') j_l(kr'). \end{aligned} \quad (17)$$

One of the most common spin-dependent interactions involves a simple spin-orbit coupling term

$$V(\vec{r}', \vec{s}) = V_0(r') + V_1(r')(\vec{l} \cdot \vec{s}). \quad (18)$$

Because the components of the operator \vec{l} change only the components m_l and not the quantum number l , this interaction is diagonal in l . Moreover, it has the simple

form

$$\mathcal{V}_{l_f,l}^{s,j}(r') = \delta_{l_f,l} \left(V_0(r') + \frac{1}{2} V_1(r') [j(j+1) - l(l+1) - s(s+1)] \right), \quad (19)$$

leading to the first Born approximation result

$$\begin{aligned} f(\theta, \phi)_{m_{s_f} m_{s_i}} &= -\frac{2\mu}{\hbar^2} \sqrt{4\pi} \sum_{l,j} \sqrt{(2l+1)} \\ &\times \langle l0sm_{s_i} | jm_{s_i} \rangle \langle l(m_{s_i} - m_{s_f}) sm_{s_f} | jm_{s_i} \rangle Y_{l(m_{s_i} - m_{s_f})}(\theta, \phi) \\ &\times \int_0^\infty dr' r'^2 [j_l(kr')]^2 \left(V_0(r') + \frac{1}{2} V_1(r') \right) \\ &\times [j(j+1) - l(l+1) - s(s+1)], \end{aligned} \quad (20)$$

where we note the scattering process is still elastic, so the magnitude of \vec{k}_f is still the same as the magnitude k of \vec{k} . Also, matrix elements of this scattering amplitude matrix with $m_{s_f} \neq m_{s_i}$ are now ϕ -dependent. Let us consider the special case of an $s = \frac{1}{2}$ particle. First, the diagonal matrix elements with $m_{s_f} = m_{s_i}$ are independent of the sign of m_{s_i} . This result follows from the symmetry property of Clebsch–Gordan coefficients

$$[\langle l0s + m_{s_i} | j + m_{s_i} \rangle]^2 = [\langle l0s - m_{s_i} | j - m_{s_i} \rangle]^2. \quad (21)$$

Moreover, these matrix elements are of the form $\sum_l A_l Y_{l0}(\theta, \phi)$ and therefore ϕ -independent. From the similar symmetry property

$$\langle l0s + \frac{1}{2} | j + \frac{1}{2} \rangle \langle l + 1s - \frac{1}{2} | j + \frac{1}{2} \rangle = \langle l0s - \frac{1}{2} | j - \frac{1}{2} \rangle \langle l - 1s + \frac{1}{2} | j - \frac{1}{2} \rangle, \quad (22)$$

the off-diagonal elements are of the form

$$\begin{aligned} f(\theta, \phi)_{+\frac{1}{2}, -\frac{1}{2}} &= \sum_l B_l Y_{l,-1}(\theta, \phi), \\ f(\theta, \phi)_{-\frac{1}{2}, +\frac{1}{2}} &= \sum_l B_l Y_{l,+1}(\theta, \phi), \end{aligned} \quad (23)$$

with identical coefficients, B_l . Now we recall the standard spherical harmonics with $m = \pm 1$ are of the form

$$Y_{l,\pm 1}(\theta, \phi) = \mp |\mathcal{N}_{l,1}| \sin \theta \left(\frac{dP_l(\cos \theta)}{d \cos \theta} \right) e^{\pm i\phi}.$$

Therefore, we can write the scattering amplitude matrix for $s = \frac{1}{2}$ -particles in terms of two functions of θ

$$f(\theta, \phi)_{m_{s_f} m_{s_i}} = \begin{pmatrix} g(\theta) & \bar{h}(\theta) e^{-i\phi} \\ -\bar{h}(\theta) e^{+i\phi} & g(\theta) \end{pmatrix}. \quad (24)$$

Also, the functions, $g(\theta)$, and $\bar{h}(\theta)$ are real. We shall find this special property is related to the fact that we have used the first Born approximation. This result will have to be relaxed, and we shall have to examine the scattering amplitude valid for lower energies.

Scattering of Spin $\frac{1}{2}$ Particles from Spinless Target: Partial Wave Decomposition

To study the low-energy scattering of particles with spin, we shall use a partial wave decomposition. We shall restrict ourselves, however, to the simplest case of $s = \frac{1}{2}$ -particles scattering from a spinless target particle and will assume the spin-dependent interaction is given by the simple potential

$$\begin{aligned} V &= V_0(r) + V_1(r)(\vec{l} \cdot \vec{s}) \\ &= V_0(r) + \frac{1}{2}lV_1(r) \quad \text{for } j = (l + \frac{1}{2}) \\ &= V_0(r) - \frac{1}{2}(l + 1)V_1(r) \quad \text{for } j = (l - \frac{1}{2}). \end{aligned} \quad (1)$$

From eq. (11) of Chapter 52, we have

$$\begin{aligned} (2\pi)^{\frac{3}{2}}\phi_{\vec{k}}(\vec{r}, \vec{\sigma})_{m_s=\pm\frac{1}{2}} \\ = \sum_l \sqrt{4\pi} j_l(kr) \left(\sqrt{(l+1)} \mathcal{Y}_{[l\frac{1}{2}](l+\frac{1}{2}), \pm\frac{1}{2}} \mp \sqrt{l} \mathcal{Y}_{[l\frac{1}{2}](l-\frac{1}{2}), \pm\frac{1}{2}} \right), \end{aligned} \quad (2)$$

and the full solution can be expanded in the same fashion

$$\begin{aligned} (2\pi)^{\frac{3}{2}}\psi_{\vec{k}}^{(+)}(\vec{r}, \vec{\sigma})_{\pm\frac{1}{2}} &= \sqrt{4\pi} \sum_l \left(\frac{u_l^{(a)}(kr)}{kr} \sqrt{(l+1)} \mathcal{Y}_{[l\frac{1}{2}](l+\frac{1}{2}), \pm\frac{1}{2}} \right. \\ &\quad \left. + \frac{u_l^{(b)}(kr)}{kr} (\mp\sqrt{l}) \mathcal{Y}_{[l\frac{1}{2}](l-\frac{1}{2}), \pm\frac{1}{2}} \right), \end{aligned} \quad (3)$$

where the $u_l^{(a)}(kr)$ and $u_l^{(b)}(kr)$ are the one-dimensionalized radial eigenfunctions for the radial equations for $j = (l \pm \frac{1}{2})$, respectively.

$$\left(\frac{\hbar^2}{2\mu} \left(-\frac{d^2}{dr^2} + \frac{l(l+1)}{r^2} \right) + V_0(r) + \frac{1}{2}lV_1(r) \right) u_l^{(a)} = \frac{\hbar^2}{2\mu} k^2 u_l^{(a)},$$

$$\left(\frac{\hbar^2}{2\mu} \left(-\frac{d^2}{dr^2} + \frac{l(l+1)}{r^2} \right) + V_0(r) - \frac{1}{2}(l+1)V_1(r) \right) u_l^{(b)} = \frac{\hbar^2}{2\mu} k^2 u_l^{(b)}. \quad (4)$$

These radial eigenfunctions have the asymptotic form, as $r \rightarrow \infty$,

$$\begin{aligned} u_l^{(a)}(kr) &\longrightarrow a_l \sin(kr - \frac{l\pi}{2} + \delta_l^{(a)}), \\ u_l^{(b)}(kr) &\longrightarrow b_l \sin(kr - \frac{l\pi}{2} + \delta_l^{(b)}), \end{aligned} \quad (5)$$

so, as $r \rightarrow \infty$,

$$\begin{aligned} (2\pi)^{\frac{3}{2}} \psi_k^{(+)}(\vec{r}, \vec{\sigma})_{\pm\frac{1}{2}} &\rightarrow \\ \sqrt{4\pi} \sum_l &\left(\frac{a_l}{2ikr} \left(e^{i(kr - \frac{l\pi}{2} + \delta_l^{(a)})} - e^{-i(kr - \frac{l\pi}{2} + \delta_l^{(a)})} \right) \sqrt{(l+1)} \mathcal{Y}_{[l\frac{1}{2}](l+\frac{1}{2}), \pm\frac{1}{2}} \right. \\ &+ \left. \frac{b_l}{2ikr} \left(e^{i(kr - \frac{l\pi}{2} + \delta_l^{(b)})} - e^{-i(kr - \frac{l\pi}{2} + \delta_l^{(b)})} \right) (\mp\sqrt{l}) \mathcal{Y}_{[l\frac{1}{2}](l-\frac{1}{2}), \pm\frac{1}{2}} \right). \end{aligned} \quad (6)$$

With

$$a_l = e^{i\delta_l^{(a)}}, \quad b_l = e^{i\delta_l^{(b)}}, \quad (7)$$

this function goes to

$$\begin{aligned} (2\pi)^{\frac{3}{2}} \psi_k^{(+)}(\vec{r}, \vec{\sigma})_{m_s=\pm\frac{1}{2}} &\rightarrow \sqrt{4\pi} \sum_l \left[\left(\frac{(e^{2i\delta_l^{(a)}} - 1)}{2ik} \frac{e^{i(kr - \frac{l\pi}{2})}}{r} + \frac{\sin(kr - \frac{l\pi}{2})}{kr} \right) \sqrt{(l+1)} \mathcal{Y}_{[l\frac{1}{2}](l+\frac{1}{2})m_s} \right. \\ &+ \left. \left(\frac{(e^{2i\delta_l^{(b)}} - 1)}{2ik} \frac{e^{i(kr - \frac{l\pi}{2})}}{r} + \frac{\sin(kr - \frac{l\pi}{2})}{kr} \right) (\mp\sqrt{l}) \mathcal{Y}_{[l\frac{1}{2}](l-\frac{1}{2})m_s} \right] \\ &\rightarrow (2\pi)^{\frac{3}{2}} \phi_k^{(+)}(\vec{r}, \vec{\sigma})_{m_s} + \frac{\sqrt{4\pi}}{k} \frac{e^{ikr}}{r} \sum_l \\ &\left[e^{i\delta_l^{(a)}} \sin \delta_l^{(a)} \sqrt{(l+1)} (-i)^l \mathcal{Y}_{[l\frac{1}{2}](l+\frac{1}{2})m_s} \right. \\ &+ \left. e^{i\delta_l^{(b)}} \sin \delta_l^{(b)} (\mp\sqrt{l}) (-i)^l \mathcal{Y}_{[l\frac{1}{2}](l-\frac{1}{2})m_s} \right]. \end{aligned} \quad (8)$$

To compare this function with

$$(2\pi)^{\frac{3}{2}} \psi_k^{(+)}(\vec{r}, \vec{\sigma})_{m_s} \rightarrow (2\pi)^{\frac{3}{2}} \phi_k^{(+)}(\vec{r}, \vec{\sigma})_{m_s} + \frac{e^{ikr}}{r} \sum_{m'_s} \chi(\vec{\sigma})_{\frac{1}{2}m'_s} f(\theta, \phi)_{m'_s m_s}, \quad (9)$$

we need to expand the $\mathcal{Y}_{[l\frac{1}{2}]jm_s}$ through

$$(-i)^l \mathcal{Y}_{[l\frac{1}{2}]jm_s} = \sum_{m'_s} \langle l(m_s - m'_s)_{\frac{1}{2}} m'_s | jm_s \rangle Y_{l(m_s - m'_s)}(\theta, \phi) \chi(\vec{\sigma})_{\frac{1}{2}m'_s}. \quad (10)$$

The combinations of eqs. (8), (9), and (10) then give

$$f(\theta, \phi)_{m'_s m_s = \pm\frac{1}{2}}$$

$$= \frac{\sqrt{4\pi}}{k} \sum_l \left[e^{i\delta_l^{(a)}} \sin \delta_l^{(a)} \sqrt{(l+1)} \langle l(m_s - m'_s) \frac{1}{2} m'_s | (l + \frac{1}{2}) m_s \rangle \right. \\ \left. + e^{i\delta_l^{(b)}} \sin \delta_l^{(b)} (\mp \sqrt{l}) \langle l(m_s - m'_s) \frac{1}{2} m'_s | (l - \frac{1}{2}) m_s \rangle \right] Y_{l(m_s - m'_s)}(\theta, \phi). \quad (11)$$

Using the specific values of the Clebsch–Gordan coefficients, we get

$$f(\theta, \phi)_{\pm \frac{1}{2}, \pm \frac{1}{2}} = f(\theta, \phi)_{-\frac{1}{2}, -\frac{1}{2}} = \\ \frac{1}{k} \sum_l \sqrt{\frac{4\pi}{(2l+1)}} \left((l+1)e^{i\delta_l^{(a)}} \sin \delta_l^{(a)} + le^{i\delta_l^{(b)}} \sin \delta_l^{(b)} \right) Y_{l0}(\theta) = g(\theta), \quad (12)$$

$$f(\theta, \phi)_{\mp \frac{1}{2} \pm \frac{1}{2}} = \frac{\sqrt{4\pi}}{k} \sum_l \sqrt{\frac{l(l+1)}{(2l+1)}} \left(e^{i\delta_l^{(a)}} \sin \delta_l^{(a)} - e^{i\delta_l^{(b)}} \sin \delta_l^{(b)} \right) Y_{l\pm 1}(\theta, \phi) \\ = \mp \bar{h}(\theta) e^{\pm i\phi}. \quad (13)$$

This function is of the form of eq. (24) of Chapter 52 and therefore agrees in form with the result obtained in first Born approximation. Note, however, now the functions, $g(\theta)$ and $\bar{h}(\theta)$, are complex, because the quantities $e^{i\delta_l} \sin \delta_l$ are complex. [In first Born approximation, with $\delta_l = \text{Order}(V/E)$, where $E = \frac{\hbar^2 k^2}{2\mu}$, we have $e^{i\delta_l} \sin \delta_l = (1 + \dots)(\delta_l + \dots) = \text{Order}(E/V)$ (cf., problem 5), so these quantities become real.] It will now be convenient to rename $\bar{h}(\theta) = -ih(\theta)$, so

$$f(\theta, \phi)_{m'_s m_s} = \begin{pmatrix} g(\theta) & -ih(\theta)e^{-i\phi} \\ ih(\theta)e^{i\phi} & g(\theta) \end{pmatrix}. \quad (14)$$

With this notation, we can write the scattering amplitude matrix in terms of the Pauli $\vec{\sigma}$ matrices, if we introduce the unit vector, \vec{n} , normal to the scattering plane defined by the two vectors, \vec{k} and $\vec{k}_f \equiv \vec{k}_s$, the latter in the direction of the scattered beam:

$$\vec{n} = \frac{[\vec{k} \times \vec{k}_s]}{k k_s \sin \theta} = -\sin \phi \vec{e}_x + \cos \phi \vec{e}_y \quad (15)$$

(see Fig. 53.1). We note

$$(\vec{n} \cdot \vec{\sigma}) = -\sin \phi \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} + \cos \phi \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \\ = \begin{pmatrix} 0 & -ie^{-i\phi} \\ ie^{i\phi} & 0 \end{pmatrix}, \quad (16)$$

so the 2×2 scattering amplitude matrix for $s = \frac{1}{2}$ - particles can be written as

$$f(\theta, \phi) = g(\theta) \mathbf{1} + h(\theta) (\vec{n} \cdot \vec{\sigma}), \quad (17)$$

where $\mathbf{1}$ is the 2×2 unit matrix.

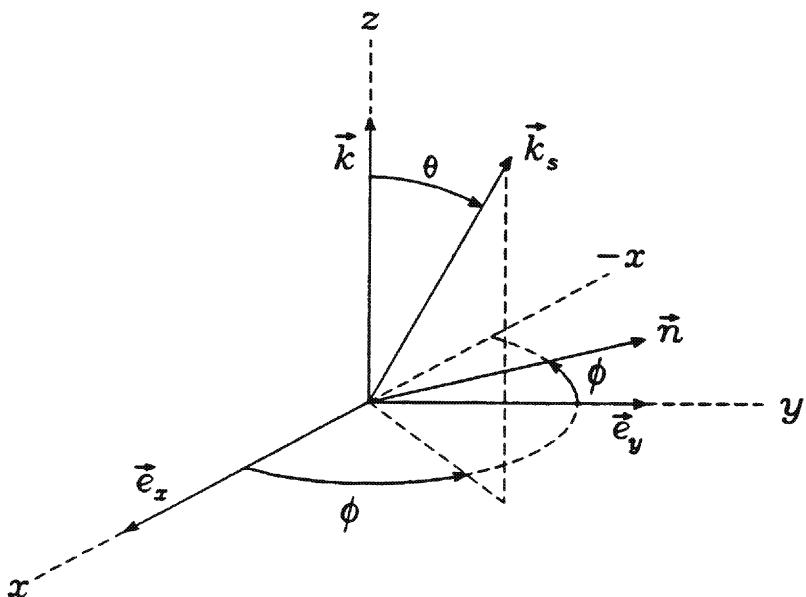


FIGURE 53.1.

