Chapter 11

Elementary Scattering Theory

As seen in the previous chapter, the bound state problem is characterized through the stationary, normalizable states in the Hilbert space. Since quantum mechanical states in principle always have to be normalized (because of the statistical interpretation of the wave functions), scattering states should be **non-stationary**, normalizable solutions of the Schrödinger equation.

An elementary, conceptually not quite satisfactory, however, in practical applications extremely successful approach, consists of dropping the normalization condition. This allows to introduce scattering states as suitably chosen **stationary**, non-normalizable solutions of the Schrödinger equation. Stationary states are in principle eigenstates of the Hamiltonian. If they are supposed to be non-normalizable, they have to be special solutions from the **continuous** spectrum of H.

11.1 Free Motion

The force free, single particle motion (free motion) is given by a Hamiltonian, often called free Hamiltonian,

$$H_0 \;=\; \frac{\vec{P}^{\,2}}{2m} \;. \tag{11.1}$$

Possible eigenvalues of H_0 are the momentum eigenstates defined by

$$\vec{P} \mid \varphi_{\vec{p}}\rangle \;=\; \vec{p} \mid \varphi_{\vec{p}}\rangle \;. \tag{11.2}$$

With (11.2) and (11.1) follows

$$H_0 \mid \varphi_{\vec{p}}\rangle \;=\; \frac{\vec{P}^{\,2}}{2m} \;\mid \varphi_{\vec{p}}\rangle \;=\; E_p \;\mid \varphi_{\vec{p}}\rangle \;, \tag{11.3}$$

the "norm" of those states can be chosen as

$$\langle \varphi_{\vec{p}\,'} \mid \varphi_{\vec{p}}\rangle \;=\; \delta(\vec{p}\,' - \vec{p}) \;. \tag{11.4}$$

The specific form of $\mid \varphi_{\vec{p}}\rangle$ is obtained when the explicit representation of the operator $\vec{P}$ in coordinate space is employed:

$$\langle \vec{x} \mid \vec{P} \mid \varphi_{\vec{p}}\rangle \;=\; \frac{\hbar}{i}\,\vec{\nabla}\,\langle \vec{x} \mid \varphi_{\vec{p}}\rangle \;=\; \frac{\hbar}{i}\,\vec{\nabla}\,\varphi_{\vec{p}}(\vec{x}) \;=\; \vec{p}\,\varphi_{\vec{p}}(\vec{x}) \;, \tag{11.5}$$

which has as solution of the differential equation

$$\varphi_{\vec{p}}(\vec{x}) \;=\; \frac{1}{(2\pi\hbar)^{3/2}}\, e^{\frac{i}{\hbar}\,\vec{p}\cdot\vec{x}} \;:=\; \langle \vec{x} \mid \vec{p}\rangle \;, \tag{11.6}$$

which corresponds to a plane wave. The norm is explicitly given as

$$\langle \varphi_{\vec{p}} \mid \varphi_{\vec{p}}\rangle \;=\; \frac{1}{(2\pi\hbar)^{3}} \int d^3x\; e^{-\frac{i}{\hbar}\,\vec{p}\,'\cdot\vec{x}}\, e^{\frac{i}{\hbar}\,\vec{p}\cdot\vec{x}} \;=\; \delta(\vec{p}\,' - \vec{p}) \;, \tag{11.7}$$

thus, the norm in a regular sense does not exist.

In general, the time evolution of solutions of the **free Schrödinger equation** is given by

$$-\frac{\hbar}{i}\,\frac{d}{dt}\;\mid \varphi(t)\rangle \;=\; H_0 \mid \varphi(t)\rangle \tag{11.8}$$

with the solution

$$\mid \varphi(t)\rangle \;=\; e^{-\frac{i}{\hbar}\,H_0 t}\;\mid \varphi\rangle \;. \tag{11.9}$$

With $\mid \varphi_{\vec{p}}\rangle$ as starting vector follows with (11.3)

$$\mid \varphi_{\vec{p}}(t)\rangle \;=\; e^{-\frac{i}{\hbar}\,E_p t}\;\mid \varphi_{\vec{p}}\rangle \;. \tag{11.10}$$

This is a stationary solution with the typical time dependence given in a phase factor. It is obviously not normalizable

$$\langle \varphi_{\vec{p}\,'}(t) \mid \varphi_{\vec{p}}(t)\rangle \;=\; \langle \varphi_{\vec{p}\,'} \mid \varphi_{\vec{p}}\rangle \;=\; \delta(\vec{p}\,' - \vec{p}) \;. \tag{11.11}$$

