Chap. VI. Quantum Theory of Potential Scattering

Ref: Roman, Chap. 3
Foderaro, Sec. 4.7

We will study two methods of analyzing potential scattering, the method of partial waves and the integral equation method which leads to the Born approximation. Basically we are still concerned with the two-body collision process analyzed in Chap. III. Recall that in the center-of-mass coordinate system the problem is to describe the motion of a particle with mass μ (the effective mass) moving in a central potential V(r). Instead of the classical mechanics approach of following the particle trajectory explicitly as it moves through the potential field, we will solve the Schroedinger wave equation for the spatial distribution of the particle and extract from this solution the relevant information for determining the differential scattering cross section $\sigma(\theta)$.

A. The Scattering Amplitude f(θ)

In treating the potential scattering problem quantum mechanically the standard approach is to define the cross section $\sigma(\theta)$ in terms of a quantity called the <u>scattering amplitude</u> and then calculate this quantity by solving the Schoredinger wave equation.

The scattering process is visualized as shown in Fig. 6.1. A beam of monoenergetic particles, mass μ and energy E, is incident upon the target located at the origin of the coordinate system. The incident beam is represented by a plane wave traveling in the +z direction,

$$\Psi_{in} = e^{i(kz - \omega t)} \tag{6.1}$$

where $\underline{k} = k\hat{\underline{z}}$ is the wave vector with magnitude given by $E = \hbar^2 k^2/2\mu = \hbar\omega$.

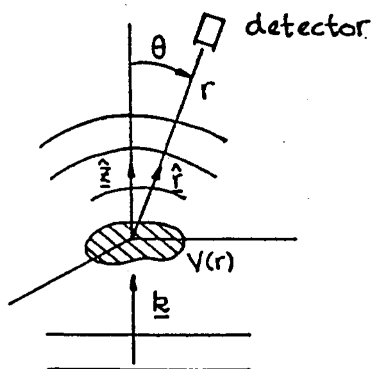

Fig. 6.1. Quantum mechanical view of scattering of a beam of particles by a central potential.

The scattered wave is purposely written in the form of a spherically outgoing wave,

$$\Psi_{sc} = f(\theta) \frac{e^{i(kr - \omega t)}}{r} \tag{6.2}$$

where the scattering amplitude $f(\theta)$ is seen to be the measure of the 'strength' of the scattering.

Once the incident and scattered waves are written down the corresponding currents can be calculated using the relation

$$\underline{J} = \frac{\hbar}{2\mu i} [\Psi^*(\underline{\nabla}\Psi) - \Psi(\underline{\nabla}\Psi^*)] \tag{6.3}$$

Thus the number of particles scattered into an element of surface area $R^2 d\Omega$ per sec as indicated in Fig. 6.1 can be written as $\underline{J} \cdot \underline{\Omega}\, R^2 d\Omega$, and the angular differential scattering cross section is

$$\boxed{\sigma(\theta) = \frac{dN/d\Omega}{J_{in}} = |f(\theta)|^2} \tag{6.4}$$

with $J_{in} = \underline{J}_{in} \cdot \hat{\underline{z}}$. This is the fundamental relation which allows us to determine $\sigma(\theta)$ whenever we know $f(\theta)$; it is analogous to (3.2) in the classical mechanics formulation of the scattering problem.

B. Method of Partial Waves

In this method one finds $f(\theta)$ from the stationary Schroedinger equation through the introduction of phase shift. Starting with (5.70) we defined the inner product $\langle r|\psi(t)\rangle = \Psi(\underline{r},t)$ which is the wave function in coordinate space. Since we are not interested in the time=dependent solution, we can set $\Psi(\underline{r},t) = \psi(\underline{r})\tau(t)$, and find from the Schroedinger equation that $\Psi(\underline{r},t)$ is indeed separable and $\tau(t) = A \exp(-itE/\hbar)$, where A is a constant and E is the separation constant. As a result, (5.70) becomes

$$H\, \psi(\underline{r}) = E\, \psi(\underline{r}) \tag{6.5}$$

where $H = p^2/2\mu + V(r)$ is the Hamiltonian operator (notice we are writing the momentum operator as p instead of P as in Chap. V). It is clear from (6.5) that the separation constant E is in fact the total energy of the particle. Observe that to find the bound states of the particle one would solve (6.5) as an eigenvalue problem with E negative. Here we are looking for scattering state solutions where E is the energy of the incident particle and is therefore manifestly positive.

Our problem is to solve (6.5) in such a way that we can relate the solution to $f(\theta)$. Explicitly (6.5) is the second-order differential equation

$$\boxed{[-\frac{\hbar^2}{2\mu}\nabla^2 + V(r)]\,\psi(\underline{r}) = E\,\psi(\underline{r}),} \tag{6.6}$$

where $E = \hbar^2k^2/2\mu$ is a positive constant. The way we relate $\psi(\underline{r})$ to $f(\theta)$ is to look for a particular solution of the form

$$\boxed{\psi_k(\underline{r}) \xrightarrow[r>>r_o]{} e^{ikz} + f(\theta)\,\frac{e^{ikr}}{r}} \tag{6.7}$$

It is appropriate to regard (6.7) as the boundary condition for the determination of the scattering amplitude. In (6.7) r_o is understood to be the range of force, that is, $V(r) = 0$ for $r > r_o$. The subscript on ψ serves to remind us that the entire analysis is carried out at constant k, thus $f(\theta)$ actually depends on the energy E although this dependence is usually not indicated explicitly.