The Polarization Vector

So far, we have calculated differential cross sections only for incident particles with a definite longitudinal polarization given by the single quantum state, $|m_{s_i}\rangle$, and being scattered into the state of definite longitudinal polarization, $|m_{s_f}\rangle$. We want to be able to calculate differential cross sections for beams of arbitrary initial polarization, and for such beams, we want to be able to calculate the polarization of the scattered beam. For this purpose, it will be useful to define first the polarization vector, \vec{P} , for a beam of particles. The polarization vector for a beam of particles with spin, s , is defined by

$$\vec{P} = \frac{1}{s} \left(\langle \vec{s} \cdot \vec{e}_x \rangle \vec{e}_x + \langle \vec{s} \cdot \vec{e}_y \rangle \vec{e}_y + \langle \vec{s} \cdot \vec{e}_z \rangle \vec{e}_z \right), \quad (1)$$

where the expectation values of $\vec{s} \cdot \vec{e}_i$ are given by, e.g.,

$$\langle \vec{s} \cdot \vec{e}_x \rangle \equiv \langle \chi_s | s_x | \chi_s \rangle, \quad (2)$$

where an arbitrary spin state can be expanded in terms of basis states $|m_s\rangle$ of definite longitudinal polarization,

$$|\chi_s\rangle = \sum_{m_s} |m_s\rangle \langle m_s| \chi_s \rangle = \sum_{m_s} |m_s\rangle c_{m_s}, \quad (3)$$

so

$$\langle s_x \rangle = \sum_{m'_s, m''_s} \langle \chi_s | m''_s \rangle \langle m''_s | s_x | m'_s \rangle \langle m'_s | \chi_s \rangle = \sum_{m'_s, m''_s} c_{m''_s}^* \langle m''_s | s_x | m'_s \rangle c_{m'_s}. \quad (4)$$

Note, in particular, if $|\chi_s\rangle = |m_s = +s\rangle$, then $\vec{P} = P_z \vec{e}_z$, with $P_z = 1$. For the special case of spin $s = \frac{1}{2}$ -particles, remembering $\vec{s} = \frac{1}{2}\vec{\sigma}$, we have

$$\vec{P} = \langle\sigma_x\rangle\vec{e}_x + \langle\sigma_y\rangle\vec{e}_y + \langle\sigma_z\rangle\vec{e}_z = P_x\vec{e}_x + P_y\vec{e}_y + P_z\vec{e}_z. \quad (5)$$

Recall a spin vector with perpendicular polarization in the x direction was given by

$$|\chi_s^{(\perp)}\rangle = \frac{1}{\sqrt{2}}|+\frac{1}{2}\rangle + \frac{1}{\sqrt{2}}|-\frac{1}{2}\rangle. \quad (6)$$

For this state,

$$\langle\sigma_x\rangle = \frac{1}{\sqrt{2}}\left(\langle+\frac{1}{2}|\sigma_x|-\frac{1}{2}\rangle + \langle-\frac{1}{2}|\sigma_x|+\frac{1}{2}\rangle\right)\frac{1}{\sqrt{2}} = \frac{1}{2}(1+1) = 1, \quad (7)$$

and $\langle\sigma_y\rangle = 0$ and $\langle\sigma_z\rangle = 0$ for this spin state. Therefore, $\vec{P} = P_x\vec{e}_x$, with $P_x = 1$ for this state. Similarly, for the spin state,

$$|\chi_s\rangle = \frac{1}{\sqrt{2}}|+\frac{1}{2}\rangle + \frac{i}{\sqrt{2}}|-\frac{1}{2}\rangle, \quad (8)$$

we have

$$\langle\sigma_y\rangle = \frac{i}{2}\langle+\frac{1}{2}|\sigma_y|-\frac{1}{2}\rangle - \frac{i}{2}\langle-\frac{1}{2}|\sigma_y|+\frac{1}{2}\rangle = 1, \quad (9)$$

whereas, now, $\langle\sigma_x\rangle = 0$, and $\langle\sigma_z\rangle = 0$, so this is a state of perpendicular polarization, with $P_y = 1$.

A Polarization of the Scattered Beam

To calculate the polarization for a scattered beam, we expand the spin vector for the scattered beam in terms of the longitudinally polarized states $|m'_s\rangle$

$$|\chi_s^{\text{scatt.}}\rangle = \sum_{m'_s} |m'_s\rangle \langle m'_s| \chi_s^{\text{scatt.}}. \quad (10)$$

Let us assume for the moment the incident beam is longitudinally polarized, with

$$\langle m_s | \chi_s^{\text{inc.}} \rangle = 1, \quad \text{for either } m_s = +\frac{1}{2} \text{ or } m_s = -\frac{1}{2}. \quad (11)$$

Then, we can take

$$\langle m'_s | \chi_s^{\text{scatt.}} \rangle = \left(f(\theta, \phi) \right)_{m'_s, m_s} \frac{1}{\sqrt{N(\theta, \phi)}}, \quad (12)$$

where $N(\theta, \phi)$ is the total number of particles scattered into the detector of cross-sectional area $r^2 d\Omega$ normal to the scattering direction, θ, ϕ , so

$$N(\theta, \phi) = \sum_{m'_s} |(f(\theta, \phi))_{m'_s, m_s}|^2. \quad (13)$$

Then,

$$\vec{P}^{\text{scatt.}} = \frac{1}{N(\theta, \phi)} \sum_{\alpha} \sum_{m'_s, m''_s} \vec{e}_{\alpha} \langle \chi_s^{\text{scatt.}} | m''_s \rangle \langle m''_s | \sigma_{\alpha} | m'_s \rangle \langle m'_s | \chi_s^{\text{scatt.}} \rangle$$

$$\begin{aligned}
&= \frac{1}{N(\theta, \phi)} \sum_{\alpha} \sum_{m_s', m_s''} \vec{e}_{\alpha} (f(\theta, \phi))_{m_s', m_s}^* (\sigma_{\alpha})_{m_s'' m_s'} (f(\theta, \phi))_{m_s', m_s} \\
&= \frac{1}{N(\theta, \phi)} \sum_{\alpha} \sum_{m_s' m_s''} \vec{e}_{\alpha} (f^\dagger)_{m_s m_s''} (\sigma_{\alpha})_{m_s'' m_s'} (f)_{m_s', m_s} \\
&= \frac{1}{N(\theta, \phi)} \sum_{\alpha} \vec{e}_{\alpha} (f^\dagger \sigma_{\alpha} f)_{m_s, m_s}.
\end{aligned} \tag{14}$$

We could also write $N(\theta, \phi)$ by utilizing the matrix form employed in the last line of this equation.

$$N(\theta, \phi) = \sum_{m_s'} (f(\theta, \phi))_{m_s', m_s}^* (f(\theta, \phi))_{m_s', m_s} = (f^\dagger f)_{m_s, m_s}. \tag{15}$$

We shall be most interested in the following question: If the incident beam is completely unpolarized, what is the polarization of the scattered beam? For an unpolarized incident beam, an equal probability of $\frac{1}{2}$ exists that the incident longitudinal polarization be $m_s = +\frac{1}{2}$ or $m_s = -\frac{1}{2}$. Thus,

$$\vec{P}^{\text{scatt.}} = \frac{1}{N(\theta, \phi)} \frac{1}{2} \sum_{\alpha} \vec{e}_{\alpha} \sum_{m_s} (f^\dagger \sigma_{\alpha} f)_{m_s, m_s} = \frac{1}{N(\theta, \phi)} \frac{1}{2} \sum_{\alpha} \vec{e}_{\alpha} \text{trace}(f^\dagger \sigma_{\alpha} f), \tag{16}$$

where, now,

$$N(\theta, \phi) = \frac{1}{2} \sum_{m_s} (f^\dagger f)_{m_s, m_s} = \frac{1}{2} \text{trace}(f^\dagger f). \tag{17}$$

To take the necessary taces, we now use the trivial identity

$$\text{trace}(M_1 M_2 M_3) = \text{trace}(M_2 M_3 M_1) = \text{trace}(M_3 M_1 M_2), \tag{18}$$

and the properties of the Pauli σ matrices

$$\sigma_j \sigma_k = i \epsilon_{jkl} \sigma_l + \delta_{jk} \mathbf{1}, \tag{19}$$

or

$$\sigma_x \sigma_y = i \sigma_z \quad \text{and cyclically,} \quad (\sigma_x)^2 = (\sigma_y)^2 = (\sigma_z)^2 = \mathbf{1}. \tag{20}$$

Also,

$$\text{trace}(\sigma_x) = \text{trace}(\sigma_y) = \text{trace}(\sigma_z) = 0; \quad \text{trace}(\mathbf{1}) = 2. \tag{21}$$

Also, recall

$$\begin{aligned}
f(\theta, \phi) &= g(\theta) \mathbf{1} + h(\theta) (\vec{n} \cdot \vec{\sigma}) = g(\theta) \mathbf{1} + h(\theta) \sigma_{y'}, \\
\text{with } \sigma_{y'} &= -\sin \phi \sigma_x + \cos \phi \sigma_y.
\end{aligned} \tag{22}$$

Thus,

$$\begin{aligned}
\frac{1}{2} \text{trace}(f^\dagger \sigma_{\alpha} f) &= \frac{1}{2} \text{trace}(\sigma_{\alpha} f f^\dagger) \\
&= \frac{1}{2} \text{trace}(\sigma_{\alpha} (g(\theta) \mathbf{1} + h(\theta) \sigma_{y'})(g(\theta)^* \mathbf{1} + h(\theta)^* \sigma_{y'})) \\
&= \frac{1}{2} \text{trace}(\sigma_{\alpha} (|g(\theta)|^2 + |h(\theta)|^2) + (\sigma_{\alpha} \sigma_{y'})(g(\theta) h^*(\theta) + g^*(\theta) h(\theta)))
\end{aligned}$$

$$\begin{aligned}
&= \frac{1}{2} \left(0 + 2\delta_{\alpha,y'}(g(\theta)h^*(\theta) + g^*(\theta)h(\theta)) \right) \\
&= \delta_{\alpha,y'}(g(\theta)h^*(\theta) + g^*(\theta)h(\theta)) = \delta_{\alpha,y'} 2\text{Real}(g(\theta)h^*(\theta)).
\end{aligned} \tag{23}$$

Also,

$$\begin{aligned}
N(\theta, \phi) &= \frac{1}{2} \left(\text{trace}(\mathbf{1})(|g(\theta)|^2 + |h(\theta)|^2) + \text{trace}(\sigma_{y'})(g(\theta)h^*(\theta) + g(\theta)^*h(\theta)) \right) \\
&= (|g(\theta)|^2 + |h(\theta)|^2).
\end{aligned} \tag{24}$$

Putting these together, we have the polarization vector for the scattered beam,

$$\vec{P}^{\text{scatt.}} = \vec{e}_y \frac{2\text{Real}(g(\theta)h^*(\theta))}{(|g(\theta)|^2 + |h(\theta)|^2)} = \vec{n} \frac{2\text{Real}(g(\theta)h^*(\theta))}{(|g(\theta)|^2 + |h(\theta)|^2)}. \tag{25}$$

The polarization of this scattered beam has only a component perpendicular to the scattering plane. This fact can be understood in terms of a semiclassical picture. The orbital angular-momentum vector, \vec{l} , is normal to the scattering plane. Thus, if the \vec{s} vector lies in the scattering plane, either in the z or x direction, the $\vec{l} \cdot \vec{s}$ term of the interaction would be zero. Only the y component of \vec{s} , normal to the scattering plane, is affected by the $\vec{l} \cdot \vec{s}$ interaction. Before seeing how we would detect the polarization of this scattered beam, perhaps in a double-scattering experimental setup, let us introduce the density matrix for a beam of particles with spin.

Density Matrices

In the last chapter, we considered an incident beam completely unpolarized. Now, let us consider an incident beam of definite polarization, either a pure beam, perfectly polarized along some specific direction, z' , or an incident beam with a statistical distribution of spin orientations giving the beam a partial polarization. For this purpose, it will be useful to introduce the so-called density matrix for the spin orientation of the beam. Recall, for an incident particle with definite spin orientation given by

$$|\chi_s^{\text{inc.}}\rangle = \sum_{m_s} |m_s\rangle c_{m_s} \quad (1)$$

the incident polarization vector, with components, P_α , is given by

$$P_\alpha = \langle \sigma_\alpha \rangle = \sum_{m_s, m'_s} c_{m'_s}^* \langle m'_s | \sigma_\alpha | m_s \rangle c_{m_s} = \sum_{m_s, m'_s} (\sigma_\alpha)_{m'_s m_s} c_{m_s} c_{m'_s}^*. \quad (2)$$

We define the density matrix

$$\rho_{m_s, m'_s} = c_{m_s} c_{m'_s}^*, \quad (3)$$

so

$$\langle \sigma_\alpha \rangle = \sum_{m_s, m'_s} (\sigma_\alpha)_{m'_s m_s} \rho_{m_s, m'_s} = \text{trace}(\sigma_\alpha \rho), \quad (4)$$

and

$$\vec{P} = \sum_\alpha \vec{e}_\alpha \text{trace}(\sigma_\alpha \rho). \quad (5)$$

For a single spin- $\frac{1}{2}$ -particle in a pure spin state, that is, a state with a definite m'_s along a specific z' direction, with $c_{+\frac{1}{2}} = \alpha$, $c_{-\frac{1}{2}} = \beta$, we would have

$$\rho = \begin{pmatrix} \alpha\alpha^* & \alpha\beta^* \\ \beta\alpha^* & \beta\beta^* \end{pmatrix}. \quad (6)$$

For such a pure state, the trace of the density matrix is unity, and the determinant of the density matrix is zero:

$$\text{trace } \rho = |\alpha|^2 + |\beta|^2 = 1 \quad \text{and } \det \rho = 0. \quad (7)$$

Specific examples would be: (1) a beam with longitudinal polarization with pure $m_s = +\frac{1}{2}$, i.e., with $\alpha = 1, \beta = 0$,

$$\rho = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}; \quad (8)$$

(2) a beam with perpendicular polarization in the x direction, with $\alpha = \beta = \frac{1}{\sqrt{2}}$,

$$\rho = \begin{pmatrix} \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} \end{pmatrix}; \quad (9)$$

(3) a beam with perpendicular polarization in the y direction, with $\alpha = \frac{1}{\sqrt{2}}$, $\beta = \frac{i}{\sqrt{2}}$,

$$\rho = \begin{pmatrix} \frac{1}{2} & -\frac{i}{2} \\ \frac{i}{2} & \frac{1}{2} \end{pmatrix}. \quad (10)$$

In terms of such density matrices, the polarization of the incident beam can be given by

$$\vec{P} = \sum_{\alpha} \vec{e}_{\alpha} \sum_{m_s, m'_s} (\sigma_{\alpha})_{m'_s m_s} \rho_{m_s m'_s} = \sum_{\alpha} \vec{e}_{\alpha} \text{trace}(\sigma_{\alpha} \rho). \quad (11)$$

The differential scattering cross section can be given by

$$\begin{aligned} \frac{d\sigma}{d\Omega} &= \sum_{m_s, m'_s, m''_s} f^*(\theta, \phi)_{m'_s m''_s} c_{m''_s}^* f(\theta, \phi)_{m'_s m_s} c_{m_s} \\ &= \sum_{m_s, m'_s, m''_s} f_{m''_s m'_s}^{\dagger} f_{m'_s m_s} \rho_{m_s m''_s} = \text{trace}(f^{\dagger} f \rho), \end{aligned} \quad (12)$$

and, finally, the polarization of the scattered beam is given by

$$\vec{P}_{\text{scatt.}} = \frac{1}{\text{trace}(f^{\dagger} f \rho)} \sum_{\alpha} \vec{e}_{\alpha} \text{trace}(f^{\dagger} \sigma_{\alpha} f \rho). \quad (13)$$

All physically interesting quantities are given in terms of traces involving the density matrix of the incident beam. For spin $\frac{1}{2}$ -particles, the taking of these traces is particularly simple. The great advantage of the density matrix formalism, however, is that it applies not only for incident beams of pure spin orientation, for which every particle has exactly the same spin state, but also for a statistical distribution of initial spin states, the usual experimental situation. Suppose the n^{th} incident

particle is in a spin state given by the $c_{m_s}^{(n)} = c_{+\frac{1}{2}}^{(n)}, c_{-\frac{1}{2}}^{(n)}$, and the probability for this spin orientation is given by w_n . Suppose there are a large number of incident particles, given by N . Then

$$\sum_{n=1}^N w_n = 1, \quad (14)$$

and the density matrix for this statistical distribution of spin states is given by

$$(\rho)_{m_s m'_s} = \sum_n w_n c_{m_s}^{(n)} c_{m'_s}^{(n)*}, \quad (15)$$

and with

$$c_{+\frac{1}{2}}^{(n)} = \alpha^{(n)}, \quad c_{-\frac{1}{2}}^{(n)} = \beta^{(n)}, \quad (16)$$

$$\rho = \begin{pmatrix} \sum_n w_n \alpha^{(n)} \alpha^{(n)*} & \sum_n w_n \alpha^{(n)} \beta^{(n)*} \\ \sum_n w_n \beta^{(n)} \alpha^{(n)*} & \sum_n w_n \beta^{(n)} \beta^{(n)*} \end{pmatrix}. \quad (17)$$

The trace of this matrix is still unity, since $|\alpha^{(n)}|^2 + |\beta^{(n)}|^2 = 1$, and $\sum_n w_n = 1$. But, now, the determinant of ρ is no longer equal to zero. Because the hermitian 2×2 matrix ρ for $s = \frac{1}{2}$ -particles is specified by four independent parameters, ρ can be given in terms of the 2×2 unit matrix and the three Pauli σ -matrices, by

$$\rho = A\mathbf{1} + B\sigma_x + C\sigma_y + D\sigma_z. \quad (18)$$

From $\text{trace}(\rho) = 2A$, $\text{trace}(\sigma_x \rho) = P_x = 2B$, and so on, we have

$$\rho = \frac{1}{2}(\mathbf{1} + \vec{P} \cdot \vec{\sigma}). \quad (19)$$

For example, with $P_z = \frac{1}{2}$, $P_x = 0$, $P_y = 0$,

$$\rho = \begin{pmatrix} \frac{3}{4} & 0 \\ 0 & \frac{1}{4} \end{pmatrix}, \quad (20)$$

whereas, with $P_x = \frac{1}{2}$, $P_y = 0$, $P_z = 0$

$$\rho = \begin{pmatrix} \frac{1}{2} & \frac{1}{4} \\ \frac{1}{4} & \frac{1}{2} \end{pmatrix}, \quad (21)$$

and an unpolarized beam has

$$\rho = \begin{pmatrix} \frac{1}{2} & 0 \\ 0 & \frac{1}{2} \end{pmatrix}. \quad (22)$$

In the last chapter, we saw such an unpolarized incident beam can lead to a polarized scattered beam, where the polarization vector has only a component perpendicular to the scattering plane formed by \vec{k} and \vec{k}_s . One way to detect this polarization of the scattered beam is through a double scattering experiment.