Inserting (11.6) into (11.10) gives the explicit representation

$$\varphi_{\vec{p}}(\vec{x},t) \;=\; e^{-\frac{i}{\hbar}\,E_p t}\,\varphi_{\vec{p}}(\vec{x}) \;=\; \frac{1}{(2\pi\hbar)^{3/2}}\, e^{\frac{i}{\hbar}\,(\vec{p}\cdot\vec{x} - E_p t)} \;, \tag{11.12}$$

which is just the De-Broglie wave. In coordinate space, the physical interpretation of (11.12) can be readily studied. We have a plane wave. Positions with the same phase

$$\vec{p}\cdot\vec{x} \ - \ E_p t \ = \ \text{constant} \tag{11.13}$$

spread with the phase velocity

$$\vec{v}_{ph} \ = \ \frac{d\vec{x}}{dt} \ = \ \frac{E_p}{p}\,\hat{p} \ = \ \frac{1}{p}\,\frac{p^2}{2m}\,\hat{p} \ = \ \frac{p}{2m}\,\hat{p} \ = \ \frac{v}{2}\,\hat{p} \ , \tag{11.14}$$

where $\hat{p} = \vec{p}/ \mid \vec{p} \mid$ indicates the direction of the spread. This leads intuitively to the fact that plane waves are used to describe the motion of quanta with a definite starting momentum $\vec{p}$.

11.2 Free Wave Packets

Especially at the beginning, it is useful to understand that in principle we should have described the free motion with a normalizable state $\mid \varphi_a\rangle$. We should work with a packet

$$\mid \varphi_a\rangle \ = \ \int d^3p \ \mid \varphi_{\vec{p}}\rangle\langle\varphi_{\vec{p}} \mid \varphi_a\rangle \ = \ \int d^3p \ \mid \varphi_{\vec{p}}\rangle \ \tilde{\varphi}_a(\vec{p}) \ , \tag{11.15}$$

where $\tilde{\varphi}_a(\vec{p})$ is the **experimentally** given distribution of momenta, e.g., around a specific value $\vec{p}_a$. Of course, we can assume that this distribution is finite, so that the integral over $\mid \tilde{\varphi}_a(\vec{p}) \mid^2$ exists and can be set to one. This means, we can require

$$\parallel \varphi_a \parallel^2 = \ \langle\varphi_a \mid \varphi_a\rangle \ = \ \int d^3p \ \langle\varphi_a \mid \varphi_{\vec{p}}\rangle\langle\varphi_{\vec{p}} \mid \varphi_a\rangle \ = \ \int d^3p \ \mid \tilde{\varphi}_a(\vec{p}) \mid^2 = \ 1 \ . \tag{11.16}$$

In contrast to $\mid \varphi_{\vec{p}}\rangle$ this normalizable state $\mid \varphi_a\rangle$ is **not** an eigenvector of H_0 to a definite energy E, since

$$H_0 \mid \varphi_a\rangle \ = \ \int d^3p \ H_0 \mid \varphi_{\vec{p}}\rangle \ \tilde{\varphi}_a(\vec{p}) \ = \ \int d^3p \ \frac{p^2}{2m} \ \mid \varphi_{\vec{p}}\rangle \ \tilde{\varphi}_a(\vec{p}) \ \neq \ E \mid \varphi_a\rangle \ . \tag{11.17}$$

The general solution (11.9) of the time-dependent Schrödinger equation (11.8) reads with the initial state $\mid \varphi_a\rangle$:

$$\mid \varphi_a(t)\rangle \ = \ \int d^3p \ e^{-\frac{i}{\hbar}H_0 t} \ \mid \varphi_{\vec{p}}\rangle \ \tilde{\varphi}_a(\vec{p}) \ = \ \int d^3p^{-\frac{i}{\hbar}\ \frac{p^2}{2m}\ t} \ \mid \varphi_{\vec{p}}\rangle \ \tilde{\varphi}_a(\vec{p}) \ , \tag{11.18}$$

and similarly to (11.17) the time dependence cannot be pulled in front of the integral. One has instead

$$\mid \varphi_a(t)\rangle \ \neq \ e^{-\frac{i}{\hbar}\ Et} \ \mid \varphi_a\rangle \ . \tag{11.19}$$