According to (6.7) in the asymptotic region far away from the scattering potential the wave function is a superposition of an incident plane wave and a spherically outgoing scattered wave. In this region the wave equation is simpler because in (6.6) V(r) can be set equal to zero, and the resulting equation is that of a free particle moving with energy E. Therefore it is the solution to this free-particle equation that we want to match up with the boundary condition in (6.7). It is not difficult to solve the free-particle equation, but our interest really lies in putting the solution in a convenient form to be compared with the right hand side of (6.7). What this means is that we should expand the solution $\psi(\underline{r})$ into a set of partial waves.

It should be evident that the natural coordinate system for the central potential scattering problem is the spherical coordinate, $\underline{r} \longrightarrow (r,\theta,\varphi)$. If the potential is spherically symmetric, then the azimuthal angle φ becomes irrelevant or ignorable. This means that $\psi(\underline{r})$ is only a function of r and θ, and the expansion we want is

$$\psi(r,\theta) = \sum_{\ell} R_\ell(r)\; P_\ell(\cos\theta) \tag{6.8}$$

where $P_\ell(\cos\theta)$ is the Legendre polynomial of order ℓ. Eq.(6.8) is the partial wave expansion of $\psi(\underline{r})$. Each term in this sum is a partial wave which has a definite value of the orbital angular momentum. The set of functions $\{P_\ell(x)\}$ is known to be orthogonal and complete on the interval $-1 \leq x \leq 1$. Some of the properties of $P_\ell(x)$ are:

$$\int_{-1}^{1} dx\, P_\ell(x)\, P_{\ell'}(x) = \frac{2}{2\ell+1}\,\delta_{\ell\ell'} \qquad (6.9)$$

$$P_\ell(1) = 1, \quad P_\ell(-1) = (-1)^\ell \qquad (6.10)$$

$$P_o(x) = 1$$

$$P_1(x) = x$$

$$P_2(x) = \frac{1}{2}(3x^2 - 1)$$

$$P_3(x) = \frac{1}{2}(5x^3 - 3x)$$

Inserting the expansion (6.8) into (6.6) and making a change of dependent variable,

$$R_\ell(r) = u_\ell(r)/r \qquad (6.11)$$

we find the wave equation can be reduced to

$$\boxed{\frac{d^2u_\ell(r)}{dr^2} + [k^2 - \frac{2\mu}{\hbar^2}V(r) - \frac{\ell(\ell+1)}{r^2}]\,u_\ell(r) = 0} \qquad (6.12)$$

with the condition that $u_\ell(0) = 0$ so the wave function $\psi(r,\theta)$ is finite at the origin. Eq.(6.12) is called the radial wave equation; it is a one-dimensional equation whose solution determines the scattering process in three dimensions.

Now we want to look at the solution in the exterior region $(r > r_o)$ where (6.12) becomes the equation for a free particle,

u_ℓ

$$\frac{d^2u}{dr^2} + [k^2 - \frac{\ell(\ell+1)}{r^2}]\,u_\ell = 0 \qquad (6.13)$$

The general solution of (6.13) is known to be of the form

$$u_\ell(r) = B_\ell\, rj_\ell(kr) + C_\ell\, rn_\ell(kr) \qquad (6.14)$$

where B_ℓ and C_ℓ are integration constants to be determined, and j_ℓ and n_ℓ are the spherical Bessel and Neumann functions respectively. The properties of j_ℓ and n_ℓ are well tabulated; for our purposes it is sufficient to note the following:

$$j_o(x) = \frac{\sin x}{x} \qquad\qquad n_o(x) = -\frac{\cos x}{x}$$

$$j_1(x) = \frac{\sin x}{x^2} - \frac{\cos x}{x} \qquad\qquad n_1(x) = -\frac{\cos x}{x^2} - \frac{\sin x}{x}$$

$$j_\ell(x) \xrightarrow[x \to 0]{} \frac{x^\ell}{1\cdot 3\cdot 5 \ldots (2\ell+1)} \qquad\qquad n_\ell(x) \xrightarrow[x \to 0]{} \frac{1\cdot 3\cdot 5 \ldots (2\ell-1)}{x^{\ell+1}}$$

$$j_\ell(x) \xrightarrow[x \to \infty]{} \frac{1}{x} \sin(x - \ell\pi/2) \qquad\qquad n_\ell(x) \xrightarrow[x \to \infty]{} -\frac{1}{x} \cos(x - \ell\pi/2)$$