A Detection of Polarization via Double Scattering

If the incident beam is unpolarized, no preferred direction exists in the x - y plane normal to the incident \vec{k} vector, and we can place \vec{k}_s in the x - z plane, at a position with $\phi = 0$, without loss of generality. We saw the scattered beam then has a polarization vector, with

$$\vec{P} = \vec{e}_y \frac{\text{Real}(g(\theta_1)h(\theta_1)^*)}{(|g(\theta_1)|^2 + |h(\theta_1)|^2)}. \quad (23)$$

This polarization can be detected by scattering the scattered spin $s = \frac{1}{2}$ -particles from a second $s = 0$ target particle of the same kind as the first $s = 0$ particle, in particular, by comparing the differential scattering cross sections in two detectors, placed at angles θ_2 in the x - z plane, symmetrically to the left and right of the direction of the \vec{k}_s vector of the first scattering process. (See Fig. 55.1.) The “left” detector is placed at the angular position, $\theta_2, \phi_2 = 0$, and the “right” detector is placed at the angular position, $\theta_2, \phi_2 = \pi$. Thus, with $\vec{n}_2 = -\sin \phi_2 \vec{e}_x + \cos \phi_2 \vec{e}_y$, we have $\vec{n}_2 = \pm \vec{e}_y$ for the left (upper sign) and right (lower sign) detectors. Hence,

$$f(\theta_2, \phi_2) = g(\theta_2)\mathbf{1} \pm \sigma_y h(\theta_2), \quad (24)$$

where the upper (lower) signs refer to left (right) detector, respectively. Now, using $\frac{d\sigma}{d\Omega} = \text{trace}(f^\dagger f \rho)$, we get

$$\begin{aligned} \frac{d\sigma}{d\Omega} &= \text{trace}\left((g^*(\theta_2)\mathbf{1} \pm h^*(\theta_2)\sigma_y)(g(\theta_2)\mathbf{1} \pm h(\theta_2)\sigma_y)\left(\frac{1}{2}(\mathbf{1} + P_y(\theta_1)\sigma_y)\right)\right) \\ &= \frac{1}{2}\text{trace}\left(\left[|g(\theta_2)|^2 + |h(\theta_2)|^2\right]\mathbf{1} \pm (g(\theta_2)h^*(\theta_2) + g^*(\theta_2)h(\theta_2))\sigma_y\right] \\ &\quad \times (\mathbf{1} + P_y(\theta_1)\sigma_y) \\ &= \frac{1}{2}\text{trace}\left(\mathbf{1}\left[|g(\theta_2)|^2 + |h(\theta_2)|^2\right] \pm 2\text{Real}(g(\theta_2)h^*(\theta_2))P_y(\theta_1)\right. \\ &\quad \left.+ \sigma_y[\dots]\right) \\ &= (|g(\theta_2)|^2 + |h(\theta_2)|^2) \pm P_y(\theta_1)2\text{Real}(g(\theta_2)h^*(\theta_2)), \end{aligned} \quad (25)$$

where the upper (lower) signs refer to left (right) detectors and we have again used: $\text{trace}(\sigma_y) = 0$; $\text{trace}(\mathbf{1}) = 2$. Using eq. (23) for $P_y(\theta_1)$, we can then get the left-right asymmetry parameter

$$\frac{d\sigma_L - d\sigma_R}{d\sigma_L + d\sigma_R} = \frac{2\text{Real}(g(\theta_1)h^*(\theta_1))}{(|g(\theta_1)|^2 + |h(\theta_1)|^2)} \times \frac{2\text{Real}(g(\theta_2)h^*(\theta_2))}{(|g(\theta_2)|^2 + |h(\theta_2)|^2)}. \quad (26)$$

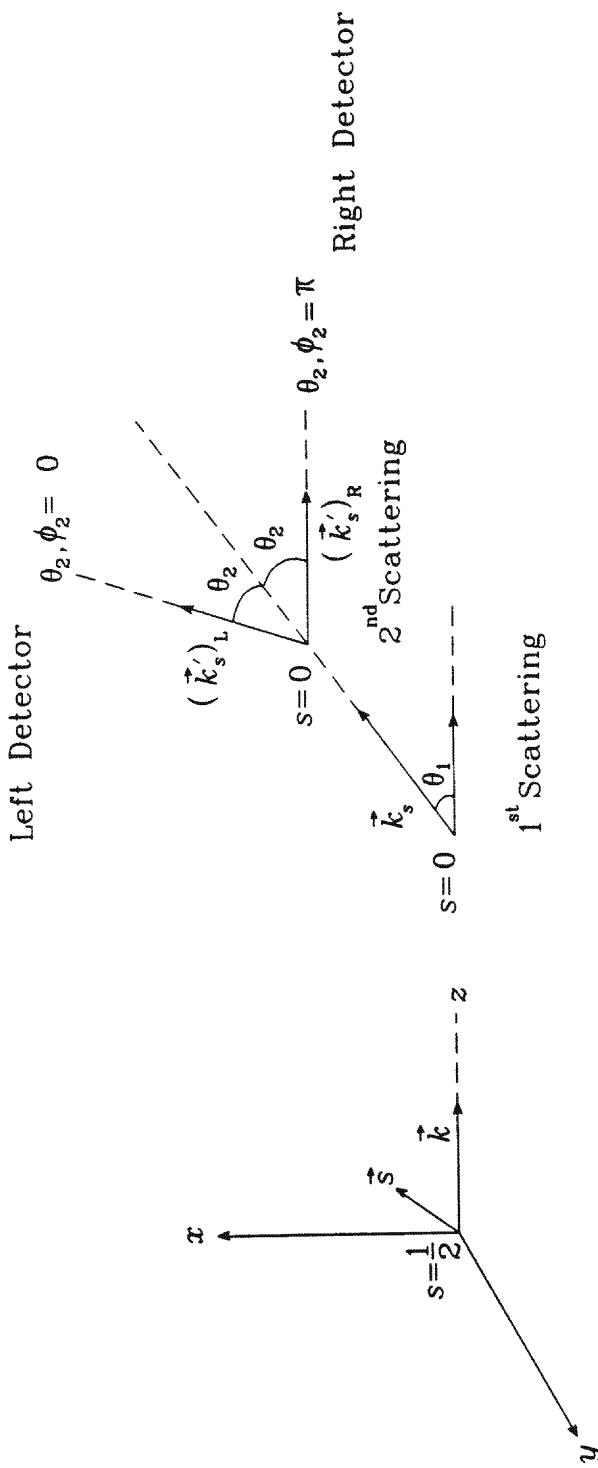


FIGURE 55.1. Double scattering of an $s = \frac{1}{2}$ particle from identical $s = 0$ target particles.

B Differential Scattering Cross Section of a Beam with Arbitrary Incident Polarization

As a final exercise, let us calculate the differential cross section for an incident beam of arbitrary polarization, \vec{P} . Because the initial polarization vector will define the directions of the x and y axes, we want to place our detector at an arbitrary azimuth angle, ϕ , relative to the x - z plane. Now, the normal to the scattering plane defined by \vec{k} and \vec{k}_s is given by $\vec{n} = -\sin \phi \vec{e}_x + \cos \phi \vec{e}_y$, and

$$(\vec{n} \cdot \vec{\sigma}) = -\sin \phi \sigma_x + \cos \phi \sigma_y = \sigma_y. \quad (27)$$

With $\rho = \frac{1}{2}(\mathbf{1} + \sum_{\alpha} \sigma_{\alpha} P_{\alpha})$, we now get

$$\begin{aligned} \frac{d\sigma}{d\Omega} &= \text{trace}(f^* f \rho) \\ &= \text{trace}\left((g^*(\theta)\mathbf{1} + h^*(\theta)\sigma_y)(g(\theta)\mathbf{1} + h(\theta)\sigma_y)\frac{1}{2}(\mathbf{1} + \sum_{\alpha} P_{\alpha}\sigma_{\alpha})\right) \\ &= \frac{1}{2}\text{trace}\left(\left[|g(\theta)|^2 + |h(\theta)|^2\right]\mathbf{1} + 2\text{Real}(g(\theta)h^*(\theta)) \right. \\ &\quad \times \left.(-\sin \phi \sigma_x + \cos \phi \sigma_y)\right](\mathbf{1} + \sum_{\alpha} \sigma_{\alpha} P_{\alpha}) \\ &= \left[|g(\theta)|^2 + |h(\theta)|^2 + 2\text{Real}(g(\theta)h^*(\theta))(-\sin \phi P_x + \cos \phi P_y)\right]. \end{aligned} \quad (28)$$

A ϕ -dependence in the differential cross section exists if either P_x or $P_y \neq 0$ in the incident beam.

C Generalizations to More Complicated Cases

Scattering of Spin $s = 1$ Projectile from $s = 0$ Target Particles

For the scattering of a $s = 1$ projectile from a $s = 0$ target particle, we shall need 3×3 scattering amplitude matrices and 3×3 density matrices. The most general density matrix will require nine parameters. The density matrix ρ can now be given in terms of the 3×3 unit matrix, the three components of S_{α} , and the five components of the spherical tensors of spherical rank 2, $[S^1 \times S^1]_M^2$, with $M = +2, +1, 0, -1, -2$,

$$\rho = \frac{1}{3}\mathbf{1} + \frac{1}{2}(P_x S_x + P_y S_y + P_z S_z) + \sum_M (-1)^M \mathcal{P}_M^2 [S^1 \times S^1]_{-M}^2, \quad (29)$$

where P_x, P_y, P_z are the three components of the polarization vector defined in Chapter 54, and the \mathcal{P}_M^2 are the five components of the tensor polarization. The incident beam may have both vector and tensor polarizations, or may have vector polarizations only with zero tensor polarizations. The 3×3 matrices for S_x, S_y, S_z

are well known (see Chapter 8)

$$S_x = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \quad S_y = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix}, \quad S_z = \begin{pmatrix} +1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}.$$

The matrix algebra is somewhat more complicated, but the process of trace-taking is very similar to that of the simpler case of $s = \frac{1}{2}$ particles.

Scattering of Spin $s = \frac{1}{2}$ Projectile from $s = \frac{1}{2}$ Target Particles

Now, the density matrix can be given by the $c_{m_{s,1}}$ of projectile and $c_{m_{s,2}}$ of target, with

$$|\chi_s^{\text{proj.}}\rangle = \sum_{m_{s,1}} |m_{s,1}\rangle c_{m_{s,1}}^{\text{proj.}}, \quad (30)$$

$$|\chi_s^{\text{targ.}}\rangle = \sum_{m_{s,2}} |m_{s,2}\rangle c_{m_{s,2}}^{\text{targ.}}. \quad (31)$$

The density matrix is a 4×4 hermitian matrix, with

$$\rho_{\mu\mu'} = c_{m_{s,1}}^{\text{proj.}} c_{m_{s,2}}^{\text{targ.}} c_{m'_{s,1}}^{\text{proj.*}} c_{m'_{s,2}}^{\text{targ.*}}, \quad (32)$$

where the row and column indices $\mu = m_{s,1} m_{s,2}$ and $\mu' = m'_{s,1} m'_{s,2}$ now have four possible values, viz., $+\frac{1}{2}, +\frac{1}{2}; -\frac{1}{2}, +\frac{1}{2}; +\frac{1}{2}, -\frac{1}{2}; -\frac{1}{2}, -\frac{1}{2}$. The most general density matrix now requires 16 parameters. It could be written as

$$\rho = \frac{1}{2} (A \mathbf{1} + \vec{P}_1 \cdot \vec{\sigma}_1 + \vec{P}_2 \cdot \vec{\sigma}_2 + A' (\vec{\sigma}_1 \cdot \vec{\sigma}_2) + \vec{B} \cdot [\vec{\sigma}_1 \times \vec{\sigma}_2] + \sum_M (-1)^M C_M^2 [\vec{\sigma}_1 \times \vec{\sigma}_2]_M^2), \quad (33)$$

with $(1 + 3 + 3 + 1 + 3 + 5) = 16$ components. In actual practice, of course, the projectile may be given a vector polarization, \vec{P}_1 , and the target may be given a vector polarization, \vec{P}_2 . The additional combined scalar, vector, and tensor polarizations may be difficult to realize experimentally, but the additional coefficients A , A' , \vec{B} , and C_M^2 are needed for the analysis, which again involves trace-taking and the algebra of the two sets of Pauli σ matrices.

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Isospin

The simplicity of the algebra for the case of $s = \frac{1}{2}$ -particles, involving the algebra of the Pauli σ matrices, makes this chapter a good place to introduce a brief remark about isospin.

For proton–proton, proton–neutron, or neutron–neutron scattering, the essential charge independence of the nuclear force must be taken into account. (This charge independence of the nucleon–nucleon interaction does not include the Coulomb term in the proton–proton interaction. This is a relatively small part, however, of the full proton–proton interaction at energies high enough that the protons are far above the proton–proton Coulomb barrier for $r \approx 1\text{ fermi}$.) It is useful to introduce the isospin formalism and consider the neutron and proton as the two possible charge states of a nucleon. Being a spin $s = \frac{1}{2}$ particle, the nucleon is a fermion. Besides the internal degree of freedom associated with the spin of the nucleon, another internal degree of freedom is associated with the charge of the nucleon. Thus, the wave function associated with the internal degrees of freedom of our point nucleon must include besides the spin function, $\chi(\vec{\sigma})_{m_s}$, with two quantum states, $m_s = +\frac{1}{2}$ and $m_s = -\frac{1}{2}$, a similar charge function, also with two quantum states. Even though nothing is “spinning” in this charge space, we can use the mathematics of a system with two internal quantum states to make a one-to-one parallel between the two-spin state system and the two-charge state system. We therefore can name the neutron as the state of the system with a new spin, the “isospin,” with a new quantum number with value $+\frac{1}{2}$, whereas the proton is the state of the system for which the new quantum number has the value $-\frac{1}{2}$. We introduce the isospin vector operator \vec{i} in analogy with \vec{s} . Just as it is useful to

introduce $\vec{\sigma}$ via $\vec{s} = \frac{1}{2}\vec{\sigma}$, we now let $\vec{i} = \frac{1}{2}\vec{\tau}$, where

$$\begin{aligned} i_z |\text{neutron}\rangle &= \frac{1}{2}\tau_z |\text{neutron}\rangle = +\frac{1}{2}|\text{neutron}\rangle = +\frac{1}{2}|m_i = +\frac{1}{2}\rangle \\ i_z |\text{proton}\rangle &= \frac{1}{2}\tau_z |\text{proton}\rangle = -\frac{1}{2}|\text{proton}\rangle = -\frac{1}{2}|m_i = -\frac{1}{2}\rangle. \end{aligned} \quad (1)$$

(Note: It is of course quite arbitrary as to whether a neutron or proton is designated as the $m_i = +\frac{1}{2}$ particle. This is illustrated by the fact that nuclear physicists and particle physicists do not agree on this choice. The above is the nuclear convention. Particle physicists name the proton the $m_i = +\frac{1}{2}$ particle.) In analogy with the operators, $\vec{\sigma}$, we can introduce the operators $\vec{\tau}$, with

$$\tau_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \tau_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \tau_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \quad (2)$$

Now, just as the operator $s_+ = \frac{1}{2}(\sigma_x + i\sigma_y)$, when acting on a state with $m_s = -\frac{1}{2}$ converts it to a state with $m_s = +\frac{1}{2}$, so the operator $i_+ = \frac{1}{2}(\tau_x + i\tau_y)$, when acting on a proton state with $m_i = -\frac{1}{2}$ converts it to a neutron state with $m_i = +\frac{1}{2}$. This operator is needed in the theory of beta-decay, where a proton may be converted to a neutron.

Just as we found it convenient to write spin functions in terms of internal variables, $\vec{\xi} \equiv \vec{\sigma}$, namely, $\chi(\vec{\sigma})_{m_s}$, we will now write the internal charge functions in terms of the internal variable designated by $\vec{\tau}$, namely, $\bar{\chi}(\vec{\tau})_{m_i}$. This will be particularly useful for a discussion of the symmetry of two-particle functions. For the two-particle spin functions, it was convenient to make a transformation from the two-particle functions in the $m_{s,1}m_{s,2}$ representation to the SM_S representation, via

$$\chi(\vec{\sigma}_1)_{m_{s,1}}\chi(\vec{\sigma}_2)_{m_{s,2}} = \sum_S \langle \frac{1}{2}m_{s,1}\frac{1}{2}m_{s,2}|SM_S\rangle \chi(\vec{\sigma}_1, \vec{\sigma}_2)_{SM_S}, \quad (3)$$

where the three functions with $S = 1, M_S = +1, 0, -1$ are symmetric under the interchange of indices 1 and 2 of the two fermions, whereas the single function with $S = 0$ and $M_S = 0$ is antisymmetric (changes sign) under interchange of the indices 1 and 2. In the same fashion, the charge function for two neutrons, for two protons, and one linear combination of the neutron-proton function are symmetric under the interchange of the indices 1 and 2 of the two-particle charge functions, and can be considered members of a triplet with two-particle quantum numbers, $I = 1$, with $M_I = +1, -1, 0$, where $\vec{I} = \vec{i}_1 + \vec{i}_2$ [in analogy with $\vec{S} = \vec{s}_1 + \vec{s}_2$, with the same vector-coupling (or Clebsch-Gordan coefficients) in isospin space as in ordinary spin space.] Thus,

$$\begin{aligned} \bar{\chi}(\vec{\tau}_1)_{+\frac{1}{2}}\bar{\chi}(\vec{\tau}_2)_{+\frac{1}{2}} &= \bar{\chi}(\vec{\tau}_1, \vec{\tau}_2)_{I=1, M_I=+1}, \\ \bar{\chi}(\vec{\tau}_1)_{-\frac{1}{2}}\bar{\chi}(\vec{\tau}_2)_{-\frac{1}{2}} &= \bar{\chi}(\vec{\tau}_1, \vec{\tau}_2)_{I=1, M_I=-1}, \\ \frac{1}{\sqrt{2}} \left(\bar{\chi}(\vec{\tau}_1)_{+\frac{1}{2}}\bar{\chi}(\vec{\tau}_2)_{-\frac{1}{2}} + \bar{\chi}(\vec{\tau}_1)_{-\frac{1}{2}}\bar{\chi}(\vec{\tau}_2)_{+\frac{1}{2}} \right) &= \bar{\chi}(\vec{\tau}_1, \vec{\tau}_2)_{I=1, M_I=0}, \end{aligned} \quad (4)$$

and

$$\frac{1}{\sqrt{2}} \left(\bar{\chi}(\vec{\tau}_1)_{+\frac{1}{2}} \bar{\chi}(\vec{\tau}_2)_{-\frac{1}{2}} - \bar{\chi}(\vec{\tau}_1)_{-\frac{1}{2}} \bar{\chi}(\vec{\tau}_2)_{+\frac{1}{2}} \right) = \bar{\chi}(\vec{\tau}_1, \vec{\tau}_2)_{I=0, M_I=0}. \quad (5)$$

For nucleon–nucleon scattering, therefore, the total two-particle function can be considered a product of a relative motion orbital function, a two-particle spin function, and a two-particle charge function

$$\psi_{\text{total}} = \psi_{\text{orbital}}(\vec{r}_1 - \vec{r}_2) \chi(\vec{\sigma}_1, \vec{\sigma}_2)_{S, M_S} \bar{\chi}(\vec{\tau}_1, \vec{\tau}_2)_{I, M_I}. \quad (6)$$

Because the $s = \frac{1}{2}$ nucleons are fermions, this total wave function must be antisymmetric under interchange of particle indices. In a partial wave decomposition where the orbital functions with even l do not change sign under the $\vec{r}_1 \leftrightarrow \vec{r}_2$ interchange and the orbital functions with odd l do change sign, the partial waves with even l are therefore restricted to terms with $S = 1, I = 0$, or with $S = 0, I = 1$, whereas the partial waves with odd l are restricted to terms with $S = 1, I = 1$ or with $S = 0, I = 0$. The scattering amplitude matrix must now be designated by the initial m_s and the initial m_i quantum numbers of the two particles in the incident beam, and the final m'_s and m'_i of the two particles in the scattered beam, that is, the scattering amplitude matrix, will be of the form

$$f(\theta, \phi)_{m'_{s,1} m'_{s,2} m'_{i,1} m'_{i,2}; m_{s,1} m_{s,2} m_{i,1} m_{i,2}}.$$

To take account of the required antisymmetry of the two-particle wave function in a partial wave decomposition, however, it will be necessary to transform from the $m_{s,1} m_{s,2} m_{i,1} m_{i,2}$ basis into an S, M_S, I, M_I basis (via standard and very simple Clebsch–Gordan coefficients), and expand the scattering amplitude in partial waves in the matrix form

$$f(\theta, \phi)_{S' M'_S I' M'_I; S M_S I M_I}$$

to be able to observe the S, I value restrictions for even and odd l . In addition, the dominant part of the nucleon–nucleon interaction has terms of the form