Using (11.12) we obtain for the wave packet in coordinate space representation

$$\varphi_a(\vec{x},t) \;=\; \frac{1}{(2\pi\hbar)^{3/2}} \int d^3p \; e^{\frac{i}{\hbar}\,(\vec{p}\cdot\vec{x}-E_p t)}\; \tilde{\varphi}_a(\vec{p}) \; . \tag{11.20}$$

It can be shown that for a general initial state $\mid \varphi(0)\rangle$ the explicit time evolution is given by

$$\varphi(\vec{x},t) \;=\; \left(\frac{m}{2\pi i\hbar t}\right)^{3/2} \int d^3x' \; e^{\frac{i}{\hbar}\,\frac{m}{2t}\,(\vec{x}-\vec{x}\;')^2}\; \varphi(\vec{x},0) \; . \tag{11.21}$$

Estimating the absolute value gives

$$\begin{aligned} \mid \varphi(\vec{x},t) \mid \;&\leq\; \frac{1}{\mid t \mid^{3/2}} \left|\frac{m}{2\pi i\hbar}\right|^{3/2} \int d^3x' \;\; \mid e^{\frac{im}{2\pi t}(\vec{x}-\vec{x}')^2} \mid \mid \varphi(\vec{x}) \mid \\ &=\; \frac{\text{constant}}{\mid t \mid^{3/2}} \; . \end{aligned} \tag{11.22}$$

Thus for the probability density, we obtain

$$\rho(\vec{x},t) \;= \mid \varphi(\vec{x},t) \mid^2 \leq \frac{\text{constant}}{\mid t \mid^{3/2}} \; . \tag{11.23}$$

However, the total probability, which corresponds to the conservation of the number of particles is given by

$$\begin{aligned} \| \varphi(t) \|^2 \;&=\; \langle\varphi(t) \mid \varphi(t)\rangle \;=\; \langle e^{-\frac{i}{\hbar}\,H_0 t}\,\varphi(0) \mid \; e^{-\frac{i}{\hbar}\,H_0 t}\,\varphi(0)\rangle \\ &=\; \langle\varphi(0) \mid \varphi(0)\rangle \;= \| \varphi(0) \|^2 \; . \end{aligned} \tag{11.24}$$

This means that the total probability is independent of t; however, in (11.21) one has to integrate over increasingly larger areas in order to compensate the $\frac{1}{|t|^{3/2}}$ behavior.

11.3 Scattering States

As we saw with respect to the free motion, the energy eigenvalues in the continuous spectrum are infinitely degenerate. In this simple case, it was possible to **explicitly** give the physically realized solutions, the plane waves. If a potential V is present, this is in general no longer the case. Here we need **boundary conditions** in order to pick the physically relevant solutions among the infinitely many possible solutions.

Asymptotic Conditions:
If we assume that the region of the interaction V is specially restricted (short-ranged

potential), then it seems plausible to assume that the scattering solution $|\,\psi_{\vec{p}}^{(+)}\rangle$ consists of a superposition of the free solution and a scattering piece $|\,\psi_{p}^{sc}\rangle$, which is given by the potential. According to the previous discussion, one chooses as the free solution the momentum state $|\,\varphi_{\vec{p}}\rangle$. We, therefore, assume that the solution of the **full** eigenvalue equation, which is associated with an incoming particle with sharp momentum $\vec{p}$,

$$H\,|\,\psi_{\vec{p}}^{(+)}\,\rangle \;=\; E\,|\,\psi_{\vec{p}}^{(+)}\rangle \;=\; \frac{p^2}{2m}\;|\,\psi_{\vec{p}}^{(+)}\rangle \tag{11.25}$$

can be written as

$$|\,\psi_{\vec{p}}^{(+)}\rangle \;=|\,\varphi_{\vec{p}}\rangle \,+\; |\,\psi_{\vec{p}}^{sc}\rangle\;. \tag{11.26}$$

In principle, this is not yet a real statement, since one can always separate a piece $|\,\varphi_{\vec{p}}\rangle$ off any vector (which is normalized on a δ function). The ansatz (11.26) becomes less trivial if we assume that the piece $|\,\psi_{\vec{p}}^{sc}\rangle$ is caused by the potential, and thus vanishes if the potential vanishes. This transition can be achieved by multiplying a given potential with a factor λ and one studies the limit $\lambda \to 0$.