Using the asymptotic expressions for j_ℓ and n_ℓ with large arguments, we can rewrite the general solution (6.14) as

$$\begin{aligned} u_\ell(r) &\xrightarrow[kr \gg 1]{} \frac{B_\ell}{k} \sin(kr - \ell\pi/2) - \frac{C_\ell}{k} \cos(kr - \ell\pi/2) \\ &= \frac{1}{kr} \sin\left(kr - \frac{\ell\pi}{2} + \delta_\ell\right) \end{aligned} \tag{6.15}$$

where although δ_ℓ is introduced formally as another integration constant, it has the physical significance of the phase shift for the partial wave u_ℓ. Given the result (6.15) the partial wave expansion of $\psi(\underline{r})$ in the asymptotic region becomes

$$\psi(r,\theta) \xrightarrow[kr \gg 1]{} \sum_\ell a_\ell P_\ell(\cos\theta) \frac{\sin(kr - \ell\pi/2 + \delta_\ell)}{kr} \tag{6.16}$$

This is an appropriate form for the left hand side of (6.7). The right hand side also can be put into the same form by expansion in terms of Legendre polynomials. First,

$$\begin{aligned} e^{ikr\cos\theta} &= \sum_\ell i^\ell (2\ell+1)\, j_\ell(kr)\, P_\ell(\cos\theta) \\ &\xrightarrow[kr \gg 1]{} \sum_\ell i^\ell (2\ell+1)\, P_\ell(\cos\theta) \frac{\sin(kr - \ell\pi/2)}{kr} \end{aligned} \tag{6.17}$$

Secondly,

$$f(\theta) = \sum_\ell f_\ell P_\ell(\cos\theta) \tag{6.18}$$

Inserting these expansions into (6.7) and comparing with (6.16), we see that terms on both sides of (6.7) are proportional to either exp(ikr) or exp(−ikr). If (6.7) is to hold in general, the coefficients of each exponential have to be equal. Thus we find

$$f_\ell = \frac{1}{2ik} (-i)^\ell \, [a_\ell \, e^{i\delta_\ell} - i^\ell (2\ell+1)] \tag{6.19}$$

$$a_\ell = i^\ell (2\ell+1) \, e^{i\delta_\ell} \tag{6.20}$$

With these result we can go back to (6.18) and obtain an expression for the scattering amplitude in terms of the phase shifts,

$$\boxed{f(\theta) = \frac{1}{k} \sum_{\ell=0}^{\infty} (2\ell+1) \, e^{i\delta_\ell} \sin \delta_\ell \, P_\ell(\cos\theta)} \tag{6.21}$$

This is the desired resut which relates the phase shifts to the scattering cross sections. Using (6.4) we obtain

$$\sigma(\theta) = \lambdabar^2 \left| \sum_{\ell=0}^{\infty} (2\ell+1) \, e^{i\delta_\ell} \sin \delta_\ell \, P_\ell(\cos\theta) \right|^2 \tag{6.22}$$

and

$$\boxed{\sigma = \int d\Omega \, \sigma(\theta) = 4\pi\lambdabar^2 \sum_{\ell=0}^{\infty} (2\ell+1) \sin^2 \delta_\ell} \tag{6.23}$$

where we have set $\lambdabar = 1/k$. These are well-known expressions in the quantum theory of potential scattering. They are quite general in that there are no restrictions on the incident energy.

We now take up the question of how the phase shift δ_ℓ is to be determined in an actual calculation. Although δ_ℓ was introduced as an integration constant in the solution to the wave equation in the exterior region, its physical meaning indicates that its numerical value depends on the wave function in the interior region as well, since it is the shift in the phase of the wave function in going from the interior region to the exterior region. Recall from the bound state energy level calculations discussed in 22.111 that the phase shift is obtained by matching the interior and exterior solutions to the radial wave equation at $r = r_o$, the range of the interaction. This boundary condition at $r = r_o$ is most

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conveniently applied in terms of the loarithmic derivative g

$$q_\ell \equiv \left[\frac{r}{u_\ell} \frac{du_\ell}{dr} \right]_{r=r_o} \tag{6.24}$$

The equation which determines δ_ℓ is therefore

$$\boxed{q_\ell^{int} = q_\ell^{ext}} \tag{6.25}$$

where q_ℓ^{int} and q_ℓ^{ext} are both defined by (6.24) with u_ℓ being the interior and exterior region solutions respectively. Notice that thus far we have written the exterior region solution as (6.14) but have said nothing yet about the interior region solution which has to come from (6.12).