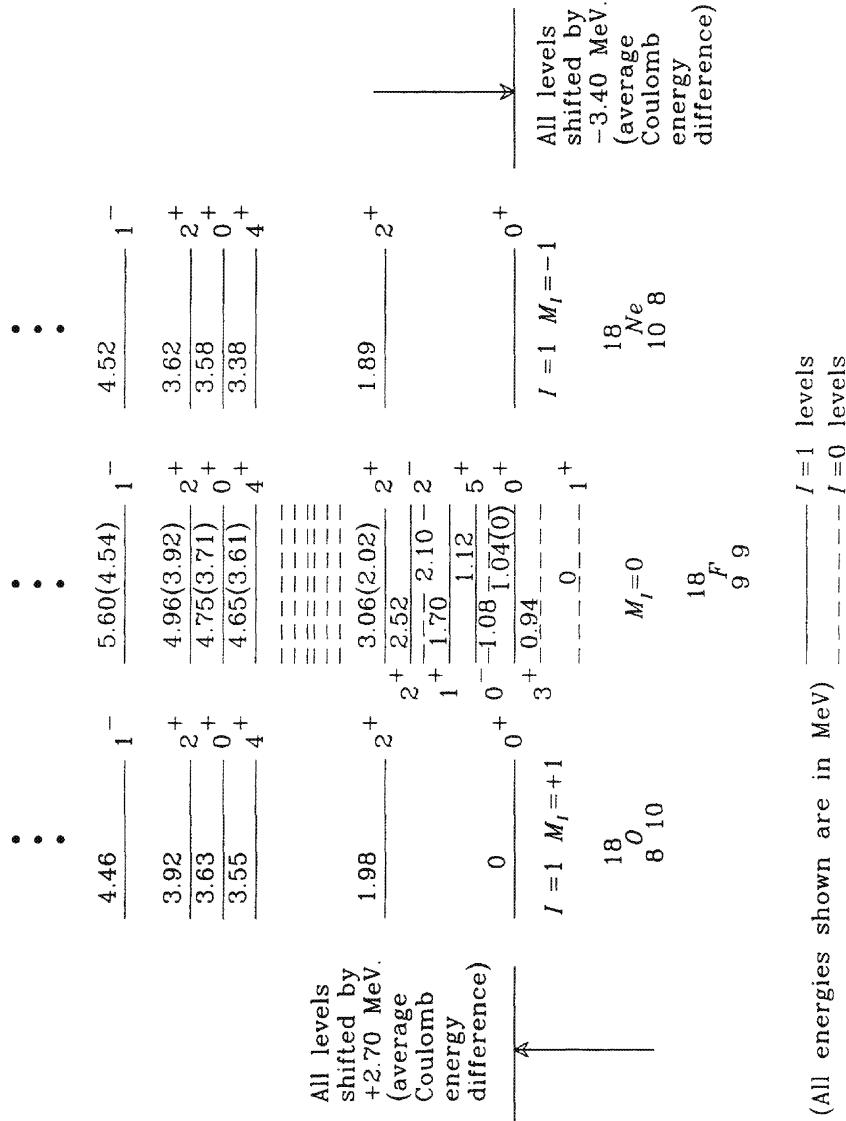
$$V = V_0(r) + V_1(r)(\vec{\sigma}_1 \cdot \vec{\sigma}_2) + V_2(r)(\vec{\tau}_1 \cdot \vec{\tau}_2) + V_3(r)(\vec{\sigma}_1 \cdot \vec{\sigma}_2)(\vec{\tau}_1 \cdot \vec{\tau}_2), \quad (7)$$

where $r = |\vec{r}_1 - \vec{r}_2|$. The four terms of this potential are scalars separately in orbital space, in spin space, and in isospin space. Hence, they cannot induce a change in the total spin quantum number S or the total isospin quantum number I . Thus, the above f -scattering amplitude matrix must be diagonal in S and I , i.e., $S' = S$ and $I' = I$.

A Spectra of Two-Valence Nucleon Nuclei

The isospin quantum number also plays an important role in the energy level scheme of nuclei. Let us consider briefly two-valence nucleon nuclei with mass number, $A = 18$, that is, the nuclei $^{18}_8 O_{10}$, $^{18}_9 F_9$, and $^{18}_{10} Ne_8$, which have two-valence shell nucleons outside the doubly magic nucleus, $^{16}_8 O_8$, two neutrons for

$^{18}_8O_{10}$, one proton and one neutron for $^{18}_9F_9$, and two protons for $^{18}_{10}Ne_8$. These nuclei have $M_I = +1, 0$, and -1 , respectively. All three nuclei have states with $I = 1$. In addition, $^{18}_9F_9$ has states with $I = 0$. Thus, we are dealing with isospin triplets and an isospin singlet of energy levels. The total Coulomb energy separates the energy levels of the triplet. It is, however, easy to make an average Coulomb energy correction by considering the 8, 9, or 10 proton cloud as a spherically symmetric charge cloud of the experimentally observed radius. Because the greatest Coulomb repulsion occurs in $^{18}_{10}Ne_8$ with its 10 protons, the levels of this nucleus should be shifted down by 3.40 MeV to put them into correspondence with the companion levels in $^{18}_9F_9$. Similarly, the smaller Coulomb repulsion in $^{18}_8O_{10}$ requires an upward shift of 2.70 MeV. With these shifts, the members of the $I = 1$ triplet at once become apparent. The lowest levels in both $^{18}_8O_{10}$ and $^{18}_{10}Ne_8$ are $0^+, 2^+, 4^+$, $0^+, 2^+$, and 1^- . The required companion levels are also found in the $M_I = 0$ nucleus, $^{18}_9F_9$. The 2^+ level lies at 1.98, 2.02, and 1.89 MeV above the 0^+ level in these three nuclei. Similarly, the 4^+ level lies at 3.55, 3.61, and 3.38 MeV above the 0^+ level. For the approximate triplet nature of the other excited states, see Fig. 56.1. Moreover, these are the levels predicted by the nuclear shell model. The lowest states are those in which the two-valence nucleons are both in a $2d_{\frac{5}{2}}$ single particle state, with the same principal quantum number, $n = 2$, and orbital angular-momentum quantum number, $l = 2$, coupled to $j = \frac{5}{2}$. For such a two-particle configuration, states with J even, $J = 0, 2, 4$, are antisymmetric in the combined spin-orbital part of the space, and hence must be symmetric in the isospin-space part of the two-nucleon wave function. Hence, this is restricted to $I = 1$. The states of this configuration, with J odd, $J = 1, 3, 5$, are symmetric in the combined spin-orbital part of the full space, and must be antisymmetric in the isospin part of the space. Hence, such states are restricted to two-particle isospin quantum number, $I = 0$, and can occur only in the $M_I = 0$ member of the triplet, $^{18}_9F_9$. In fact, the 1^+ state is the ground state of $^{18}_9F_9$. The 3^+ state also lies below the lowest 0^+ state in this nucleus. The remaining $I = 0$ states in this nucleus have mainly positive parity for odd J , and negative parity for even J , just the opposite of the low-lying states with $I = 1$, which have positive parity for even J and negative parity for odd J , a strong indication they have the opposite symmetry in the combined orbital-spin part of the full space. (Note, however, two-nucleon configurations such as $2s_{\frac{1}{2}} 2d_{\frac{5}{2}}$, with different single-particle l 's can have both (orbital-spin) symmetric and antisymmetric combinations, so they can have both $I = 0$ and $I = 1$. The 2^+ level at 2.52-MeV excitation energy in $^{18}_9F_9$ with $I = 0$ is such a level. Although the isospin quantum number in nuclei is only an approximately good quantum number (largely because of the additional Coulomb force between protons), Fig. 56.1 gives a clear indication of the importance of the isospin quantum number in nuclei.)

FIGURE 56.1. Energy levels of $A = 18$ nuclei. (All energies shown are in MeV.)

Problems

- 17.** A low-energy beam of $s = \frac{1}{2}$ particles is scattered from an $S = 0$ target particle. The interaction can be approximated by the potential

$$V = V_0(r) + V_1(r)(\vec{l} \cdot \vec{s}),$$

where $V_1(r) = \frac{1}{2}V_0(r)$ and $V_0(r) = -V_0$, for $r \leq a$ and $V(r) = 0$ for $r > a$. Assume further V_0 has a value such that to order (ka) the s wave phase shift is zero,

$$\sqrt{\frac{2\mu a^2 |V_0|}{\hbar^2}} = \rho_0 = 4.493, \quad \text{so } \frac{\tan \rho_0}{\rho_0} = 1.$$

(a) Calculate the differential scattering cross section to lowest nonzero order in (ka) , assuming $(ka) \ll 1$, for an unpolarized incident beam.

(b) To this order, investigate whether the scattered beam remains unpolarized.

- 18.** The scattering of $s = \frac{1}{2}$ particles from a spinless target is governed by the scattering amplitude matrix

$$(f(\theta, \phi))_{m'_s m_s} = \begin{pmatrix} a(2 + \cos \theta) & \frac{1}{2}a(1 + i)\sin \theta e^{-i\phi} \\ -\frac{1}{2}a(1 + i)\sin \theta e^{i\phi} & a(2 + \cos \theta) \end{pmatrix},$$

where a is an energy-dependent real amplitude. Calculate the polarization of the scattered beam for the two cases:

(a) The incident beam has longitudinal polarization with $\vec{P} = \frac{2}{3}\vec{e}_z$.

(b) The incident beam has transverse polarization with $\vec{P} = \frac{2}{3}\vec{e}_x$.

- 19.** An unpolarized beam of $s = \frac{1}{2}$ particles is scattered from a spinless target. An analysis of the scattering data yields the following phase shifts:

$$\delta(s_{\frac{1}{2}}) = 350^\circ, \quad \delta(p_{\frac{1}{2}}) = 220^\circ, \quad \delta(p_{\frac{1}{2}}) = 180^\circ,$$

$$\delta(d_{\frac{1}{2}}) = 20^\circ, \quad \delta(d_{\frac{3}{2}}) = 30^\circ, \quad \delta_{l,j} = 0 \text{ for } l > 2.$$

Calculate the differential scattering cross section and the polarization vector of the scattered beam as a function of θ . In a double scattering experiment, the second target is placed at an angle of 30° relative to the incident beam. The left and right detectors are placed in the initial scattering plane at angles of 45° relative to the first scattered beam. Calculate the left-right asymmetry in the second scattering:

$$\frac{d\sigma_L - d\sigma_R}{d\sigma_L + d\sigma_R}.$$

- 20. (a)** The following are density matrices for $s = \frac{1}{2}$ particles:

$$\rho = \begin{pmatrix} \frac{1}{3} & -\frac{i\sqrt{2}}{3} \\ \frac{i\sqrt{2}}{3} & \frac{2}{3} \end{pmatrix}, \quad \rho = \begin{pmatrix} \frac{1}{3} & -\frac{i}{3} \\ \frac{i}{3} & \frac{2}{3} \end{pmatrix}.$$

Show one of these represents a pure state with particles with 100% polarization along a specific direction and find this direction. What is \vec{P}^{inc} for these two cases?

(b) Calculate the polarization of the scattered beam of $s = \frac{1}{2}$ particles into directions, θ, ϕ by an $S = 0$ target particle for the three cases:

$$(i) : P_x^{\text{inc.}} \neq 0; P_y^{\text{inc.}} = P_z^{\text{inc.}} = 0.$$

$$(ii) : P_y^{\text{inc.}} \neq 0; P_x^{\text{inc.}} = P_z^{\text{inc.}} = 0..$$

$$(iii) : P_z^{\text{inc.}} \neq 0; P_x^{\text{inc.}} = P_y^{\text{inc.}} = 0$$

Express your answer in terms of $g(\theta), h(\theta)$.

21. Calculate the scattering amplitude matrix $(f(\theta, \phi))_{m'_s m_s}$ for a beam of $s = 1$ particles being scattered from an $S = 0$ target particle assuming an interaction of the form, $V(r) = V_0(r) + V_1(r)(\vec{l} \cdot \vec{s})$.

(a) Calculate this scattering amplitude matrix first by a partial wave expansion, and show it must have the form

$$(f(\theta, \phi))_{m'_s m_s} = \begin{pmatrix} g_1(\theta) & -ih_1(\theta)e^{-i\phi} & l(\theta)e^{-2i\phi} \\ ih_2(\theta)e^{i\phi} & g_0(\theta) & -ih_2(\theta)e^{-i\phi} \\ l(\theta)e^{2i\phi} & ih_1(\theta)e^{i\phi} & g_1(\theta) \end{pmatrix}.$$

(b) Show in first Born approximation this $(f(\theta, \phi))_{m'_s m_s}$ has the simpler form

$$\begin{pmatrix} g(\theta) & -ih(\theta)e^{-i\phi} & 0 \\ ih(\theta)e^{i\phi} & g(\theta) & -ih(\theta)e^{-i\phi} \\ 0 & ih(\theta)e^{i\phi} & g(\theta) \end{pmatrix}.$$

Show this relation can be expressed as a linear combination of the 3×3 unit matrix and the 3×3 matrices S_x and S_y in the linear combination, $S_{y'} = -S_x \sin \phi + S_y \cos \phi$.

$$(f(\theta, \phi))_{m'_s m_s} = (g(\theta)\mathbf{1} + \sqrt{2}h(\theta)S_{y'})_{m'_s m_s}.$$

(c) For this latter case, find the differential cross section and the polarization vector for the scattered beam as a function of $g(\theta)$ and $h(\theta)$ for an unpolarized incident beam, assuming the detector is placed in the $x-z$ plane, so $\phi = 0$.

22. (a) For the scattering of a beam of particles with spin, s , from a spinless, $S = 0$, target particle with an incident beam density matrix, $\rho^{\text{inc.}}$, show the density matrix of the scattered beam is given by

$$(\rho^{\text{scatt.}})_{m'_s m_s} = \frac{(f\rho^{\text{inc.}} f^\dagger)_{m'_s m_s}}{\text{trace}(f\rho^{\text{inc.}} f^\dagger)},$$

where $(f(\theta, \phi))_{m'_s m_s}$ is the scattering amplitude matrix.

For the case of $s = 1$ particles and the scattering amplitude of part (b) of problem 21, show this gives

$$\rho^{\text{scatt.}} = \frac{[|g(\theta)|^2 \mathbf{1} + \sqrt{2}(g(\theta)h^*(\theta) + g^*(\theta)h(\theta))S_y + 2|h(\theta)|^2 S_y^2]}{3|g(\theta)|^2 + 4|h(\theta)|^2}$$

for an unpolarized incident beam, with $\rho^{\text{inc.}} = \frac{1}{3}\mathbf{1}$, where the scattering plane has been chosen as the $x-z$ plane, so $\phi = 0$.

(b) Calculate the left-right asymmetry

$$\frac{d\sigma_L - d\sigma_R}{d\sigma_L + d\sigma_R}$$

as a function of $g(\theta)$ and $h(\theta)$ for a double scattering experiment for this case, if the left and right detectors are also placed in the x - z plane at angles, θ , which are identical to the scattering angle, θ , for the first scattering process.

23. For a beam of $s = 1$ particles with perfect polarization, show both a tensor polarization and a vector polarization must exist with $|\vec{P}| = 1$. In particular, with perfect perpendicular polarization in the y direction, perpendicular to the x - z scattering plane, i.e., with (S_y) – eigenvalue = +1 for all particles, show the density matrix for such a beam is given by

$$\rho = \frac{1}{2}S_y + \frac{1}{2}S_y^2 = \frac{1}{3}\mathbf{1} + \frac{1}{2}S_y - \frac{1}{4}(S_x^2 - S_y^2) + \frac{1}{12}(S_x^2 + S_y^2 - 2S_z^2).$$

Using the result of (a) of problem 22 show the scattering of a beam with perfect polarization in the y direction, normal to the scattering plane, will not alter this perfect polarization. That is, show

$$\rho^{\text{scatt.}} = \rho^{\text{inc.}} = \frac{1}{2}S_y + \frac{1}{2}S_y^2$$

in this case. Recall the simple 3×3 matrix for S_y has the property: $S_y^3 = S_y$ and $S_y^4 = S_y^2$.

24. Assume at a certain energy the nucleon–nucleon interaction is effectively spin-independent, and, although “charge-independent” (a “charge-independent” potential is a scalar in isospin space; it is independent of M_I , but may be I -dependent), it does depend on the total isospin of the two-particle system through a potential of the form

$$V(r) = V_a(r) + V_b(r)(\vec{\tau}_1 \cdot \vec{\tau}_2),$$

where $\frac{1}{2}\vec{\tau}_1 = \vec{i}_1$ and $\frac{1}{2}\vec{\tau}_2 = \vec{i}_2$ are the isospin operators of nucleons labelled by the subscripts 1 and 2. Assume V_a and V_b have strengths and signs such that

$$V_a + \frac{1}{2}V_b \left(4[I(I+1) - \frac{3}{4} - \frac{3}{4}] \right)$$

is attractive when the two-particle isospin quantum number $I = 0$ and repulsive when $I = 1$ such that the scattering can be parameterized by the phase shifts:

$$\begin{aligned} \text{For } I = 0 : \quad & \delta_{l=0}^{S=1} = -\frac{\pi}{4} \quad \delta_{l=1}^{S=0} = -\frac{\pi}{4}, \\ \text{For } I = 1 : \quad & \delta_{l=0}^{S=0} = +\frac{\pi}{2} \quad \delta_{l=1}^{S=1} = +\frac{\pi}{2}, \end{aligned}$$

and

$$\delta_l^S = 0 \quad \text{for all } l \geq 2.$$

Although V is spin-independent, the phase shifts depend on all three quantum numbers, the two-particle I , S , and the relative motion orbital angular momentum l . Show the I , S , l combinations with nonzero phase shifts are consistent with the required antisymmetry of the two-particle wave functions.

Assume the nucleons in the incident beam and in the target are unpolarized. Calculate the relative strengths of the following differential cross sections for $\theta = 30^\circ$ (center of mass system):

- (a) proton–proton scattering;
- (b) proton–neutron scattering (scattered proton forward 30°);
- (c) proton–neutron exchange scattering (target neutron forward 30°).