In order to obtain a detailed requirement for $|\,\psi_{\vec{p}}^{sc}\rangle$, we use the coordinate space representation. Here (11.26) reads

$$\psi_{\vec{p}}^{(+)}(\vec{x}) \;=\; \frac{1}{(2\pi\hbar)^{3/2}}\;e^{\frac{i}{\hbar}\;\vec{p}\cdot\vec{x}} \;+\; \psi_{\vec{p}}^{sc}(\vec{x})\;. \tag{11.27}$$

As already mentioned, $\psi_{\vec{p}}^{sc}(\vec{x})$ is in general in a complicated way given by the potential V. If one considers how the influence of a perturbation (here a short-ranged potential) influences a plane wave, it is reasonable to require as physically motivated boundary condition that $\psi_{\vec{p}}^{(+)}(\vec{x})$ behaves asymptotically as an outgoing spherical wave, i.e.,

$$\psi_{\vec{p}}^{sc}(\vec{x}) \;\overset{r\to\infty}{\longrightarrow}\; \frac{1}{(2\pi\hbar)^{3/2}}\;f_E(\hat{x},\hat{p})\;\frac{e^{\frac{i}{\hbar}\;pr}}{r}\;, \tag{11.28}$$

where $E = \frac{p^2}{2m}$. With this we fix the scattering solution as the specific solution of (11.25) for which in the coordinate space representation the condition (11.28) holds. This means they are defined by the following requirements

$$\left[-\,\frac{\hbar^2}{2m}\;\vec{\nabla}^2 \;+\; V(\vec{x})\right]\;\psi_{\vec{p}}^{(+)}(\vec{x}) \;=\; E\;\psi_{\vec{p}}^{(+)}(\vec{x}) \tag{11.29}$$

$$\psi_{\vec{p}}^{(+)}(\vec{x}) \;\overset{r\to\infty}{\longrightarrow}\; \frac{1}{(2\pi\hbar)^{3/2}}\;\left[e^{\frac{i}{\hbar}\;\vec{p}\cdot\vec{x}} \;+\; f_E(\hat{x},\hat{p})\;\frac{e^{\frac{i}{\hbar}\;pr}}{r}\right]\;. \tag{11.30}$$

The factor $f_E(\hat{x},\hat{p})$ is a measure for the magnitude of the scattering part $\psi_{\vec{p}}^{sc}(\vec{x})$ of the scattering solution and is called **scattering amplitude**. According to our assumptions $f_E(\hat{x},\hat{p})$ has to vanish if the potential is zero. The condition (11.30) is also known as **Sommerfeld Radiation Condition**.

11.4 Cross Section

The scattering of a particle under the influence of a potential can be described in the following fashion. From the incoming current $\vec{j}_0$ of particles the scattering process creates a current $\vec{j}^{sc}$ of scattered particles.

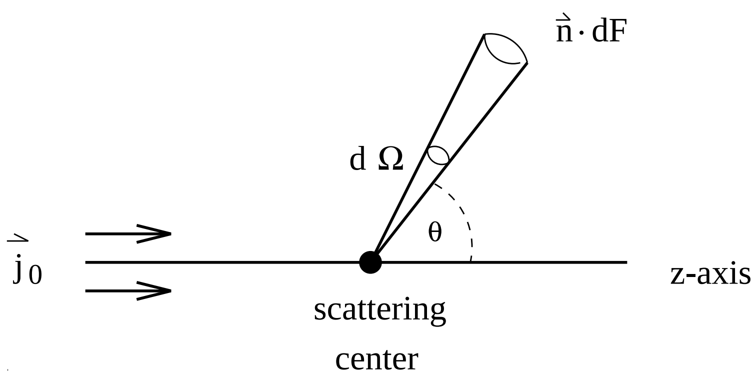

Fig. 11.1

Explanation of the differential cross section.