It is useful to manipulate the exterior region solution further in order to obtain a direct expression for $\exp(i\delta_\ell)\sin\delta_\ell$, the quantity which appears in the differential scattering cross section (6.22). Going back to (6.15) we see that for the chsen normalization of u_ℓ the two integration constants must satisfy $B_\ell = \cos\delta_\ell$ and $C_\ell = -\sin\delta_\ell$. Inserting these relations into (6.15) and defining the quantities

o

a_ℓ a_ℓ

$$u_\ell^{(\pm)} = kr\,[n_\ell(kr) \pm i j_\ell(kr)] \tag{6.26}$$

we can rewrite (6.15) as

a_ℓ/k

$$u_\ell^{ext} = \mathrm{Im}\left[u_\ell^{(+)}\, e^{-i\delta_\ell} \right] \tag{6.27}$$

Therefore the ~~left~~ hand side of (6.25) becomes

right

$$q_\ell^{ext} = \xi\, \frac{\mathrm{Im}\{e^{-i\delta_\ell}\,[du_\ell^{(+)}/d\xi]\}}{\mathrm{Im}[e^{-i\delta_\ell}\, u_\ell^{(+)}]} \tag{6.28}$$

where $\xi = kr_o$. We can avoid writing the imaginary part of a complex quantity in (6.28) by defining still another pair of quantities,

$$q_\ell^{(+)} \equiv \frac{\xi}{u_\ell^{(-)}} \frac{du_\ell^{(-)}}{d\xi} \tag{6.29}$$

and a corresponding definition for $q_\ell^{(-)}$. Notice the reversal of the (±) sign between $q_\ell^{(\pm)}$ and $u_\ell^{(\pm)}$. This is only convention and nothing more! After some algebra we find that (6.28) becomes

$$q_\ell^{ext} = \frac{u_\ell^{(+)} q_\ell^{(-)} - e^{2i\delta_\ell} u_\ell^{(-)} q_\ell^{(+)}}{u_\ell^{(+)} - e^{2i\delta_\ell} u_\ell^{(-)}} \tag{6.30}$$

Eq.(6.30) shows a certain symmetry in the appearance of the quantities $u_\ell^{(\pm)}$. Since they are a conjugate pair, we can express their ratio in terms of a phase angle τ_ℓ by writing

$$u_\ell^{(\pm)} = \frac{1}{\sqrt{v_\ell}} e^{\mp i\tau_\ell} \tag{6.31}$$

or, equivalently,

$$\boxed{\tau_\ell = -\tan^{-1}[j_\ell/n_\ell] = \tan^{-1}[j_\ell/n_\ell]} \tag{6.32}$$

In (6.31) the amplitude $1/\sqrt{v_\ell}$ is of no interest in this discussion, in the literature of nuclear reactions, it is sometimes called the penetration factor. Using (6.31) we can eliminate $u_\ell^{(\pm)}$ in favor of τ_ℓ in (6.30). Then equating the result to q_ℓ^{int} which is still yet to be determined, we obtain

$$\boxed{\eta_\ell \equiv e^{2i\delta_\ell} = e^{-2i\tau_\ell} \frac{q_\ell^{int} - q_\ell^{(-)}}{q_\ell^{int} - q_\ell^{(+)}}} \tag{6.33}$$

This is a classic result in the quantum theory of scattering. Considering all the definitions and manipulations, and the intermediate quantities that we have eliminated, it is a marvelously compact expression. The quantity η_ℓ is related to the so-called scattering matrix which is well-known in scattering theory. For our present interest it is sufficient to note that this form of η_ℓ has a useful interpretation, namely, the effects of scattering can be decomposed into two contributions, one having to do with scattering at the potential surface and is represented by the factor $\exp(2i\tau_\ell)$, and the other arising from interactions within the potential thus involving q_ℓ^{int}. We can expect that it is the second part that will allow us to describe resonances in the cross section.

A direct expression for the factor $\exp(i\delta_\ell)\sin\delta_\ell$ in (6.22) now can be obtained by noting that this combination is just $[\exp(2i\delta_\ell) - 1]/2i$ and using (6.33). One finds

$$e^{i\delta_\ell} \sin \delta_\ell = e^{-2i\tau_\ell} \left[\frac{s_\ell}{q_\ell^{int} - \Delta_\ell - is_\ell} - e^{i\tau_\ell} \sin \tau_\ell \right] \qquad (6.34)$$

where Δ_ℓ and s_ℓ are the real and imaginary parts of $q_\ell^{(\pm)}$,

$$q_\ell^{(\pm)} \equiv \Delta_\ell \pm is_\ell \qquad (6.35)$$

Eq.(6.34) is the expression one should use in an actual calculation. The two kinds of scattering contributions we mentioned are even more evident in this result; the first term in the bracket clearly has a resonance form. If the wave function does not penetrate inside the potential, which is the case for hard sphere scattering, we would expect the first term to be absent and the scattering is entirely due to the second term. For later purposes we remark here that the two terms in (6.34) should be interpreted as the respective contributions from resonance and potential (or shape elastic) scattering.

Hard Sphere Scattering

We have already discussed the classcal mechanics result for this case in Sec. 3.E. For the quantum mechanical treatment this is a degenerate case since physically one has the boundary condition that the wave function must vanish at the range cutoff $r = r_o$ and does not penetrate inside the potential. (Notice that r_o is the range of the potential, and if one is thinking of an actual collision between two hard spheres, then r_o is the diameter of the hard sphere.) Since the logarithmic derivative (6.24) is now infinite, (6.33) reduces to $\delta_\ell = -\tau_\ell$ which confirms our earlier interpretation that to within a sign τ_ℓ is the phase shift due to interaction at the potential surface, or conversely, one can say that shape elastic scattering is the same as scattering from a hard-sphere potential.