Time-Dependent Perturbation Theory

Time-Dependent Perturbation Expansion

We recall from Chapter 19 the time evolution of a quantum system is given by

$$|\psi(t)\rangle = U(t, t_0)|\psi(t_0)\rangle, \quad (1)$$

where the time evolution operator, $U(t, t_0)$, is unitary, with

$$UU^\dagger = U^\dagger U = 1, \quad \text{with} \quad U(t_0, t_0) = 1, \quad (2)$$

and

$$-\frac{\hbar}{i} \frac{dU}{dt} = HU(t, t_0), \quad (3)$$

where $H(t)$ may now be time dependent. We can express the solution, $U(t, t_0)$, in terms of the integral equation,

$$U(t, t_0) = 1 - \frac{i}{\hbar} \int_{t_0}^t d\tau H(\tau)U(\tau, t_0). \quad (4)$$

For general $H(t)$, this integral equation cannot be solved, but if

$$H = H_0 + \lambda h(t), \quad (5)$$

where H_0 is time independent with known eigenvectors and eigenvalues and λ is a parameter of smallness, $\lambda \ll 1$, then we may be able to find $U(t, t_0)$ by perturbation theory in a power series in λ . The zeroth-order solution for the time evolution is now known

$$U^{(0)}(t, t_0) = e^{-\frac{i}{\hbar} H_0(t-t_0)}. \quad (6)$$

It may now be useful to go from the Heisenberg picture to the Schrödinger picture (see Chapter 19) via an intermediate representation, through the so-called

interaction picture, by transforming the time-independent Heisenberg state vector, $|\psi_H\rangle \equiv |\psi(t_0)\rangle$, to the time-dependent Schrödinger state vector, $|\psi_S\rangle \equiv |\psi(t)\rangle$, via an intermediate state vector, the interaction representation state vector, $|\psi_I(t)\rangle$, where

$$|\psi(t)\rangle = U^{(0)}(t, t_0)|\psi_I(t)\rangle = U^{(0)}(t, t_0)U'(t, t_0)|\psi(t_0)\rangle, \quad (7)$$

where, again, $U'(t_0, t_0) = 1$. Substituting into eq. (3), we get

$$\begin{aligned} -\frac{\hbar}{i} \left(\frac{dU^{(0)}}{dt} \right) U' - \frac{\hbar}{i} U^{(0)} \left(\frac{dU'}{dt} \right) &= (H_0 + \lambda h) U^{(0)} U' \\ H_0 U^{(0)} U' - \frac{\hbar}{i} U^{(0)} \left(\frac{dU'}{dt} \right) &= H_0 U^{(0)} U' + \lambda h U^{(0)} U' \\ -\frac{\hbar}{i} U^{(0)} \left(\frac{dU'}{dt} \right) &= \lambda h U^{(0)} U', \end{aligned} \quad (8)$$

so, after left-multiplication with $U^{(0)\dagger}$, we have the equation for U' ,

$$-\frac{\hbar}{i} \frac{dU'}{dt} = \lambda \left(U^{(0)\dagger} h U^{(0)} \right) U' = \lambda h_I(t) U', \quad (9)$$

where the interaction representation, h_I , is given by

$$h_I(t) = U^{(0)\dagger} h(t) U^{(0)} = e^{+\frac{i}{\hbar} H_0(t-t_0)} h(t) e^{-\frac{i}{\hbar} H_0(t-t_0)}, \quad (10)$$

and we are now led to the integral equation

$$U'(t, t_0) = 1 - \frac{i}{\hbar} \lambda \int_{t_0}^t d\tau h_I(\tau) U'(\tau, t_0). \quad (11)$$

Because λ is a parameter of smallness, this equation is now in a form that can be iterated:

$$U'(t, t_0) = 1 - \frac{i}{\hbar} \lambda \int_{t_0}^t d\tau h_I(\tau) \left(1 - \frac{i}{\hbar} \lambda \int_{t_0}^\tau d\tau_1 h_I(\tau_1) \left(1 - \dots \right) \right), \quad (12)$$

with

$$\begin{aligned} U'^{(0)}(t, t_0) &= 1, \\ U'^{(1)}(t, t_0) &= -\frac{i}{\hbar} \lambda \int_{t_0}^t d\tau_1 h_I(\tau_1), \\ U'^{(2)}(t, t_0) &= \left(\frac{i}{\hbar} \right)^2 \lambda^2 \int_{t_0}^t d\tau_2 h_I(\tau_2) \int_{t_0}^{\tau_2} d\tau_1 h_I(\tau_1), \end{aligned} \quad (13)$$

or, in general,

$$U'(t, t_0) = 1 + \sum_{n=1}^{\infty} \left(\frac{-i}{\hbar} \right)^n \lambda^n I_n, \quad (14)$$

with

$$I_n = \int_{t_0}^t d\tau_n h_I(\tau_n) \int_{t_0}^{\tau_n} d\tau_{n-1} h_I(\tau_{n-1}) \int_{t_0}^{\tau_{n-1}} d\tau_{n-2} h_I(\tau_{n-2})$$

$$\times \int_{t_0}^{\tau_{n-2}} d\tau_{n-3} h_I(\tau_{n-3}) \int_{t_0}^{\tau_{n-3}} d\tau_{n-4} \dots \dots \int_{t_0}^{\tau_2} d\tau_1 h_I(\tau_1), \quad (15)$$

where

$$h_I(\tau_k) = e^{+\frac{i}{\hbar} H_0 (\tau_k - t_0)} h(\tau_k) e^{-\frac{i}{\hbar} H_0 (\tau_k - t_0)}. \quad (16)$$

We are assuming the eigenvectors, $|a\rangle, |b\rangle, \dots, |m\rangle, \dots$, of H_0 are known, together with their eigenvalues, $E_a^{(0)}, E_b^{(0)}, \dots$, where

$$H_0 |b\rangle = E_b^{(0)} |b\rangle. \quad (17)$$

The type of question we want to answer is the following: Given our quantum system was initially in a state $|\psi(t_0)\rangle = |i\rangle$, where $|i\rangle$ is an eigenstate of H_0 with energy $E_i^{(0)}$, what is the probability the system, as a result of the time-dependent perturbation, be in the final state, $|\psi(t)\rangle = |k\rangle$, which is a different eigenstate of H_0 ? For this purpose, we need to calculate

$$\begin{aligned} \langle k | \psi(t) \rangle &= \langle k | U^{(0)}(t, t_0) U'(t, t_0) | i \rangle \\ &= e^{-\frac{i}{\hbar} E_k^{(0)}(t-t_0)} \langle k | U'(t, t_0) | i \rangle \\ &= e^{-\frac{i}{\hbar} E_k^{(0)}(t-t_0)} \sum_n \lambda^n \langle k | U'^{(n)}(t, t_0) | i \rangle \\ &= e^{-\frac{i}{\hbar} E_k^{(0)}(t-t_0)} \sum_n \left(\frac{-i}{\hbar} \right)^n \lambda^n \langle k | I_n | i \rangle. \end{aligned} \quad (18)$$

The needed probability is of course the square of the absolute value of this matrix element, and we shall be interested in this number in the limit in which the final time, t , is such that $(t - t_0)$ is large compared with the characteristic periods of the quantum system.

To first order in λ , we have

$$\begin{aligned} \langle k | U^{(0)}(t, t_0) U'(t, t_0) | i \rangle &= -\frac{i}{\hbar} \lambda e^{-\frac{i}{\hbar} E_k^{(0)}(t-t_0)} \int_{t_0}^t d\tau_1 e^{+\frac{i}{\hbar} E_k^{(0)}(\tau_1-t_0)} \langle k | h(\tau_1) | i \rangle e^{-\frac{i}{\hbar} E_i^{(0)}(\tau_1-t_0)} \\ &= -\frac{i}{\hbar} \lambda \int_{t_0}^t d\tau_1 e^{-\frac{i}{\hbar} E_k^{(0)}(t-\tau_1)} \langle k | h(\tau_1) | i \rangle e^{-\frac{i}{\hbar} E_i^{(0)}(\tau_1-t_0)}. \end{aligned} \quad (19)$$

By inserting a set of unit operators of the type $\sum_a |a\rangle \langle a|$, the n^{th} order term can be written as

$$\begin{aligned} \langle k | U^{(0)}(t, t_0) U'^{(n)}(t, t_0) | i \rangle &= \lambda^n \left(\frac{-i}{\hbar} \right)^n \times \\ &\sum_{a,b,\dots,u} \int_{t_0}^t d\tau_n e^{-\frac{i}{\hbar} E_k^{(0)}(t-\tau_n)} \langle k | h(\tau_n) | a \rangle \int_{t_0}^{\tau_n} d\tau_{n-1} e^{-\frac{i}{\hbar} E_a^{(0)}(\tau_n-\tau_{n-1})} \langle a | h(\tau_{n-1}) | b \rangle \\ &\int_{t_0}^{\tau_{n-1}} d\tau_{n-2} e^{-\frac{i}{\hbar} E_b^{(0)}(\tau_{n-1}-\tau_{n-2})} \langle b | h(\tau_{n-2}) | c \rangle \int_{t_0}^{\tau_{n-2}} d\tau_{n-3} e^{-\frac{i}{\hbar} E_c^{(0)}(\tau_{n-2}-\tau_{n-3})} \\ &\times \langle c | h(\tau_{n-3}) | d \rangle \dots \dots \int_{t_0}^{\tau_2} d\tau_1 e^{-\frac{i}{\hbar} E_u^{(0)}(\tau_2-\tau_1)} \langle u | h(\tau_1) | i \rangle e^{-\frac{i}{\hbar} E_i^{(0)}(\tau_1-t_0)}. \end{aligned} \quad (20)$$

The various factors of this n^{th} order term can be remembered via a diagram of the type used by A. Messiah, *Quantum Mechanics. Vol. II*, New York: John Wiley,

1965, and illustrated in Fig. 57.1 via a sixth-order diagram, with time running upward, $t > \tau_n > \tau_{n-1} > \dots > \tau_2 > \tau_1 > t_0$. Each vertex with its wiggly line stands for the matrix element at that time, e.g., at time τ_n , the matrix element is $\langle k|h(\tau_n)|a\rangle$. Each solid line, e.g., the line labeled b , connecting times τ_{n-1} and τ_{n-2} stands for an exponential, in this case $e^{-\frac{i}{\hbar}E_b^{(0)}(\tau_{n-1}-\tau_{n-2})}$.

A First-Order Probability Amplitude: The Golden Rule

Let us, as a first example, calculate the probability amplitude a quantum system initially in the state $|i\rangle$ at time, t_0 , be in the state $|f\rangle$ at a later time, t , assuming the perturbation, $\lambda h(t)$, is weak enough that first-order perturbation theory is sufficient, and even more, choosing first a time-independent perturbation, λh . Then, the general

$$\langle f|U(t, t_0)|i\rangle = -\frac{i}{\hbar}\lambda \int_{t_0}^t d\tau e^{-\frac{i}{\hbar}E_f^{(0)}(t-\tau)} \langle f|h(\tau)|i\rangle e^{-\frac{i}{\hbar}E_i^{(0)}(\tau-t_0)} \quad (21)$$

leads to

$$|\langle f|U(t, t_0)|i\rangle| = \frac{\lambda}{\hbar} |\langle f|h|i\rangle \int_{t_0}^t d\tau e^{+\frac{i}{\hbar}(E_f^{(0)} - E_i^{(0)})\tau}|, \quad (22)$$

where we have used the assumed time-independence of h and have taken the absolute value of this transition probability amplitude, because the quantity of physical interest is the square of this absolute value. Then,

$$\begin{aligned} |\langle f|U(t, t_0)|i\rangle| &= \frac{\lambda}{\hbar} |\langle f|h|i\rangle \int_{t_0}^t d\tau e^{i\omega_{fi}\tau}| \\ &= \frac{\lambda}{\hbar} \left| \langle f|h|i\rangle \frac{(e^{i\omega_{fi}(t-t_0)} - 1)}{i\omega_{fi}} e^{i\omega_{fi}t_0} \right| \\ &= \frac{\lambda}{\hbar} \left| \langle f|h|i\rangle \frac{\sin\left[\frac{\omega_{fi}}{2}(t-t_0)\right]}{\left(\frac{\omega_{fi}}{2}\right)^2} e^{i\frac{\omega_{fi}}{2}(t+t_0)} \right|, \end{aligned} \quad (23)$$

so

$$|\langle f|U(t, t_0)|i\rangle|^2 = \frac{\lambda^2}{\hbar^2} |\langle f|h|i\rangle|^2 \frac{\sin^2\left[\frac{\omega_{fi}}{2}(t-t_0)\right]}{\left(\frac{\omega_{fi}}{2}\right)^2}. \quad (24)$$

We shall be interested in this quantity in the limit when the time interval $(t - t_0)$ is large compared with characteristic periods of the quantum system. We shall therefore go to the macroscopic time limit $(t - t_0) \rightarrow \infty$. Recalling the Dirac delta function can be given by

$$\delta(\omega) = \lim_{t \rightarrow \infty} \frac{1}{2\pi} \int_{-t}^{+t} dt' e^{i\omega t'} = \lim_{t \rightarrow \infty} \frac{\sin \omega t}{\pi \omega}, \quad (25)$$

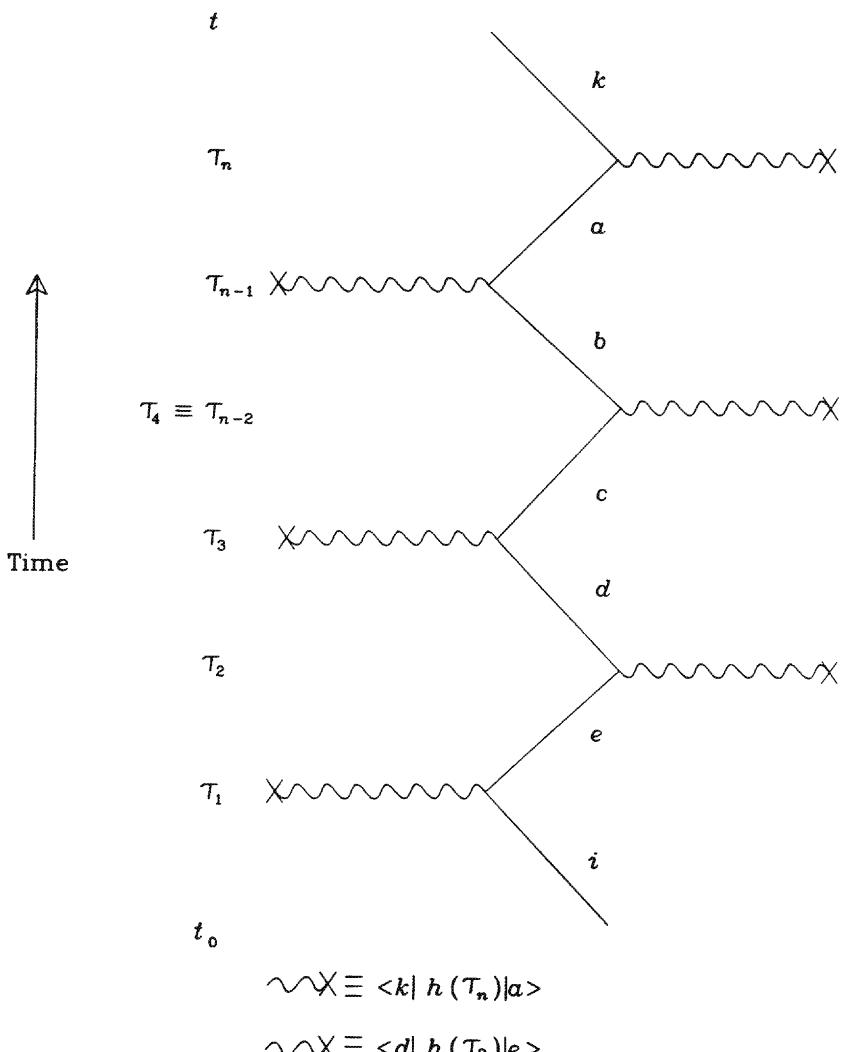


FIGURE 57.1.

we can express the large time limit of the time-dependent function above by using the identity

$$\lim_{t \rightarrow \infty} \left(\frac{\sin\left[\frac{\omega}{2}t\right]}{\pi \frac{\omega}{2}} \right) \left(\frac{\sin\left[\frac{\omega}{2}t\right]}{\frac{\omega}{2}t} \right) = \delta(\frac{1}{2}\omega) = 2\delta(\omega), \quad (26)$$

where we have used: $\delta(\omega)f(\omega) = \delta(\omega)f(0)$ and $\delta(\frac{1}{a}\omega) = a\delta(\omega)$. Using this identity, we get

$$\lim_{t \rightarrow \infty} \frac{\sin^2\left[\frac{\omega_f}{2}t\right]}{\left(\frac{\omega_f}{2}\right)^2} = 2\pi t\delta(\omega_{fi}). \quad (27)$$

Therefore,

$$\begin{aligned} \lim_{t \rightarrow \infty} |\langle f | U(t, t_0) | i \rangle|^2 &= \frac{\lambda^2}{\hbar^2} |\langle f | h | i \rangle|^2 2\pi(t - t_0) \delta\left(\frac{1}{\hbar}(E_f^{(0)} - E_i^{(0)})\right) \\ &= 2\pi\hbar(t - t_0) \frac{\lambda^2}{\hbar^2} |\langle f | h | i \rangle|^2 \delta(E_f^{(0)} - E_i^{(0)}), \end{aligned} \quad (28)$$

or

$$\lim_{t \rightarrow \infty} \frac{|\langle f | U(t, t_0) | i \rangle|^2}{(t - t_0)} = \frac{2\pi}{\hbar} \delta(E_f^{(0)} - E_i^{(0)}) |\langle f | \lambda h | i \rangle|^2 = \left[\frac{\text{probability}}{\text{unit time}} \right]_{i \rightarrow f}. \quad (29)$$

That is, the expression gives the probability per unit time the quantum system, initially in state $|i\rangle$ end in the state $|f\rangle$, where the time interval is a macroscopic one. We will be likely to satisfy the Dirac delta function condition of conservation of energy only if the initial and final total energy of the system lies in the continuum, so a group of states in an energy interval dE about $E = E_f$ exists. Let $|E_f\rangle$ be an eigenvector of H_0 with eigenvalue E_f , part of an energy continuum for the total system.

$$H_0|E_f\rangle = E_f|E_f\rangle, \quad (30)$$

with a similar relation for E_i . Let $\rho(E_f)$ be the number of states between E_f and $E_f + dE$. Then,

$$\begin{aligned} \left[\frac{\text{Transition Prob.}}{\text{unit time}} \right]_{i \rightarrow f} &= \lim_{t \rightarrow \infty} \int dE_f \rho(E_f) \frac{|\langle f | U(t, t_0) | i \rangle|^2}{(t - t_0)} \\ &= \frac{2\pi}{\hbar} \int dE_f \rho(E_f) |\langle f | \lambda h | i \rangle|^2 \delta(E_f - E_i), \end{aligned} \quad (31)$$

so, with $E_f = E_i$,

$$\left[\frac{\text{Transition Probability}}{\text{second}} \right]_{i \rightarrow f} = \frac{2\pi}{\hbar} \rho(E_i) |\langle f | \lambda h | i \rangle|^2. \quad (32)$$

This important result was named Golden Rule II by Fermi. Fermi claimed almost all important results in quantum theory could be obtained from the two Golden Rules. (Recall Golden Rule I was the energy correction, through second order, using stationary state perturbation theory.)