Experimentally one measures at a distance r from the scattering center the probability current which penetrates through an area

$$dF \;=\; r^2 \, d\Omega \; . \tag{11.31}$$

Here $d\Omega$ is a solid angle which is given by the resolution of the detector (ideally $d\Omega$ is infinitesimally small). This current is then related to the incoming current, i.e., one considers the quantity

$$d\sigma \;=\; \frac{\vec{j}^{sc} \cdot \vec{n} \; dF}{\mid \vec{j}_0 \mid} \;=\; \frac{\vec{j}^{sc} \cdot \vec{n} \; r^2 \; d\Omega}{\mid \vec{j}_0 \mid} \; . \tag{11.32}$$

Here $\vec{n}$ characterizes the location of the areal element dF through which the scattered particles penetrate. This definition (11.32) shows that $d\sigma$ has the dimension of an **area**. The current is given by the probability density multiplied by the velocity. For the incoming plane wave, this means

$$\vec{j}_0 \;=\; \left| \frac{1}{(2\pi\hbar)^{3/2}} \, e^{\frac{i}{\hbar} \; \vec{p}\cdot\vec{x}} \right|^2 \vec{v} \;=\; \frac{\vec{v}}{(2\pi\hbar)^{3/2}} \; , \tag{11.33}$$

whereas for the scattered wave

$$\vec{j}^{sc} = |\, \psi^{sc}\,|^2 \;\; v' \cdot \vec{n} \;=\; \left| \frac{1}{(2\pi\hbar)^{3/2}}\; f_E(\hat{x}, \hat{p})\; \frac{1}{r}\; e^{\frac{i}{\hbar}\, pr} \right|^2 \; v'\vec{n}$$
$$= \frac{|\, f_E(\hat{x}, \hat{p})\,|^2}{r^2}\; \frac{v'}{(2\pi\hbar)^3}\; \vec{n}\;. \tag{11.34}$$

Here the current points in direction of $\vec{n}$, i.e., it is perpendicular to the corresponding spheres whose center is given by the scattering center. Inserting (11.33) and (11.34) into (11.32) leads to

$$d\sigma \;=\; |\, f_E(\hat{x}, \hat{p})\,|^2 \;\; \frac{v'}{v}\; d\Omega \;=\; |\, f_E(\hat{x}, \hat{p})\,|^2 \;\; \sqrt{\frac{E'}{E}}\; d\Omega\;. \tag{11.35}$$

The factor $\frac{1}{r^2}$ in (11.34) is canceled through the multiplication with the factor r^2 from the area dF in (11.31). This is important since then the result (11.35) does not depend on the distance r at which the detector is positioned. Experimentally one only has to make sure that this detector is positioned **outside** the interaction region, where the asymptotic conditions are realized. When considering short-ranged potentials, this is trivially fulfilled, however, leads to complications when considering the quantum mechanical treatment of Coulomb scattering.

In (11.33) and (11.34) v and v' denote the velocity of the incoming and outgoing particles. Correspondingly the factor

$$\frac{v'}{v} \;=\; \frac{p'}{p} \;=\; \sqrt{\frac{E'}{E}} \tag{11.36}$$

occurs in (11.35). However, in the here considered case of potential scattering $v = v'$, a condition which as been assumed in the asymptotic condition (11.30). Scattering with $v = v'$ is also called **elastic scattering**. From (11.35) we derive that the **differential cross section** $\frac{d\sigma}{d\Omega}$ is given through the scattering amplitude $f_E(\hat{x}, \hat{p})$ according to

$$\frac{d\sigma}{d\Omega} \;=\; |\, f_E(\hat{x}, \hat{p})\,|^2 \;\;. \tag{11.37}$$

The amplitude f_E has obviously the dimension of a **length**, which can be immediately seen from (11.30). In (11.35) the factor (11.36) has been considered explicitly to point out that in, e.g., inelastic processes energy can be lost in the scattering process, e.g., through the excitation of composite targets, and then the factors (11.36) have to occur in the cross section.

Spatial Symmetries

if the potential is rotationally symmetric or has an axial symmetry with respect to the direction $\hat{p}$ of the incoming current, one has to expect that the scattering amplitude will only depend on the azimuthal angle θ with respect to the direction of the incoming particle. Choosing the incoming direction as z-axis, we obtain for the asymptotic condition (11.30)

$$\psi_{\vec{p}}^{(+)}(\vec{x}) \overset{r\to\infty}{\longrightarrow} \frac{1}{(2\pi\hbar)^{3/2}} \left[e^{\frac{i}{\hbar}\, pz} \;+\; f_E(\theta)\, \frac{e^{\frac{i}{\hbar}\, pr}}{r} \right] \tag{11.38}$$

and the differential cross section becomes

$$\frac{d\sigma}{d\Omega} = |\; f_E(\theta)\; |^2 \;\; . \tag{11.39}$$

Total Cross Section

If one sums up the scattering into all different directions, i.e., integrates the differential cross section over all angles, one obtains the total cross section

$$\sigma_{tot} \;=\; \int d\Omega\, \frac{d\sigma}{d\Omega} \;=\; \int d\Omega \;\; |\; f_E(\hat{x},\hat{p})\; |^2 \;\; . \tag{11.40}$$