One can show (see Mott and Massey, pp. 38 –) that under the condition of $kr_o \ll 1$ which means low incident energy, only the $\ell = 0$ partial wave, s-wave, contribution is important. Then

$$\sigma(\theta) = \sigma(\theta)\big|_{\ell=0} = r_o^2 \qquad (6.36)$$

so the total cross section in the low energy limit is

$$\boxed{\sigma = 4\pi r_o^2 \qquad kr_o \ll 1} \tag{6.37}$$

At the opposite limit of high incident energy, one finds

$$\boxed{\sigma = 2\pi r_o^2 \qquad kr_o \gg 1} \tag{6.38}$$

We see that the quantum mechanical scattering cross section for hard spheres is in general dependent on the incident energy E, and in the limits of low and high energy the cross sections are greater than the classical value of πr_o^2. This difference between the quantum and classical results lies in the effects of diffraction, sometimes known as 'shadow scattering', present in the quantum mechanical treatment; these effects are most pronounced in the forward scattering region in $\sigma(\theta)$.

Partial waves at low energy

One can make a simple semiclassical argument to show that at a given incident energy k (meaning $k = \sqrt{2\mu E}/\hbar$) only those partial waves with $\ell < kr_o$ make significant contributions to scattering. In this argument one considers an impact parameter b which translates into an angular momentum $\hbar\ell = pb$ with linear momentum p being $\hbar k$. Depending on the value of b compared to the potential range r_o, one can say whether or not there is appreciable interaction. Roughly speaking, we expect the scattering to be significant when $b < r_o$, or in other words, only those ℓ values which satisfy the condition $b = \ell/k < r_o$ will contribute to the scattering amplitude. Thus the condition for a partial wave to contribute is

$$\ell < kr_o \tag{6.39}$$

According to (6.39), if $kr_o \ll 1$, then only the $\ell = 0$ partial wave contributes to the scattering. For this case,

$$f(\theta)\Big|_{\ell=0} = \frac{1}{k} e^{i\delta_o} \sin \delta_o \tag{6.40}$$

$$\sigma(\theta) = \frac{1}{k^2} \sin^2 \delta_o \tag{6.41}$$

$$\boxed{\sigma\Big|_{\ell=0} = \frac{4\pi}{k^2} \sin^2 \delta_o \simeq 4\pi a^2} \tag{6.42}$$

From (6.41) we see that s-wave scattering is always isotropic in CMCS regardless of the central potential. In (6.42) the last equality assumes that $\sin\delta_o$ can be replaced by $-ak$, where a is a constant called scattering length. This assumption is valid unless the cross section has a resonance in the vicinity of the energy under consideration. The significance of this last relation is that the both $\sigma(\theta)$ and σ are then constant in energy.

If one includes the $\ell = 1$ (p-wave) contribution in the partial-wave expansion, then

$$f(\theta)\Big|_{s,p} = \frac{1}{k} (e^{i\delta_o} \sin\delta_o + 3e^{i\delta_1} \sin\delta_1 \cos\theta) \tag{6.43}$$

and

$$\sigma(\theta)\Big|_{s,p} = \frac{1}{k^2} (A + B \cos\theta + C \cos^2\theta) \tag{6.44}$$

with $A = \sin^2\delta_o$, $B = 6\cos(\delta_o - \delta_1)\sin\delta_o\sin\delta_1$, $C = 9\sin^2\delta_1$. Usually $\delta_1 < \delta_o$, then C is negligible and $B \simeq 3\delta_1\sin 2\delta_o$. Moreover, $|\delta_o| < \pi/2$, so B is positive. This means $\sigma(\theta)$ will be peaked in the forward direction when p-wave contribution starts to become important.

One can integrate (6.44) to obtain the total cross section,

$$\sigma\Big|_{s,p} = 4\pi\lambda\!\!\!^{-2} (\sin^2\delta_o + 3 \sin^2\delta_1) \simeq \sigma\Big|_s + \theta(\delta_1^2) \tag{6.45}$$

so the p-wave contribution is of order δ_1 in the differential cross section $\sigma(\theta)$ but of order δ_1^2 in σ. It follows that the total cross section is less sensitive to energy variation than $\sigma(\theta)$. Physically the reason for this is that the different partial waves interfere coherently in $\sigma(\theta)$ (absolute value square of sum over ℓ), whereas they interfere incoherently in σ (sum of squares).

There is a simple relation between the scattering amplitude at $\theta = 0$ and the total cross section. From (6.21) we can write

$$\mathrm{Im}[f(\theta=0)] = \frac{1}{k} \sum_{\ell} (2\ell+1) \sin^2 \delta_\ell \tag{6.46}$$

Comparing this with (6.23) we have

$$\sigma = 4\pi\lambda\!\!\!^{-} \,\mathrm{Im}[f(\theta=0)] \tag{6.47}$$

a relation which is called the optical theroem in analogy with a similar relation in optics between the imaginary part of the complex index of refraction and the absorption coefficient; it is a direct consequence of the conservation of probability (cf. Roman, p. 337). Eq.(6.47) holds even when inelastic scattering is present, thus at any energy the scattering amplitude for elastic scattering in the forward direction determines the complete scattering cross section.