B Application: The First Born Approximation of Scattering Theory Revisited

As a first simple test of our result, let us rederive the differential cross section for the scattering of a point projectile from a point target particle interacting via a potential that is weak compared with the kinetic energy of the relative motion. The Hamiltonian for this system is

$$H = H_0 + V(\vec{r}), \quad \text{where now } V = \lambda h, \quad (33)$$

$$H_0|\phi_{\vec{k}}\rangle = E_k|\phi_{\vec{k}}\rangle = \frac{\hbar^2 k^2}{2\mu}|\phi_{\vec{k}}\rangle, \quad \text{with } |\phi_{\vec{k}}\rangle \equiv |\vec{k}\rangle, \quad (34)$$

with

$$\phi_{\vec{k}}(\vec{r}) = \langle \vec{r} | \vec{k} \rangle = \frac{e^{i\vec{k} \cdot \vec{r}}}{(2\pi)^{\frac{3}{2}}}. \quad (35)$$

With this normalization, the unit operator is $\int d\vec{k} |\vec{k}\rangle \langle \vec{k}|$, and the scalar product $\langle \vec{k}' | \vec{k} \rangle = \delta(\vec{k} - \vec{k}')$ has the standard Dirac delta function form. The number of states in this continuum between \vec{k} and $\vec{k} + d\vec{k}$ is then given by the volume element

$$dk_x dk_y dk_z = k^2 dk \sin \theta_k d\theta_k d\phi_k,$$

where k is the magnitude of \vec{k} , and θ_k, ϕ_k give the direction of \vec{k} . This must now be transformed to the form $\rho(E_f) dE_f$, so we can use Golden Rule II. From

$$E_f = \frac{\hbar^2 k_f^2}{2\mu_f}, \quad dE_f = \frac{\hbar^2}{\mu_f} k_f dk_f, \quad (36)$$

so

$$dk_x dk_y dk_z = k_f^2 dk_f d\Omega_f = k_f \frac{\mu_f}{\hbar^2} dE_f d\Omega_f = p_f \frac{\mu_f}{\hbar^3} dE_f d\Omega_f = \rho(E_f) dE_f, \quad (37)$$

and the density of states factor is given by

$$\rho(E_f) = k_f \frac{\mu_f}{\hbar^2} d\Omega_f = p_f \frac{\mu_f}{\hbar^3} d\Omega_f = [2\mu_f E_f]^{\frac{1}{2}} \frac{\mu_f}{\hbar^3} d\Omega_f, \quad (38)$$

where $d\Omega_f$ is the element of solid angle about the direction of the scattering vector \vec{k}_f . Now, Golden Rule II says

$$\begin{aligned} \left[\frac{\text{Transition probability}}{\text{sec.}} \right]_{\vec{k}_i \rightarrow \vec{k}_f} &= \frac{\text{Nr. of part. scattered into } d\Omega_f}{\text{sec.}} \\ &= \frac{2\pi}{\hbar} \frac{k_f \mu_f d\Omega_f}{\hbar^2} |\langle \vec{k}_f | V | \vec{k}_i \rangle|^2. \end{aligned} \quad (39)$$

To get the differential cross section, we need to divide this quantity by the magnitude of the incident flux. With $\langle \vec{r} | \vec{k}_i \rangle = 1/(2\pi)^{\frac{3}{2}} e^{i\vec{k}_i \cdot \vec{r}}$, the incident flux has the

magnitude

$$|\vec{S}_i| = \frac{\hbar k_i}{\mu_i} \frac{1}{(2\pi)^3},$$

so

$$\begin{aligned} d\sigma &= \frac{(\text{Transition Prob./sec.})_{\vec{k}_i \rightarrow \vec{k}_f}}{\text{Inc. Flux}} = \frac{2\pi}{\hbar} \frac{k_f \mu_f d\Omega_f}{\hbar^2} \frac{\mu_i (2\pi)^3}{\hbar k_i} |\langle \vec{k}_f | V | \vec{k}_i \rangle|^2 \\ &= \left(\frac{2\pi}{\hbar} \right)^4 \mu_f \mu_i \frac{k_f}{k_i} d\Omega_f \left| \int d\vec{r}' \frac{e^{-i\vec{k}_f \cdot \vec{r}'}}{(2\pi)^{\frac{3}{2}}} V(\vec{r}') \frac{e^{i\vec{k}_i \cdot \vec{r}'}}{(2\pi)^{\frac{3}{2}}} \right|^2, \end{aligned} \quad (40)$$

and

$$\frac{d\sigma}{d\Omega} = \frac{\mu_f \mu_i}{(2\pi\hbar^2)^2} \frac{k_f}{k_i} \left| \int d\vec{r}' e^{-i\vec{k}_f \cdot \vec{r}'} V(\vec{r}') e^{i\vec{k}_i \cdot \vec{r}'} \right|^2. \quad (41)$$

For the purely elastic scattering process, of course, $k_f = k_i$ and $\mu_f = \mu_i$. This equation agrees with our earlier first Born approximation result. Also, the time-dependent perturbation theory result is easily adapted to the case of a rearrangement collision, where $\mu_f \neq \mu_i$ and $k_f \neq k_i$.

C Box Normalization: An Alternative Approach

It may be useful to show that the first Born approximation result also follows directly from the Golden Rule II, if we use the finely discrete spectrum of box normalization in place of the true continuous spectrum of our plane wave states. For a cubical macroscopic laboratory of side L , we have the eigenfunctions of H_0 , given by

$$\phi_i(\vec{r}) = \frac{e^{i\vec{k}_i \cdot \vec{r}}}{L^{\frac{3}{2}}}, \quad (42)$$

with \vec{k}_i and \vec{k}_f both given by a triple of integers $(n_1, n_2, n_3) \equiv \vec{n}$, with n_s , integers, both positive and negative, such that

$$k_x = \frac{2\pi}{L} n_1, \quad k_y = \frac{2\pi}{L} n_2, \quad k_z = \frac{2\pi}{L} n_3, \quad \text{or } \vec{k} = \frac{2\pi}{L} \vec{n}, \quad (43)$$

with

$$k^2 = \left(\frac{2\pi}{L} \right)^2 \vec{n} \cdot \vec{n} = \left(\frac{2\pi}{L} \right)^2 (n_1^2 + n_2^2 + n_3^2) = \left(\frac{2\pi}{L} \right)^2 n^2(k). \quad (44)$$

In n space, each allowed state given by the triple of integers, (n_1, n_2, n_3) , takes a cubical volume, where the elementary cube has a side of length 1, hence, a volume of 1^3 . For large $n(k)$, the total number of discrete states with $k' < k$ is then given approximately by the volume of a sphere of radius $n(k)$

$$\text{Nr. of states with } k' < k = \frac{4\pi}{3} n^3 = \frac{4\pi}{3} \left(\frac{L}{2\pi} \right)^3 k^3, \quad (45)$$

and the total number of discrete states between k and $k + dk$ is

$$N(k)dk = 4\pi \left(\frac{L}{2\pi}\right)^3 k^2 dk. \quad (46)$$

The total number of discrete states between k and $k + dk$, but directions in an element of solid angle $d\Omega$ about a specific direction, θ, ϕ , of the \vec{k} vector, is

$$N(k)dk \frac{d\Omega}{4\pi} = \left(\frac{L}{2\pi}\right)^3 k^2 dk d\Omega = \left(\frac{L}{2\pi}\right)^3 k \frac{\mu}{\hbar^2} d\Omega dE, \quad (47)$$

so

$$\rho(E_f) = \left(\frac{L}{2\pi}\right)^3 \left(\frac{k_f \mu_f}{\hbar^2}\right) d\Omega_f. \quad (48)$$

Now,

$$\left[\frac{\text{Transition Prob.}}{\text{sec.}} \right]_{i \rightarrow f} = \frac{2\pi}{\hbar} \rho(E_f) \left| \int d\vec{r}' \phi_f^*(\vec{r}') V(\vec{r}') \phi_i(\vec{r}') \right|^2. \quad (49)$$

$$\text{With } \phi_i(\vec{r}) = \frac{e^{i\vec{k}_i \cdot \vec{r}}}{L^{\frac{3}{2}}}, \quad (50)$$

the magnitude of the incident flux is given by

$$\frac{\hbar k_i}{\mu_i} \frac{1}{L^3},$$

so

$$d\sigma = \frac{2\pi}{\hbar} \left(\frac{L}{2\pi}\right)^3 \left(\frac{k_f \mu_f}{\hbar^2}\right) d\Omega_f \left(\frac{\mu_i L^3}{\hbar k_i}\right) \left| \int d\vec{r}' \frac{e^{-i\vec{k}_f \cdot \vec{r}'}}{L^{\frac{3}{2}}} V(\vec{r}') \frac{e^{i\vec{k}_i \cdot \vec{r}'}}{L^{\frac{3}{2}}} \right|^2, \quad (51)$$

$$\frac{d\sigma}{d\Omega} = \frac{\mu_f \mu_i}{(2\pi \hbar^2)^2} \frac{k_f}{k_i} \left| \int d\vec{r}' e^{-i\vec{k}_f \cdot \vec{r}'} V(\vec{r}') e^{i\vec{k}_i \cdot \vec{r}'} \right|^2, \quad (52)$$

in agreement with the earlier results. We note, in particular, the volume L^3 has disappeared from the final result, as it must!

D Second-Order Effects

Second-order terms may be particularly significant if the matrix element of the perturbation, λh , between states i and f happen to vanish. From our diagram, the second-order contribution to $\langle f | U(t, t_0) | i \rangle$ is given by

$$\begin{aligned} \langle f | U^{(2)}(t, t_0) | i \rangle &= \frac{(-i)^2 \lambda^2}{\hbar^2} \sum_a \int_{t_0}^t d\tau_2 e^{-\frac{i}{\hbar} E_f^{(0)}(t-\tau_2)} \langle f | h(\tau_2) | a \rangle \\ &\times \int_{t_0}^{\tau_2} d\tau_1 e^{-\frac{i}{\hbar} E_a^{(0)}(\tau_2-\tau_1)} \langle a | h(\tau_1) | i \rangle e^{-\frac{i}{\hbar} E_i^{(0)}(\tau_1-t_0)}. \end{aligned} \quad (53)$$

We shall again start with the special case, where \hbar is assumed to be independent of the time. Then,

$$\begin{aligned}
 & \langle f | U^{(2)}(t, t_0) | i \rangle \frac{\hbar^2}{(-i)^2 \lambda^2} e^{+\frac{i}{\hbar}(E_f^{(0)} t - E_i^{(0)} t_0)} \\
 &= \sum_a \langle f | h | a \rangle \langle a | h | i \rangle \int_{t_0}^t d\tau_2 e^{i\omega_{fa}\tau_2} \int_{t_0}^{\tau_2} d\tau_1 e^{i\omega_{ai}\tau_1} \\
 &= \sum_a \langle f | h | a \rangle \langle a | h | i \rangle \int_{t_0}^t d\tau_2 e^{i\omega_{fa}\tau_2} \frac{(e^{i\omega_{ai}\tau_2} - e^{i\omega_{fi}t_0})}{i\omega_{ai}} \\
 &= \sum_a \frac{\langle f | h | a \rangle \langle a | h | i \rangle}{i\omega_{ai}} \left[\frac{(e^{i\omega_{fi}t} - e^{i\omega_{fi}t_0})}{i\omega_{fi}} - \frac{(e^{i\omega_{fa}(t-t_0)} - 1)}{i\omega_{fa}} e^{i(\omega_{fa} + \omega_{fi})t_0} \right]. \tag{54}
 \end{aligned}$$

Now the last time-dependent factor can be written as

$$\frac{(e^{i\omega_{fa}(t-t_0)} - 1)}{i\omega_{fa}} = e^{i\frac{\omega_{fa}}{2}(t-t_0)} \frac{\sin\left[\frac{\omega_{fa}}{2}(t-t_0)\right]}{\left(\frac{\omega_{fa}}{2}\right)}. \tag{55}$$

We shall deal first with the case where *nonzero* matrix elements exist only between states f and a and i and a such that $\omega_{fa} \neq 0$ and $\omega_{ai} \neq 0$. In this case, the

$$\frac{\sin\left[\frac{\omega_{fa}}{2}(t-t_0)\right]}{\frac{\omega_{fa}}{2}}$$

term is proportional to $\approx \frac{1}{\omega_{fa}}$; i.e., it is a time of the order of a period of the quantum system, viz., the period associated with ω_{fa} . The term we shall retain, however, will be proportional to the macroscopic time difference $(t - t_0)$. Hence, we will be able to neglect this ω_{fa} -term. Now, we use (as before) for the ω_{fi} term

$$\frac{(e^{i\omega_{fi}t} - e^{i\omega_{fi}t_0})}{i\omega_{fi}} = e^{i\frac{\omega_{fi}}{2}(t+t_0)} \frac{\sin\left[\frac{\omega_{fi}}{2}(t-t_0)\right]}{\left(\frac{\omega_{fi}}{2}\right)}. \tag{56}$$

The absolute value squared of this term will lead to the factor $2\pi\hbar(t-t_0)\delta(E_f^{(0)} - E_i^{(0)})$, as before. The additional factor $(-i)/\hbar$ arising from the second-order term in the perturbation expansion can be combined with the denominator factor, $i\omega_{ai}$, to give the denominator factor, $+(E_i^{(0)} - E_a^{(0)})$, so through second order the transition probability per unit time is given by

$$\begin{aligned}
 & \frac{\left| \langle f | U^{(1)}(t, t_0) + U^{(2)}(t, t_0) | i \rangle \right|^2}{(t-t_0)} = \\
 & \frac{2\pi}{\hbar} \delta(E_f^{(0)} - E_i^{(0)}) \left| \langle f | \lambda h | i \rangle + \sum_a \frac{\langle f | \lambda h | a \rangle \langle a | \lambda h | i \rangle}{(E_i^{(0)} - E_a^{(0)})} \right|^2. \tag{57}
 \end{aligned}$$

Finally, combining the energy conservation delta function with the density of states factor, and renaming, $\lambda h = V$, we have the extension of Fermi's Golden

Rule through next order in the perturbation expansion

$$\left[\frac{\text{Transition Prob.}}{\text{second}} \right]_{i \rightarrow f} = \frac{2\pi}{\hbar} \rho(E_f) \left| \langle f | V | i \rangle + \sum_a \frac{\langle f | V | a \rangle \langle a | V | i \rangle}{(E_i^{(0)} - E_a^{(0)})} \right|^2, \quad (58)$$

where again, $E_f^{(0)} = E_i^{(0)}$, and it is assumed the matrix element $\langle a | V | i \rangle$ vanishes for $E_a^{(0)} = E_i^{(0)}$. Note the similarity between this result and the corresponding result for stationary-state perturbation theory, which was Fermi's other Golden Rule.

E Case 2: A Periodic Perturbation

So far, our perturbation, λh , has been assumed to be time independent. Let us now look at a truly time-dependent perturbation, of periodic form

$$h(t) = h(0)e^{-i\omega t} + h^\dagger(0)e^{i\omega t}, \quad (59)$$

where we assume h is hermitian. For simplicity, we shall assume $h^\dagger(0) = h(0)$. Now,

$$\langle f | U^{(1)}(t, t_0) | i \rangle = -i \frac{\lambda}{\hbar} \int_{t_0}^t d\tau e^{-\frac{i}{\hbar} E_f^{(0)}(t-\tau)} \langle f | h(0) | i \rangle (e^{-i\omega\tau} + e^{i\omega\tau}) e^{-\frac{i}{\hbar} E_i^{(0)}(\tau-t_0)}, \quad (60)$$

so

$$\begin{aligned} & \left| \langle f | U^{(1)}(t, t_0) | i \rangle \right| \frac{\hbar}{\lambda} = \left| \langle f | h(0) | i \rangle \int_{t_0}^t d\tau (e^{i(\omega_{fi}-\omega)\tau} + e^{i(\omega_{fi}+\omega)\tau}) \right| \\ &= \left| \langle f | h(0) | i \rangle \left[\frac{(e^{i(\omega_{fi}-\omega)t} - e^{i(\omega_{fi}-\omega)t_0})}{i(\omega_{fi}-\omega)} + \frac{(e^{i(\omega_{fi}+\omega)t} - e^{i(\omega_{fi}+\omega)t_0})}{i(\omega_{fi}+\omega)} \right] \right| \\ &= \left| \langle f | h(0) | i \rangle \left[e^{i\frac{1}{2}(\omega_{fi}-\omega)(t+t_0)} \left(\frac{\sin\left[\frac{(\omega_{fi}-\omega)}{2}(t-t_0)\right]}{\frac{(\omega_{fi}-\omega)}{2}} \right) \right. \right. \\ & \quad \left. \left. + e^{i\frac{1}{2}(\omega_{fi}+\omega)(t+t_0)} \left(\frac{\sin\left[\frac{(\omega_{fi}+\omega)}{2}(t-t_0)\right]}{\frac{(\omega_{fi}+\omega)}{2}} \right) \right] \right|. \end{aligned} \quad (61)$$

Now, for very large values of $(t - t_0)$, the first term is strongly peaked when $\omega_{fi} = \omega$, and the second term is negligible for this value of ω_{fi} . Conversely, for large values of $(t - t_0)$, the second term is strongly peaked when $\omega_{fi} = -\omega$, and the first term is negligible for this value of ω_{fi} . Thus,

$$\text{either or } \left| \langle f | U(t, t_0) | i \rangle \right|^2 = \frac{\lambda^2}{\hbar^2} |\langle f | h(0) | i \rangle|^2 f((\omega_{fi} \mp \omega), (t - t_0)), \quad (62)$$

where the peaked function, $f(\Omega, t)$, has the limiting value

$$\lim_{t \rightarrow \infty} f(\Omega, t) = 2\pi t \delta(\Omega). \quad (63)$$

Thus, again renaming, $\lambda h(0) = V(0)$, we have now

$$\left[\frac{\text{Transition prob.}}{\text{second}} \right]_{i \rightarrow f} = \frac{2\pi}{\hbar} \left(\delta(E_f^{(0)} - E_i^{(0)} - \hbar\omega) + \delta(E_f^{(0)} - E_i^{(0)} + \hbar\omega) \right) |\langle f | V(0) | i \rangle|^2. \quad (64)$$

If we consider ω to be a positive quantity, we can get a strong transition probability, either if $\hbar\omega = E_f^{(0)} - E_i^{(0)}$ or if $\hbar\omega = E_i^{(0)} - E_f^{(0)}$. [Note, in the case, when $V(0)^\dagger \neq V(0)$, the second term that applies for the case with $\hbar\omega = E_i^{(0)} - E_f^{(0)}$ would be proportional to the square of the absolute value of the matrix element of $V^\dagger(0)$, rather than $V(0)$.]