If the potential has the symmetries leading to (11.39), then this definition simplifies to

$$\begin{aligned} \sigma_{tot} \;=\; \int d\Omega \;\; |\; f_E(\theta)\; |^2 \;&=\; \int_0^{\pi} \int_0^{2\pi} \sin\theta\; d\theta\; d\varphi \;\; |\; f_E(\theta)\; |^2 \\ &=\; 2\pi \int_{-1}^{1} d\cos\theta \;\; |\; f_E(\theta)\; |^2 \;\; . \end{aligned} \tag{11.41}$$

In the preceding discussion we introduce the probability current densities by multiplying the probabilities with the corresponding velocities, as is customary in electro dynamics, where charge density times velocity is introduced as current density. This is a quite intuitive procedure and leads quickly to the desired results. However, we could also have used the more formal definition of a current density

$$\vec{j}(\vec{x},t) \;=\; \frac{\hbar}{m} \Im m(\psi^*(\vec{x},t)\vec{\nabla}\; \psi(\vec{x},t)) \; . \tag{11.42}$$

The current of the incoming particles is then obtained by inserting the plane wave:

$$\begin{aligned} \vec{j}_0(\vec{x},t) \;&=\; \frac{\hbar}{m} \Im m \left[\frac{1}{(2\pi\hbar)^3}\; e^{-\frac{i}{\hbar}\, \vec{p}\cdot\vec{x}}\; \vec{\nabla}\; e^{\frac{i}{\hbar}\, \vec{p}\cdot\vec{x}} \right] \\ &=\; \frac{\hbar}{m}\, \frac{1}{(2\pi\hbar)^3}\; \Im m \left(\frac{i}{\hbar}\; \vec{p} \right) \;=\; \frac{\vec{p}/m}{(2\pi\hbar)^3} \; , \end{aligned} \tag{11.43}$$

a result which coincides with (11.33). Similarly, we can determine the current of scattering particles in direction $\vec{n}$ and obtain

$$
\begin{aligned}
j_r^{sc} \;=\; \vec{n}\cdot\vec{j}^{sc}(\vec{x},t) \;&=\; \frac{\hbar}{m}\Im m\left[\psi^{sc*}(\vec{x},t)\vec{n}\cdot\vec{\nabla}\;\psi^{sc}(\vec{x},t)\right] \\
&=\; \frac{\hbar}{m}\Im m\left[\psi^{sc*}(\vec{x},t)\;\frac{\partial}{\partial r}\;\psi^{sc}(\vec{x},t)\right]\;.
\end{aligned}
\tag{11.44}
$$

Here we used that $\vec{n} = \frac{\vec{x}}{r}$, from which follows $\vec{n}\cdot\vec{\nabla} = \frac{\vec{x}}{r}\cdot\vec{\nabla} = \frac{\partial}{\partial r}$. Now we need the scattered current at the place of the detector, i.e., large r, and thus can use (11.30). This gives

$$
\begin{aligned}
j_r^{sc} \;&=\; \vec{n}\cdot\vec{j}^{sc}(\vec{x},t) \;\overset{r\to\infty}{\longrightarrow}\; \frac{\hbar}{m}\,\frac{1}{(2\pi\hbar)^3}\Im m\left[\frac{f_E^*(\hat{x},\hat{p})}{r}\;\frac{i}{\hbar}\;p\;\frac{f_E(\hat{x},\hat{p})}{r}\right] \\
&+\;\text{higher orders in}\;\left(\frac{1}{r}\right)\;.
\end{aligned}
\tag{11.45}
$$

Aside from higher orders, which are negligible for sufficiently large r, we obtain

$$
\vec{n}\cdot\vec{j}^{sc} \;\overset{r\to\infty}{\longrightarrow}\; \frac{1}{(2\pi\hbar)^3}\;\frac{|\;f_E(\hat{x},\hat{p})\;|^2}{r^2}\;\frac{p}{m}\;,
\tag{11.46}
$$

which corresponds to (11.34). Inserting (11.43) and (11.45) into (11.32), where now automatically $p' = p$, we obtain the differential cross section (11.37).