There are other related topics which one can take up to round out the discussion of the partial-wave analysis of scattering cross section. In particular, some disucssions of the scattering length a and the so-called effective range theory would be quite appropriate. However, we will defer further discussions (to Chap. VII) to keep this section from being overly long. Interested students can read up on these topics by consulting Roman, pp. 172- and 188- .

C. Integral Equation Method and the Born Approximation

Another approach in the quantum theory of potential scattering is to convert the time-independent Schroedinger equation (6.6) into an integral equation which incorporates the desired boundary condition (6.7). We first rewrite (6.6) as

$$(\nabla^2 + k^2)\,\psi(\underline{r}) = U(r)\,\psi(\underline{r}) \tag{6.48}$$

where we have defined

$$U(r) \equiv \frac{2\mu}{\hbar^2} V(r) \tag{6.49}$$

Suppose we regard the right hand side of (6.48) as an inhomogeneous (or source) term and write the formal solution to (6.48) as the sum of the solution to the homogeneous equation

$$(\nabla^2 + k^2)\,\varphi(\underline{r}) = 0 \tag{6.50}$$

plus a particular solution due to the inhomogeneous term. So one writes

$$\boxed{\psi(\underline{r}) = \varphi(\underline{r}) - \int d^3r'\, G(\underline{r} - \underline{r}')\, U(r')\, \psi(\underline{r}')} \tag{6.51}$$

where $G(\underline{r} - \underline{r}')$ is the Green's function which obeys the equation

$$(\nabla^2 + k^2)\, G(\underline{r} - \underline{r}') = -\,\delta(\underline{r} - \underline{r}') \tag{6.52}$$

The best way to see that (6.51) is indeed a general solution to (6.48) is by direct substitution.

A solution to the homogeneous equation (6.50) is

$$\varphi(\underline{r}) = \exp(i\underline{k}\cdot\underline{r}) \equiv e^{ikz} \tag{6.53}$$

which is just the incident plane wave (cf. (6.1)). The solution to (6.52) is

$$G(\underline{r} - \underline{r}') = \exp\{ik|\underline{r} - \underline{r}'|\} / [4\pi|\underline{r} - \underline{r}'|] \tag{6.54}$$

Since the Green's function (6.54) is a result one may encounter in other problems (because $(\nabla^2 + k^2)$ is an important operator and (6.50) is called the Helmholtz equation in mathematical physics), we will show how this expression can be derived using Fourier transform.

Without any loss of generality we can set $\underline{r}' = 0$ in (6.52). Defining the Fourier transform of $G(\underline{r})$ as $F(\underline{\kappa})$,

$$F(\underline{\kappa}) = \int d^3r\, G(\underline{r}) \exp(-i\underline{\kappa}\cdot\underline{r}) \tag{6.55}$$

we take the Fourier transform of (6.52) to obtain

$$F(\underline{\kappa}) = -(k^2 - \kappa^2)^{-1} \tag{6.56}$$

To find $G(\underline{r})$ we have only to invert (6.56),

$$G(\underline{r}) = (2\pi)^{-3} \int d^3\kappa\, (\kappa^2 - k^2)^{-1} \exp(i\underline{\kappa}\cdot\underline{r}) \tag{6.57}$$

Working as usual in the spherical coordinate system we can carry out the angular integrations immediately since the only dependence is $\exp(i\cancel{k}r\cos\theta)$. κ
The remaining integral over κ becomes

$$G(r) = \frac{1}{2\pi^2}\frac{1}{r}\int_0^\infty d\kappa\, \kappa \sin\kappa r \frac{1}{\kappa^2 - k^2} \tag{6.58}$$

Notice that because $F(\underline{\kappa})$ depends only on the magnitude of $\underline{\kappa}$, its Fourier transform G depends only on the magnitude of $\underline{r}$. Since the integrand in (6.58) is manifestly an even function of κ, we can extend the lower limit of integration from 0 to $-\infty$ and write the integral as

$$G(r) = \frac{1}{4ir\pi^2}\int_{-\infty}^\infty d\kappa\, \kappa \frac{e^{i\kappa r}}{(\kappa + k)(\kappa - k)} \tag{6.59}$$

In this form it is clear that the integrand has two simple poles on the real axis at $\kappa = \pm k$. We will treat (6.59) as a contour integral along the path shown in Fig. 6.2. This choice gives a contribution from the pole at

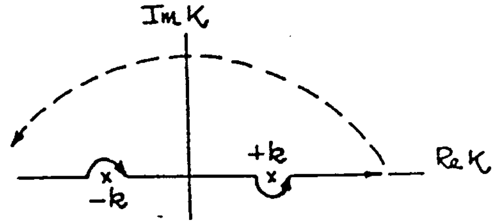

Fig. 6.2. Contour path for determining the Green's function

κ = k and no other contributions. Thus,

$$\boxed{G(r) = \frac{e^{ikr}}{4\pi r}} \tag{6.60}$$

which is the desired result (6.54). Our choice of the contour is seen to give a spherically outgoing wave for G(r) which coincides with our requirement for the boundary condition (6.7). Choosing the contour to include the pole at −k would have given a spherically incoming wave. (What would one get by including both poles?)