An example of a quantum system in which such an oscillatory perturbation might come into play is an atomic or molecular system with a magnetic moment, $\vec{\mu}$, in an external oscillating magnetic field $\vec{B}(t)$, with

$$\lambda h(t) = H_{\text{int.}} = -\vec{\mu} \cdot \vec{B}(t). \quad (65)$$

In this case, we would make a Fourier analysis of the \vec{B} field

$$\vec{B}(t) = \int_{-\infty}^{\infty} d\omega \rho(\omega) \vec{B}(0) e^{i\omega t} = \int_0^{\infty} d\omega \rho(\omega) \vec{B}(0) (e^{i\omega t} + e^{-i\omega t}), \quad (66)$$

and use

$$\begin{aligned} & \lim_{(t-t_0) \rightarrow \infty} \int_0^{\infty} d\omega f(\omega_{fi} - \omega, t - t_0) \rho(\omega) \\ &= 2\pi(t - t_0) \int_0^{\infty} d\omega \delta(\omega_{fi} - \omega) \rho(\omega) = 2\pi(t - t_0) \rho(\omega_{fi}). \end{aligned} \quad (67)$$

Thus, the transition probability induced by the oscillating magnetic field will lead to

$$\left[\frac{\text{Transition Probability}}{\text{sec.}} \right]_{i \rightarrow f} = \frac{2\pi}{\hbar^2} \rho(\omega_{fi}) |\langle f | \vec{\mu} \cdot \vec{B}(0) | i \rangle|^2. \quad (68)$$

58

Oscillating Magnetic Fields: Magnetic Resonance

For a quantum system with a magnetic moment, $\vec{\mu}$, in an external magnetic field, \vec{B} , with

$$\vec{\mu} = \frac{e\hbar}{2mc} g_J \vec{J}, \quad (1)$$

we have a Hamiltonian with the perturbing term

$$H = H_0 - \vec{\mu} \cdot \vec{B}. \quad (2)$$

Here, \vec{J} is the relevant dimensionless angular momentum vector. For an electron or a proton, we can use the Pauli $\vec{\sigma}$ operator, $\vec{J} = \frac{1}{2}\vec{\sigma}$. For a free electron the g factor is $g_s = 2$ (neglecting quantum electrodynamic corrections). This g factor may also be slightly modified because of the electron environment in a molecular or crystalline system. For the proton, the g factor is “anomalous” $g_s = 2(2.793)$. The relevant energies for electron and proton magnetic resonance experiments are given by

$$\hbar\omega(B) = \frac{e\hbar}{2mc} B g_s = -5.79 \times 10^{-5} eV \left(\frac{B}{\text{tesla}} \right) g_s \quad \text{for electrons,}$$

$$\hbar\omega(B) = \frac{e\hbar}{2mc} B g_s = +3.15 \times 10^{-8} eV \left(\frac{B}{\text{tesla}} \right) g_s \quad \text{for protons,}$$

so these are small perturbations for atomic or molecular systems.

In a typical magnetic resonance experiment, two magnetic fields are used:

- (1) A steady, time-independent, \vec{B} -field, \vec{B}_0 , where this field will be chosen to lie in the z direction, with $\hbar\omega(B_0) = \hbar\omega_0$.

(2) A perpendicular \vec{B} -field, oscillating with circular frequency, ω , and strength, \vec{B}_1 , where we define ω_1 via $\hbar\omega(B_1) = \hbar\omega_1$. This field is often linearly polarized in the x direction, or circularly polarized in the x - y plane. Because we can make a linearly polarized field from a superposition of a right and left circularly polarized field, we shall treat only the case of a right circularly polarized oscillating \vec{B}_1 -field (see Fig. 58.1) and choose our Hamiltonian as

$$\begin{aligned} H &= H_0 - [\hbar\omega_0 J_z + \hbar\omega_1 (J_x \cos \omega t + J_y \sin \omega t)] \\ &= H_0 - \hbar\omega_0 J_z - \frac{\hbar\omega_1}{2} [J_+ e^{-i\omega t} + J_- e^{i\omega t}], \end{aligned} \quad (3)$$

where $J_{\pm} = (J_x \pm i J_y)$. Our earlier perturbation theory for an oscillating field can now be used, if $\omega_1 \ll \omega_0$, so we can include the steady field part of the Hamiltonian as part of our zeroth-order problem. [Note, in this case, $h(0)^{\dagger} \neq h(0)$.] If we choose the electron-resonance case for which the $m_s = +\frac{1}{2}$ level lies above the $m_s = -\frac{1}{2}$ level and assume at $t_0 = 0$ the system is in the upper state, at excitation energy $\hbar|\omega_0|$, i.e., $|i\rangle = |m_s = +\frac{1}{2}\rangle$ at $t = 0$, to first order in ω_1 , the perturbation theory result would give

$$\begin{aligned} \left(-\frac{1}{2}|U^{(1)}(t, 0)| + \frac{1}{2}\right) &= \left(\frac{-i}{\hbar}\right)\left(-\frac{\hbar\omega_1}{2}\right)\left(-\frac{1}{2}|J_-| + \frac{1}{2}\right)e^{i\frac{(\omega_{fi}+\omega)}{2}t} \frac{\sin\left[\frac{(\omega_{fi}+\omega)}{2}t\right]}{\frac{(\omega_{fi}+\omega)}{2}} \\ &= \frac{i\omega_1}{(|\omega_0| - \omega)}e^{-i(|\omega_0| - \omega)\frac{t}{2}} \sin\left[(|\omega_0| - \omega)\frac{t}{2}\right]. \end{aligned} \quad (4)$$

In this perturbation approach, the parameter of smallness is $\omega_1/(|\omega_0| - \omega)$. The resonance condition leading to the sharply peaked function for large time t in the limit $\omega = |\omega_0|$ is considered *after* an expansion in the perturbation parameter of smallness. The magnetic resonance problem, however, is so simple we can actually solve this time-dependent problem exactly and do not need to make a perturbation expansion in powers of $\omega_1/(|\omega_0| - \omega)$.

A Exact Solution of the Magnetic Resonance Problem

We shall be able to find an exact solution for the time evolution operator for the full Hamiltonian of eq. (3). The method involves a rotation operator rotating to the frame of reference of the rotating field, \vec{B}_1 . To find $U(t, 0)$ for the solution

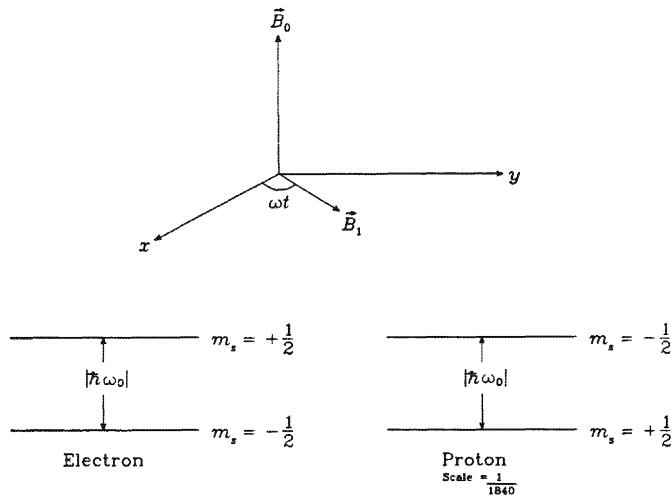
$$|\psi(t)\rangle = U(t, 0)|\psi(t_0 = 0)\rangle, \quad (5)$$

let us introduce a time-dependent rotation operator, $R_z(t)$, which rotates the system about the z axis through an angle, ωt , and look for solutions of the time evolution operator in the form

$$U(t, 0) = R_z(t)U'(t, 0) = e^{-i\omega t J_z}U'(t, 0), \quad (6)$$

where

$$-\frac{\hbar}{i} \frac{dU}{dt} = HU(t, 0) \quad (7)$$

FIGURE 58.1. Magnetic resonance \vec{B} -fields.

now leads to

$$-\frac{\hbar}{i} R_z \frac{dU'}{dt} + \hbar\omega J_z R_z U' = H(R_z U'). \quad (8)$$

Left-multiplying this equation with $R_z^\dagger = R_z^{-1}$, and noting R_z commutes with J_z , this relation leads to

$$-\frac{\hbar}{i} \frac{dU'}{dt} = R_z^\dagger (H - \hbar\omega J_z) R_z U' = H_{\text{eff.}} U', \quad (9)$$

with

$$\begin{aligned} H_{\text{eff.}} &= e^{i\omega t J_z} \left(H_0 - [\hbar(\omega_0 + \omega)J_z + \hbar\omega_1(J_x \cos \omega t + J_y \sin \omega t)] \right) e^{-i\omega t J_z} \\ &= H_0 - \hbar(\omega_0 + \omega)J_z + \hbar\omega_1 e^{i\omega t J_z} (J_x \cos \omega t + J_y \sin \omega t) e^{-i\omega t J_z}, \end{aligned} \quad (10)$$

where we have assumed H_0 is rotationally invariant, so $[H_0, J_z] = 0$; i.e., H_0 commutes with any component of \vec{J} . We also assume H_0 is time independent. Now, however, we can also show the full $H_{\text{eff.}}$ is time independent by showing the operator

$$O = e^{i\omega t J_z} (J_x \cos \omega t + J_y \sin \omega t) e^{-i\omega t J_z} \quad (11)$$

is independent of time. To show this, note

$$\begin{aligned} \frac{dO}{dt} &= e^{i\omega t J_z} \left((i\omega J_z)(J_x \cos \omega t + J_y \sin \omega t) \right. \\ &\quad \left. + (J_x \cos \omega t + J_y \sin \omega t)(-i\omega J_z) \right. \\ &\quad \left. + \omega(-J_x \sin \omega t + J_y \cos \omega t) \right) e^{-i\omega t J_z} \\ &= e^{i\omega t J_z} \omega \left((i(J_z J_x - J_x J_z) + J_y) \cos \omega t \right. \end{aligned}$$

$$= 0 \quad (12)$$

$$+ \left(i(J_z J_y - J_y J_z) - J_x \right) \sin \omega t \Big) e^{-i\omega t J_z}$$

via the angular momentum commutation relations. Because $H_{\text{eff.}}$ is independent of time, we can replace it with its value for $t = 0$,

$$H_{\text{eff.}} = H_0 - [\hbar(\omega_0 + \omega)J_z + \hbar\omega_1 J_x]. \quad (13)$$

For this time-independent $H_{\text{eff.}}$, the solution for U' is trivial

$$U' = e^{-\frac{i}{\hbar} H_{\text{eff.}} t}, \quad (14)$$

and

$$U(t, 0) = R_z(t)U'(t, 0) = e^{-i\omega t J_z} e^{-\frac{i}{\hbar} H_0 t} e^{i[(\omega_0 + \omega)J_z + \omega_1 J_x]t}, \quad (15)$$

where we have again used the fact that H_0 commutes with both J_z and J_x because of its rotational invariance. Note, however, J_z does not commute with J_x , so we cannot further simplify the final exponential in similar fashion. However, the linear combination $(\omega_0 + \omega)J_z + \omega_1 J_x$ can be reexpressed as

$$(\omega_0 + \omega)J_z + \omega_1 J_x = \Omega J_{z'} = \Omega(\cos \Theta J_z + \sin \Theta J_x), \quad (16)$$

$$\text{with } \Omega = \sqrt{(\omega_0 + \omega)^2 + \omega_1^2},$$

and

$$\cos \Theta = \frac{(\omega_0 + \omega)}{\sqrt{(\omega_0 + \omega)^2 + \omega_1^2}}, \quad \sin \Theta = \frac{\omega_1}{\sqrt{(\omega_0 + \omega)^2 + \omega_1^2}},$$

where we have made a rotation through an angle, Θ , about the y axis (see Fig. 58.2) to obtain

$$J_{z'} = \cos \Theta J_z + \sin \Theta J_x \quad (17)$$

to express $U(t, 0)$ through

$$U(t, 0) = e^{-\frac{i}{\hbar} H_0 t} e^{-i\omega t J_z} e^{i\Omega t J_{z'}}. \quad (18)$$

For the special but very important case of a spin $s = \frac{1}{2}$ particle, with $\vec{J} \equiv \vec{S} = \frac{1}{2}\vec{\sigma}$, it is easy to expand $e^{i\Omega t J_{z'}}$, via

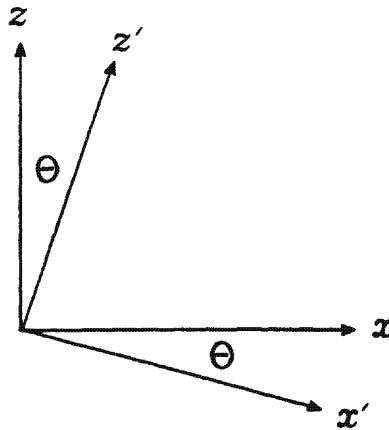
$$e^{\frac{i}{2}\Omega t \sigma_{z'}} = \cos\left(\frac{\Omega t}{2}\right) \mathbf{1} + i \sin\left(\frac{\Omega t}{2}\right) \sigma_{z'}, \quad (19)$$

where we have used

$$\sigma_{z'}^2 = \mathbf{1} = \sigma_{z'}^4 = \cdots, \quad \sigma_{z'}^3 = \sigma_{z'} = \sigma_{z'}^5 = \cdots, \quad (20)$$

and

$$\sigma_{z'} = \cos \Theta \sigma_z + \sin \Theta \sigma_x. \quad (21)$$

FIGURE 58.2. The parameter Θ of eq. (16).

With this simple expansion, we have for $s = \frac{1}{2}$ systems

$$U(t, 0) = e^{-\frac{i}{\hbar} H_0 t} e^{-i \frac{\omega}{2} t \sigma_z} \left(\cos\left(\frac{\Omega t}{2}\right) \mathbf{1} + i \sin\left(\frac{\Omega t}{2}\right) (\cos \Theta \sigma_z + \sin \Theta \sigma_x) \right). \quad (22)$$

If the initial state is given by $|i\rangle = |\alpha \frac{1}{2} m_s^{(i)}\rangle$, where α is shorthand for all quantum numbers of H_0 other than s, m_s , the final state can differ only in the quantum number, m_s , and must be of the form $|f\rangle = |\alpha \frac{1}{2} m_s^{(f)}\rangle$, and

$$\begin{aligned} & \left| \langle \alpha \frac{1}{2} m_s^{(f)} | U(t, 0) | \alpha \frac{1}{2} m_s^{(i)} \rangle \right| = \\ & \langle \alpha \frac{1}{2} m_s^{(f)} | \cos\left(\frac{\Omega t}{2}\right) \mathbf{1} + i \sin\left(\frac{\Omega t}{2}\right) (\cos \Theta \sigma_z + \sin \Theta \sigma_x) | \alpha \frac{1}{2} m_s^{(i)} \rangle. \end{aligned} \quad (23)$$

In particular,

$$\left| \langle \alpha -\frac{1}{2} - \frac{1}{2} | U(t, 0) | \alpha -\frac{1}{2} + \frac{1}{2} \rangle \right| = \sin \Theta \sin\left(\frac{\Omega t}{2}\right) = \frac{\omega_1}{\Omega} \sin\left(\frac{\Omega t}{2}\right). \quad (24)$$

The probability for a spin-flip from $m_s = +\frac{1}{2}$ to $m_s = -\frac{1}{2}$ is given by

$$\left[\text{Spin - flip Prob.}(t) \right]_{+\frac{1}{2} \rightarrow -\frac{1}{2}} = \frac{\omega_1^2}{[(\omega_0 + \omega)^2 + \omega_1^2]} \sin^2\left[\frac{t}{2} \sqrt{(\omega_0 + \omega)^2 + \omega_1^2}\right]. \quad (25)$$

We see that, at resonance, with ω such that $(\omega_0 + \omega) = 0$, this probability oscillates back and forth from zero to unity with a circular frequency of $\frac{1}{2}\omega_1$. Off resonance, with $(\omega_0 + \omega) \neq 0$, this probability oscillates back and forth from zero to a value less than unity with the circular frequency $\frac{1}{2}\Omega$. The oscillating \vec{B} -field can induce transitions both from the excited state to the lower state and from the lower state back to the excited state.

Finally, for very small values of ω_1 , for which we can expand in powers of $\omega_1/(\omega_0 + \omega)$, we have

$$\left| \langle \alpha - \frac{1}{2} | U(t, 0) | \alpha - \frac{1}{2} + \frac{1}{2} \rangle \right| \approx \frac{\omega_1}{(\omega_0 + \omega)} \sin\left[\frac{t}{2}(\omega_0 + \omega)\right], \quad (26)$$

which agrees with eq. (4) for the case of negative ω_0 .

B Density Matrices and the Magnetization Vector

So far, we have found an exact solution for the magnetic-resonance Hamiltonian for an $s = \frac{1}{2}$ -system, assuming we have an initial state that is an eigenstate of S_z , with $m_s = +\frac{1}{2}$, or $m_s = -\frac{1}{2}$. In an actual magnetic-resonance experiment, we have a system of many $s = \frac{1}{2}$ particles with different population probabilities for the states with $m_s = \pm \frac{1}{2}$. It will therefore again be advantageous to use a density matrix formulation. Suppose first the initial state at $t = 0$ is a linear combination of the eigenstates $|m_s\rangle$, given by

$$|\psi(0)\rangle = \sum_{m_s} |m_s\rangle c_{m_s}(0). \quad (27)$$

Then, the expectation value of σ_α is given by

$$\begin{aligned} \langle \sigma_\alpha \rangle &= \sum_{m_s, m'_s} c_{m'_s}^*(0) \langle m'_s | \sigma_\alpha | m_s \rangle c_{m_s}(0) = \sum_{m_s, m'_s} (\sigma_\alpha)_{m'_s m_s} c_{m_s}(0) c_{m'_s}^*(0) \\ &= \text{trace}(\sigma_\alpha \rho^i(0)). \end{aligned} \quad (28)$$

Now, we define a magnetization vector (in place of a polarization vector, bearing in mind that this is merely a change of name),

$$\vec{M} = \sum_{\alpha} \vec{e}_{\alpha} \langle \sigma_{\alpha} \rangle, \quad (29)$$

where we have

$$\vec{M} = \sum_{\alpha} \vec{e}_{\alpha} \text{trace}(\sigma_{\alpha} \rho). \quad (30)$$

The concept of the density matrix, ρ , will again be most useful when we have a statistical distribution of many $s = \frac{1}{2}$ systems in a macroscopic sample, with an initial density matrix, at $t = 0$, of the type

$$\rho^i = \sum_{n=1}^N w_n c_{m_i}^{(n)}(0) c_{m_i}^{(n)*}(0), \quad (31)$$

where w_n gives the probability the n^{th} system has the $c_{m_i}^{(n)}(0)$ and again

$$\sum_{n=1}^N w_n = 1. \quad (32)$$

For a system in thermal equilibrium, e.g., where the number of systems in the energy state E_{m_s} is proportional to the Boltzmann factor, $e^{-(E_{m_s}/kT)}$, we would have the density matrix

$$\rho = \frac{1}{(e^{-(E_{+}\frac{1}{2})/kT} + e^{-(E_{-}\frac{1}{2})/kT})} \begin{pmatrix} e^{-(E_{+}\frac{1}{2})/kT} & 0 \\ 0 & e^{-(E_{-}\frac{1}{2})/kT} \end{pmatrix}. \quad (33)$$

From the density matrix at $t = 0$, we can determine the density matrix $\rho(t)$ at a later time, t . For the n^{th} system, the time evolution gives

$$\begin{aligned} c_{m_s}^{(n)}(t) &= \sum_{m''_s} (U(t, 0))_{m_s m''_s} c_{m''_s}^{(n)}(0), \\ c_{m'_s}^{(n)*}(t) &= \sum_{m'''_s} (U^\dagger(t, 0))_{m''_s m'''_s} c_{m'''_s}^{(n)*}(0), \end{aligned} \quad (34)$$

so

$$\begin{aligned} (\rho(t))_{m_s m'_s} &= \sum_n w_n c_{m_s}^{(n)}(t) c_{m'_s}^{(n)*}(t) = \sum_{m''_s, m'''_s} U_{m_s m''_s} \rho(0)_{m''_s m'''_s} U_{m''_s m'''_s}^\dagger \\ &= (U \rho(0) U^\dagger)_{m_s m'_s}. \end{aligned} \quad (35)$$

To see how the magnetization evolves in time, we calculate $\langle \sigma_\alpha(t) \rangle$

$$\begin{aligned} \langle \sigma_\alpha(t) \rangle &= \langle \psi(t) | \sigma_\alpha | \psi(t) \rangle = \langle \psi(0) | U^\dagger(t, 0) \sigma_\alpha U(t, 0) | \psi(0) \rangle \\ &= \sum_{m_s m'_s} (U^\dagger \sigma_\alpha U)_{m'_s m_s} c_{m_s}(0) c_{m'_s}^*(0) = \text{trace}(U^\dagger \sigma_\alpha U \rho(0)), \end{aligned} \quad (36)$$

yielding

$$\vec{M}(t) = \sum_\alpha \vec{e}_\alpha \text{trace}(U^\dagger \sigma_\alpha U \rho(0)), \quad (37)$$

with a similar relation for a density matrix arising from a statistical distribution of states.