11.5 Phase Shifts

The task is to determine $f_E(\theta,\varphi)$, i.e., the solution of the Schrödinger equation

$$
-\frac{\hbar^2}{2m}\,\nabla^2\;\psi_{\vec{p}}(\vec{r})\;+\;V(|\;\vec{r}\;|)\;\psi_{\vec{p}}(\vec{r})\;=\;E_{\vec{p}}\;\psi_{\vec{p}}(\vec{r})\;.
\tag{11.47}
$$

If V is rotationally symmetric, i.e., $[H, L^2] = 0$, then we can write

$$
\psi_{\vec{p}}(\vec{r})\;=\;\sum_{\ell,m}\;\hat{a}_\ell(p)\;\frac{u_{\ell,p}(r)}{r}\;Y_{\ell m}(\theta,\varphi)\;.
\tag{11.48}
$$

For $\vec{p}$ parallel to the z-axis, θ is the angle between $\vec{p}$ and the axis, and the problem is symmetric around the z-axis, i.e., independent of φ. Thus we use

$$
\psi_{\vec{p}}(\vec{r})\;=\;\sum_{\ell=0}^{\infty}\;a_\ell(\vec{p})\;\frac{u_{\ell,p}(r)}{r}\;P_\ell(\cos\theta)\;.
\tag{11.49}
$$

Inserting in (11.47) gives as radial Schrödinger equation

$$\frac{d^2}{dr^2}\, u_{\ell,p}(r) \;+\; \left[p^2 - \;\frac{2m}{\hbar^2}\, V(r) \;-\; \frac{\ell(\ell+1)}{r^2}\right]\, u_{\ell,p}(r) \;=\; 0 \tag{11.50}$$

where we used that $E_p = \frac{p^2}{2m}$. The requirement that only the solution which is regular at the origin is physically allowed gives $u_{\ell,p}(0) = 0$ and leads to a unique solution of (11.50). Next, we need to consider the behavior of $u_{\ell,p}(r)$ for $r \to \infty$. If the potential $V(r)$ vanishes sufficiently strong for $r \to \infty$, then (11.50) goes asymptotically for large r to

$$\frac{d^2}{dr^2}\, u_{\ell,p}(r) \;+\; \left[p^2 - \;\frac{\ell(\ell+1)}{r^2}\right]\, u_{\ell,p}(r) \;=\; 0\;, \tag{11.51}$$

which has the general solution

$$u_{\ell,p}(r) \;=\; B_{\ell,p} r\; j_\ell(pr) \;+\; C_{\ell,p} r\; n_\ell(pr)\;, \tag{11.52}$$

where $j_\ell(pr)$ and $n_\ell(pr)$ are the Bessel and Neumann functions. They have the following properties:

$$\begin{aligned} pr \;<<\; 1 \;\;:\;\; & j_\ell(pr) \;\sim\; (pr)^\ell \;\hat{=}\; \text{regular solution} \\ & n_\ell(pr) \;\sim\; -(pr)^{-\ell-1} \;\hat{=}\; \text{irregular solution} \\ pr \;>>\; 1 \;\;:\;\; & j_\ell(pr) \;\rightsquigarrow\; \frac{1}{pr}\sin\left(pr - \;\frac{\ell\pi}{2}\right) \\ & n_\ell(pr) \;\rightsquigarrow\; -\frac{1}{pr}\cos\left(pr - \;\frac{\ell\pi}{2}\right)\;. \end{aligned}$$

Thus, we have the following asymptotic behavior for the radial component of the scattering solution:

$$\psi_{\ell,p}(r) \;\sim\; \frac{u_{\ell,p}(r)}{r} \;\overset{pr>>1}{\rightsquigarrow}\; B_{\ell,p}\,\frac{\sin\;\left(pr - \;\frac{\ell\pi}{2}\right)}{pr} \;-\; C_{\ell,p}\,\frac{\cos\left(pr - \;\frac{\ell\pi}{2}\right)}{pr} \tag{11.53}$$

or equivalently

$$\frac{u_{\ell,p}(r)}{r} \;\overset{pr>>1}{\rightsquigarrow}\; A_{\ell,p}\,\frac{\sin\;\left(pr - \;\frac{\ell\pi}{2} \;+\; \delta_\ell(p)\right)}{pr}\;. \tag{11.54}$$