Now that we have derived (6.54) we can insert this result into (6.51) and write out the integral equation explicitly

$$\psi(r) = e^{ikz} - \int d^3r' \; [\exp\{i\overset{k}{\cancel{\kappa}}|\underline{r} - \underline{r}'|\}/4\pi|\underline{r} - \underline{r}'|] \; U(r') \; \psi(\underline{r}') \tag{6.61}$$

We will refer to (6.61) as the integral equation of scattering; it is entirely equivalent to the Schroedinger since we have made no approximation. Its advantage is that the boundary condition (6.7) has been explicitly incorporated. However, it is not yet in a form that one can directly extract the scattering amplitude $f(\theta)$. Because we are only interested in the solution to the wave equation in the asymptotic region of large r we can simplify (6.61) by noting that the presence of U(r') means the integral over r' will be restricted to $r' \le r_o$, the potential range. Thus using the fact that $r'/r \ll 1$ we can write

$$|\underline{r} - \underline{r}'| \simeq r - \hat{\underline{r}} \cdot \underline{r}' \tag{6.62}$$

in the exponent in (6.61) and simply take r for $|\underline{r} - \underline{r}'|$ in the denominator. Then (6.61) becomes

$$\psi(\underline{r}) \xrightarrow[r \gg r_o]{} e^{ikz} - \frac{1}{4\pi}\frac{e^{ikr}}{r} \int d^3r' \; U(r') \; \psi(\underline{r}') \exp(-ik\,\hat{\underline{r}} \cdot \underline{r}') \tag{6.63}$$

Comparing this with (6.7) we obtain

$$f(\theta) = -\frac{1}{4\pi} \int d^3r \; U(r) \; \psi(\underline{r}) \exp(-i\underline{k}\cdot\underline{r}) \tag{6.64}$$

where we have defined the wavevector $\underline{k}$ as $\underline{k} \equiv k\hat{\underline{r}}$.

Eq.(6.64) is a formal expression for the scattering amplitude since it still involves the unknown wave function $\psi(\underline{r})$. To turn it into a useful result we will introduce a particular approximation for $\psi(\underline{r})$.

The Born Approximation

A well-known method of solving an inhomogeneous integral equation is to iterate with the inhomogeneous term assuming the integral kernel in the equation is 'weak' is some sense. This is a perturbation approach which generates a solution in the form of a series expansion, sometimes called the Neumann series. Under the right condition one can truncate this series and obtain a useful approximate solution directly, or one can try to sum up part of the infinite series and achieve an approximate solution which has an expansion to infinite orders in some parameter but is not the original series. For our present purposes we will adopt the former approach of truncating the series solution.

If we ignore entirely the integral term in (6.61) we would obtain the zeroth-order solution,

$$\psi^{(o)}(\underline{r}) = e^{ikz} \tag{6.65}$$

The next approximation is to insert $\psi^{(o)}$ into the integral term in (6.61) - which then gives the first-order solution, In the asymptotic region we have from (6.63),

$$\psi^{(1)}(\underline{r}) \xrightarrow[r>>r_o]{} e^{ikz} - \frac{1}{4\pi}\int d^3r' \exp(-i\underline{k}\cdot\underline{r}')U(r')\exp(i\underline{k}'\cdot\underline{r}') \tag{6.66}$$

where we have set $\underline{k}' \equiv k\hat{\underline{z}}$. Eq.(6.66) is known as the <u>first Born approximation</u>; its immediate consequence is that the scattering amplitude is now given by

$$\boxed{f(\theta) = -\frac{2\mu}{4\pi\hbar^2}\int d^3r \exp(i\underline{\kappa}\cdot\underline{r})\, V(r)} \tag{6.67}$$

where we have defined the wave vector transfer

$$\underline{\kappa} \equiv \underline{k}' - \underline{k} \tag{6.68}$$

This is a very significant result because it shows that $f(\theta)$, or the differential scattering cross section $\sigma(\theta)$, can be obtained directly from the scattering potential V(r) simply by taking its Fourier transform. Compared to the method of partial wave analysis, this is a much simpler calculation.

One should notice the physical significance of the Fourier transform variable in the Born approximation result for $f(\theta)$. According to (6.68) $\underline{\kappa}$ is the difference between $\underline{k}' = k\hat{\underline{z}}$ and $\underline{k} = k\hat{\underline{r}}$. Referring to Fig. 6.1 we see these two vectors are the incoming and outgoing (scattered) wave vectors. Thus $\hbar\underline{\kappa}$ is the momentum transfer in the scattering process. Since the scattering angle θ is the angle between incoming and outgoing directions, and $|\underline{k}| = |\underline{k}'|$, the magnitude of $\underline{\kappa}$ is

$$\kappa \;=\; 2k\,\sin(\theta/2) \tag{6.69}$$

So the angular dependence in $f(\theta)$ in the Born approximation is in the wave vector transfer κ.