It should be remarked that eqs. (35) and (37) give the time evolution of the density matrix and the magnetization vector under the action of the \vec{B} -field of our Hamiltonian and assumes the different $s = \frac{1}{2}$ systems of our sample have no additional interactions with each other (spin–spin interactions), or with the medium in which they find themselves (spin–lattice interactions). Without such interactions, the time evolution of the density matrix, given by eq. (35), would lead to

$$\begin{aligned} -\frac{\hbar}{i} \frac{d\rho}{dt} &= -\frac{\hbar}{i} \left(\frac{dU}{dt} \right) \rho(0) U^\dagger - U \rho(0) \frac{\hbar}{i} \left(\frac{dU^\dagger}{dt} \right) = H U \rho(0) U^\dagger - U \rho(0) U^\dagger H \\ &= H \rho(t) - \rho(t) H = [H, \rho(t)]. \end{aligned} \quad (38)$$

The spin–spin and spin–lattice relaxation processes caused by the spin–spin and spin–lattice interactions are taken into account by adding a relaxation term to this equation, through a relaxation matrix, $(R)_{m_s m'_s, m''_s m'''_s}$,

$$\frac{d}{dt}(\rho)_{m_s m'_s} = -\frac{i}{\hbar} [H, \rho(t)]_{m_s m'_s} - \sum_{m''_s m'''_s} (R)_{m_s m'_s, m''_s m'''_s} (\rho)_{m''_s m'''_s}. \quad (39)$$

Without this additional relaxation term, eq. (37) gives the time evolution of the magnetization vector purely under the influence of the magnetic fields, \vec{B}_0 and \vec{B}_1 .

C General Case with $J > \frac{1}{2}$

So far, we have concentrated on the $s = \frac{1}{2}$ systems. For $J \geq 1$, we could expand the operator, $e^{i\Omega t J_z'}$, by the technique used for the Pauli spin matrices. For $J = 1$, e.g., three independent 3×3 matrices are needed to expand this exponential, the 3×3 unit matrix, the 3×3 matrix for J_z' and for J_z^2 , where we now use $J_z^3 = J_z$ and $J_z^4 = J_z^2$. For the case of arbitrary J , however, it is best to use the well-known matrix elements of the rotation operator, $R_y(\Theta)$, which effects a rotation through an angle Θ about the y axis. With this rotation operator, the operator $e^{i\Omega t J_z}$ is transformed into the needed $e^{i\Omega t J_z'}$ via

$$\begin{aligned} e^{i\Omega t J_z'} &= R_y(\Theta) e^{i\Omega t J_z} R_y^{-1}(\Theta) \\ &= e^{-i\Theta J_z} e^{i\Omega t J_z} e^{i\Theta J_z}, \end{aligned} \quad (40)$$

leading to the matrix elements

$$\begin{aligned} \langle JM_J' | e^{i\Omega t J_z'} | JM_J \rangle &= \sum_{M_J'} \langle JM_J' | e^{-i\Theta J_z} | JM_J'' \rangle e^{i\Omega t M_J''} \langle JM_J'' | e^{i\Theta J_z} | JM_J \rangle \\ &= \sum_{M_J'} d_{M_J' M_J''}^J(\Theta) e^{i\Omega t M_J''} d_{M_J'' M_J}^J(-\Theta), \end{aligned} \quad (41)$$

where we have used the fact that the operator J_z is diagonal in the $|JM_J''\rangle$ basis and the d^J matrices are the rotation matrices for an Euler rotation with Euler angles, $\alpha = \gamma = 0$ and $\beta = \pm\Theta$ (see Chapter 29). As a simple test, let us rederive the matrix $\langle \frac{1}{2}m_s' | e^{i\Omega t S_z'} | \frac{1}{2}m_s \rangle$, for an $s = \frac{1}{2}$ system. Using the $d^{\frac{1}{2}}$ matrices, we have in this case

$$\begin{aligned} \langle \frac{1}{2}m_s' | e^{i\Omega t S_z'} | \frac{1}{2}m_s \rangle &= \begin{pmatrix} \cos \frac{\Theta}{2} & -\sin \frac{\Theta}{2} \\ \sin \frac{\Theta}{2} & \cos \frac{\Theta}{2} \end{pmatrix} \begin{pmatrix} e^{i\frac{\Omega}{2}t} & 0 \\ 0 & e^{-i\frac{\Omega}{2}t} \end{pmatrix} \begin{pmatrix} \cos \frac{\Theta}{2} & \sin \frac{\Theta}{2} \\ -\sin \frac{\Theta}{2} & \cos \frac{\Theta}{2} \end{pmatrix} \\ &= \begin{pmatrix} \left(\cos^2 \frac{\Theta}{2} e^{i\frac{\Omega}{2}t} + \sin^2 \frac{\Theta}{2} e^{-i\frac{\Omega}{2}t} \right) & \cos \frac{\Theta}{2} \sin \frac{\Theta}{2} \left(e^{i\frac{\Omega}{2}t} - e^{-i\frac{\Omega}{2}t} \right) \\ \cos \frac{\Theta}{2} \sin \frac{\Theta}{2} \left(e^{i\frac{\Omega}{2}t} - e^{-i\frac{\Omega}{2}t} \right) & \left(\sin^2 \frac{\Theta}{2} e^{i\frac{\Omega}{2}t} + \cos^2 \frac{\Theta}{2} e^{-i\frac{\Omega}{2}t} \right) \end{pmatrix} \\ &= \begin{pmatrix} \left(\cos \frac{\Omega t}{2} + i \sin \frac{\Omega t}{2} \cos \Theta \right) & i \sin \frac{\Omega t}{2} \sin \Theta \\ i \sin \frac{\Omega t}{2} \sin \Theta & \left(\cos \frac{\Omega t}{2} - i \sin \frac{\Omega t}{2} \cos \Theta \right) \end{pmatrix} \\ &= \cos \frac{\Omega t}{2} \mathbf{1} + i \sin \frac{\Omega t}{2} (\cos \Theta \sigma_z + \sin \Theta \sigma_x), \end{aligned} \quad (42)$$

which agrees with our earlier result.

Sudden and Adiabatic Approximations

So far, we have considered only time-independent and periodic time-dependent perturbations. One of the common time-dependent problems in quantum mechanics involves the turning on or off of a perturbing term, e.g., an external field. In general, the details of turning on or off of time-dependent perturbations are too difficult to solve. Two limiting cases exist, however, that are both important and that can be treated in detail with good accuracy: the sudden and the adiabatic approximations.

Consider a perturbation problem, with

$$H = H_0 + V, \quad (1)$$

where the perturbation, V , is off up to some time t_0 and is then turned on, so at some later time, t , with $t - t_0 = T$ the perturbation is on at full strength. In the limit for which $T \rightarrow 0$, we have the sudden approximation. In the limit $T \rightarrow \infty$, we have the adiabatic approximation.

A Sudden Approximation

We shall introduce the variable

$$s = \frac{(t - t_0)}{T}$$

such that the perturbation is off for $s = 0$ and is on at full strength for $s = 1$. With

$$U(t, t_0) = 1 - \frac{i}{\hbar} \int_{t_0}^t d\tau H(\tau) U(\tau, t_0)$$

$$= 1 - \frac{i}{\hbar} T \int_0^1 ds H(s) U_T(s). \quad (2)$$

In the limit $T \rightarrow 0$, we have

$$\lim_{T \rightarrow 0} U_T(t, t_0) = 1. \quad (3)$$

The perturbation is so sudden the quantum system cannot follow. The system stays in the state $|\psi(t_0)\rangle$ even when the perturbation is fully turned on. An example of such a sudden perturbation occurs in the beta decay of an atomic nucleus. An example of considerable recent interest is the beta decay of tritium, ${}^3_1\text{H}_2$, which is being reexamined very carefully in an attempt to pin down a possible nonzero value of the rest mass of the neutrino. The endpoint electrons are of particular interest, because the antineutrino then carries very little kinetic energy. Because the neutrino rest mass is probably much less than an atomic energy of $\sim 10\text{eV}$, the exact atomic energy of the recoiling ${}^3_2\text{He}_1$ one-electron ion must be taken into account carefully. The original one-electron tritium atom had its atomic electron in an $1s$ ground state for this $Z = 1$ nucleus. The beta decay end point energy is 18.65 keV. The e^- emitted in this beta decay traverses the atomic dimension so rapidly the original atomic electron will still have the wave function of an $1s$ $Z = 1$ atom, even though it now finds itself in the Coulomb field of a $Z = 2$ nucleus. This state at $t = t_0$ will thus be a linear combination of one-electron states $|n l m = 0\rangle$ of a $Z = 2$ one-electron ion, and the probability for all values of n will be needed for an accurate evaluation of the internal energy of the recoiling ${}^3_2\text{He}_1$ ion.

B Adiabatic Approximation: An Example: The Reversal of the Magnetic Field in a One-Electron Atom

As a second example, let us consider a one-electron atom in an external magnetic field reversed from a value, $+\vec{B}_0$, to a value, $-\vec{B}_0$, in a time interval, T . We shall consider both the sudden approximation, $T \rightarrow 0$, and the adiabatic approximation, $T \rightarrow \infty$, in particular, the latter, adiabatic case, in which we have to carry out some analysis. For simplicity, we will consider the Paschen–Back and Zeeman spectrum of an alkali atom, such as Na, to avoid the higher degeneracies of the hydrogen spectrum. The perturbing Hamiltonian consists of the external magnetic-field term and the internal magnetic-field spin-orbit term (see Chapter 26).

$$H = \beta(\vec{l} \cdot \vec{s}) + \hbar\omega_L(l_z + 2s_z), \quad (4)$$

where the Larmor frequency, ω_L , is given by

$$\hbar\omega_L(t) = \frac{|e|\hbar}{2mc} B_0(t), \quad \text{with } B_z = B_0(t) = B_0(1 - \frac{2t}{T}). \quad (5)$$

We have reversed the field \vec{B} linearly from a value $+B_0$ at $t = 0$ to a value, $-B_0$, at $t = T$ (see Fig. 59.1). The linear character of the variation is very simple. We could

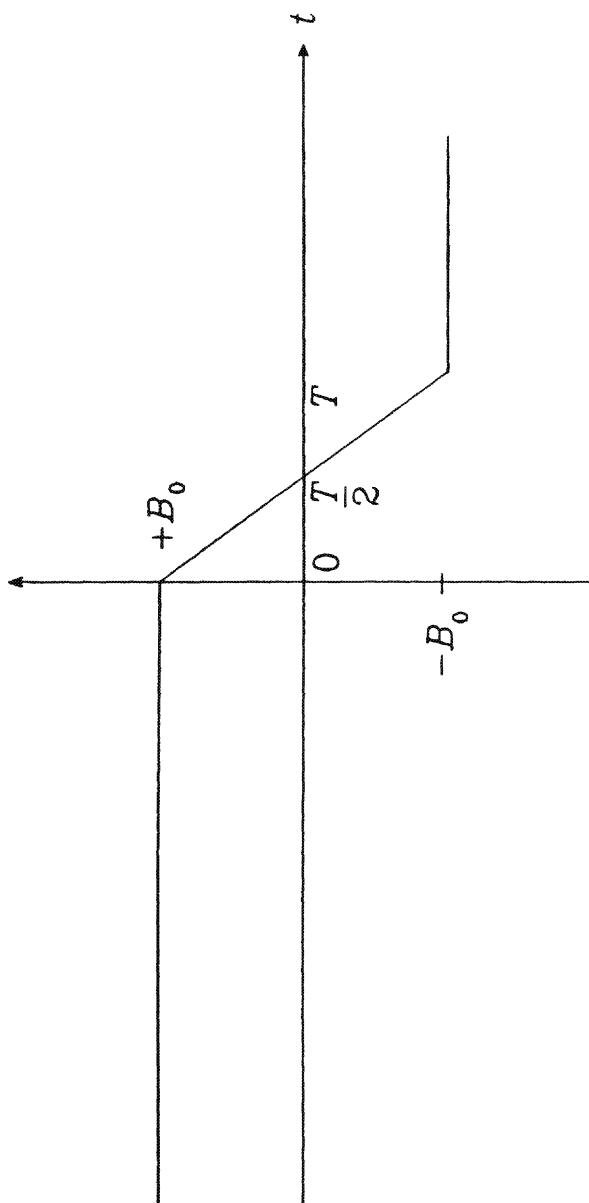


FIGURE 59.1. The linear B -field reversal of eq. (5).

have chosen a slightly more complicated function of the time. In the limits, $T \rightarrow 0$, or, $T \rightarrow \infty$, however, the exact form of the time variation is unimportant. Fig. 59.2 shows the energy level splitting for an $l = 1$ six-fold degenerate level, such as the $3p$ level in Na, as a function of B_0 for both positive and negative values of B_0 , starting with the huge-field or Paschen-Back case (for positive B_z on the right of the diagram, and for negative values of B_z on the left of the diagram). The above Hamiltonian leads to a matrix in the $|m_l m_s\rangle$ scheme, diagonal in $m_j = m_l + m_s$, and, except for the two states with $m_j = \pm(l + \frac{1}{2})$, the above Hamiltonian leads to 2×2 submatrices with fixed m_j of the form (see Chapter 26)

$$\begin{aligned} m_s &= +\frac{1}{2} & m_s &= -\frac{1}{2} \\ m_s = +\frac{1}{2} & \left(\begin{array}{cc} \hbar\omega_L(t)(m_j + \frac{1}{2}) + \frac{\beta m_j}{2} - \frac{\beta}{4} & \frac{\beta}{2}\sqrt{(l + \frac{1}{2})^2 - m_j^2} \\ \frac{\beta}{2}\sqrt{(l + \frac{1}{2})^2 - m_j^2} & \hbar\omega_L(t)(m_j - \frac{1}{2}) - \frac{\beta m_j}{2} - \frac{\beta}{4} \end{array} \right), \\ m_s = -\frac{1}{2} & \end{aligned}$$

where $m_l = m_j \mp \frac{1}{2}$ for the states with $m_s = \pm \frac{1}{2}$. This Hamiltonian submatrix, with rows and columns specified by $m_s = \pm \frac{1}{2}$, can be written in terms of a 2×2 unit matrix and the Pauli σ matrices, via

$$\begin{aligned} H &= \left[\hbar\omega_L(0)\left(1 - \frac{2t}{T}\right)m_j - \frac{\beta}{4} \right] \mathbf{1} + \left[\frac{\hbar\omega_L(0)}{2}\left(1 - \frac{2t}{T}\right) + \frac{\beta m_j}{2} \right] \sigma_z \\ &\quad + \frac{\beta}{2}\sqrt{[(l + \frac{1}{2})^2 - m_j^2]} \sigma_x \\ &= a(t)\mathbf{1} + b(t)\sigma_z + C\sigma_x \\ &= (a_0 + a_1 t)\mathbf{1} + (b_0 + b_1 t)\sigma_z + C\sigma_x. \end{aligned} \tag{6}$$

For the two levels with $m_j = \pm(l + \frac{1}{2})$, the state vectors, $|m_l = +l, m_s = +\frac{1}{2}\rangle$ and $|m_l = -l, m_s = -\frac{1}{2}\rangle$, are eigenvectors of our H for all values of B_z and independent of the time. For these two special states, therefore, $U(t, 0) = 1$, for all values of the switching time, T . For all other values of m_j , however, the results of the sudden switching are different from those of the adiabatic case. For example, if the one-electron system is in the second-highest energy state, with asymptotic quantum numbers $m_l = 0, m_s = +\frac{1}{2}$ in the huge-field limit at time, $t = 0$, a sudden switching of the direction of the \vec{B} -field to reverse the direction of \vec{B} will leave the one-electron atom in a state with $m_l = 0, m_s = +\frac{1}{2}$, but for negative B_0 , this is now the second-lowest energy state. In the extremely short time of the sudden switching of \vec{B} -field direction, the one-electron atom has jumped over the energy gap between the $p_{\frac{3}{2}}$ and $p_{\frac{1}{2}}$ levels at field strength zero to end in the second-lowest energy state. That is, the one-electron atom initially in the upper of the two energy eigenstates with $m_j = +\frac{1}{2}$ will in the sudden process end in the lower of the two energy eigenstates with $m_j = +\frac{1}{2}$.

Conversely, if the direction of the \vec{B} -field is reversed very slowly (in the adiabatic limit for which $T \rightarrow \infty$), we shall show the one-electron system follows the second-highest energy level with $m_j = +\frac{1}{2}$ through the zero B-field $p_{\frac{3}{2}}$ level and then follows the $m_j = +\frac{1}{2}$ level to the huge negative B_z -field limit with asymptotic quantum numbers $m_l = +1, m_s = -\frac{1}{2}$. That is, we shall show the one-electron