Validity of the Born Approximation

Given the remarkable simplicity of the Born approximation and the apparently wide applicability potential of the result (6.67), it is important to consider the conditions where the approximation should be valid. We will find that there exist a high-energy condition and a low-energy condition. Also it is possible to establish a connection between the Born approximation approach and the method of partial wave analysis.

For the Born series to converge, clearly the successive terms generated by iterating the lower-order solutions must be small compared to the leading term in the approximation. This means we can set

$$|\psi^{(1)}(r) - \psi^{(o)}(r)| \;\ll\; \psi^{(o)}(r) \tag{6.70}$$

n as the condition for validity. Instead of using (6.66) for $\psi^{(1)}$ we will go ~~be even more approximate by going~~ back to (6.6~~3~~1) ~~and ignoring the exponential $\exp(-ik\hat{r}\cdot\underline{r}')$ in the integrand.~~ Then by evaluating both sides in (6.70) at $r = 0$, we have

$$\Delta \;\equiv\; \left|\frac{1}{4\pi}\int \frac{d^3\underline{r}}{r}\, \exp(ikr + i\underline{k}'\cdot\underline{r})\, U(r)\right| \;\ll\; 1 \tag{6.71}$$

$\hookrightarrow |\underline{k}'| = k$

For the evaluation of (6.71) we will consider a square-well potential (cf. Sec. 3.E) of depth V_o and range r_o. With this potential one can readily carry out the angular and radial integrations to give

$$\Delta \;=\; \frac{\mu V_o}{\hbar^2 k}\left|\int_o^{r_o} dr\,(e^{2ikr} - 1)\right|$$

$$=\; \frac{\mu V_o}{2\hbar^2 k^2}\left|e^{2ikr_o} - 2ikr_o - 1\right|$$

$$=\; \frac{\mu V_o}{2\hbar^2 k^2}\,(y^2 + 2 - 2y\sin y - 2\cos y)^{1/2} \;\ll\; 1 \tag{6.72}$$

where $y \equiv 2kr_o$.

The inequality (6.72) can be satisfied for either small or large y. For $kr_o \gg 1$, the square root quantity behaves like y. Then (6.72) gives

$$\boxed{\frac{V_o r_o}{\hbar v} \ll 1} \tag{6.73}$$

where we have introduced the particle velocity $v = \hbar k/\mu$. This is the high–energy condition. In the opposite limit of $kr_o \ll 1$, the square root becomes $y^4/4$ to lowest order. Thus condition (6.72) gives

$y^2/2$

$$\boxed{\frac{\mu V_o r_o^2}{\hbar^2} \ll 1} \tag{6.74}$$

which is the low–energy condition. We will see later that in the case of electron scattering (Chap. VIII) the use of the Born approximation is justified on the basis of (6.73), whereas in the case of thermal neutron scattering (Chap. IX) the Born approximation is justified on the basis of (6.74).

It is helpful to know that there is a way to connect the Born approximation result with the method of partial waves (see Mott and Massey, p. 119). We can rewrite (6.61) as

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$$f(\theta) = -\frac{2\mu}{\hbar^2}\int_o^\infty V(r)\,\frac{\sin \kappa r}{\kappa r}\, r^2\, dr \tag{6.75}$$

and (6.21) as

$$f(\theta) = \frac{1}{2ik}\sum_{\ell=0}^{\infty} (2\ell+1)(e^{2i\delta_\ell} - 1)\, P_\ell(\cos\theta) \tag{6.76}$$

It can be shown (Mott and Massey, p. 28) that when δ_ℓ is small, it may be calculated from

$$\delta_\ell \simeq -\frac{2\mu k}{\hbar^2}\int_o^\infty V(r)\,[f_n(r)]^2\, r^2\, dr \tag{6.77}$$

with

$$f_n(r) = (\pi/2kr)^{1/2}\, J_{n+1/2}(kr) \tag{6.78}$$

where $J_n(x)$ is the Besse function. Combining (6.77) with (6.76) one obtains the same expression as (6.75) because of the following identity (Watson, <u>Theory of Bessel Functions</u>, p. 363)

$$\sum (2\ell+1)\ P_\ell(\cos\theta)[f_n(r)]^2 \ = \ \frac{\sin \kappa r}{\kappa r} \tag{6.79}$$

This connection is possible only if one can replace $\exp(2i\delta_\ell) - 1$ in (6.76) by $2i\delta_\ell$, and this is justified if $\delta_\ell << 1$. Thus we have found equivalence between the two methods of calculating $f(\theta)$ when the phase shift is small, or in other words, when the scattering is weak. This condition is quite reasonable in view of our preceding discussion about the validity of the Born approximation.