Thus $\delta_\ell(p)$ in (11.54) is a **phase shift** originating from the potential, which describes a shift with respect to the free wave (solution). The phase shifts δ_ℓ do not only depend on the potential but also on the scattering energy E_p, thus $\delta_\ell \equiv \delta_\ell(p)$. (11.54) can be rewritten as

$$\begin{aligned} A_{\ell,p}\;\cdot\;\frac{1}{pr}\sin\;\left(pr - \;\frac{\ell\pi}{2} \;+\; \delta_\ell(p)\right) \;\;=\;\; & A_{\ell,p}\,\frac{1}{pr}\;\left[\sin\left(pr - \;\frac{\ell\pi}{2}\right)\cos\delta_\ell(p)\right. \\ & \left.+\;\;\cos\left(pr - \;\frac{\ell\pi}{2}\right)\;\sin\delta_\ell(p)\right]\;, \end{aligned} \tag{11.55}$$

and thus we have

$$\frac{u_{\ell,p}(r)}{r} \rightsquigarrow A_{\ell,p}\cos\delta_\ell \, \frac{\sin\left(pr - \frac{\ell\pi}{2}\right)}{pr} + A_{\ell,p}\sin\delta_\ell \, \frac{\cos\left(pr - \frac{\ell\pi}{2}\right)}{pr} \ . \tag{11.56}$$

A comparison of the coefficients of (11.56) and (11.53) gives

$$\begin{aligned} B_{\ell,p} &= A_{\ell,p}\cos\delta_\ell \\ C_{\ell,p} &= -A_{\ell,p}\sin\delta_\ell \end{aligned} \tag{11.57}$$

with $A_{\ell,p}$ being a free parameter, which is determined by the overall normalization of the wave function. Thus, the radial solution can be written as

$$\frac{u_{\ell,p}(r)}{r} = A_{\ell,p}[\cos\delta_\ell \; j_\ell(pr) - \sin\delta_\ell \; n_\ell(pr)] \ . \tag{11.58}$$

Through this equation (11.58) the phase shifts δ_ℓ are defined. The radial solution $R_{\ell,p}(r)$ can be further rewritten as

$$R_{\ell,p}(r) = \frac{u_{\ell,p}(r)}{r} = \bar{A}_{\ell,p} \; [\; j_\ell(pr) - \tan\delta_\ell \; n_\ell(pr)] \tag{11.59}$$

with

$$\bar{A}_{\ell,p} = A_{\ell,p}\cos\delta_\ell = B_{\ell,p} \tag{11.60}$$

and

$$\tan\delta_\ell = \frac{\sin\delta_\ell}{\cos\delta_\ell} = -\frac{C_{\ell,p}}{B_{\ell,p}} \ . \tag{11.61}$$

In practical applications, one obtains the phase shift $\tan\delta_\ell$ by solving the radial Schrödinger equation (11.50) up to a value of r where the potential has sufficiently fallen off (in case of V being the nucleon-nucleon (nn) interaction typical values of r are $15fm$). Eq. (11.59), together with its derivative, gives two equations to determine $\tan\delta_\ell$ as

$$\tan\delta_\ell = \frac{p \; j'_\ell(pr) - \gamma \; j_\ell(pr)}{p \; n'_\ell(pr) - \gamma \; n_\ell(pr)} \tag{11.62}$$

where γ is the logarithmic derivative of the solution $R_{\ell,p}(r)$

$$\gamma = \frac{1}{R_{\ell,p}(r)} \frac{d}{dr} R_{\ell,p}(r) \ . \tag{11.63}$$

Once the phase shift δ_ℓ is obtained, the asymptotic behavior of the scattering solution is given as (cp. 11.49)

$$\psi_{\vec{p}}(\vec{r}) \rightsquigarrow \sum_{\ell=0}^{\infty} a_\ell(p) \left[\cos\delta_\ell \, \frac{\sin\left(pr - \frac{\ell\pi}{2}\right)}{pr} + \sin\delta_\ell \, \frac{\cos\left(pr - \frac{\ell\pi}{2}\right)}{pr}\right] P_\ell(\cos\theta) \ . \tag{11.64}$$

Since we are looking for a solution with a definite asymptotic behavior (11.30), we have to decompose (11.30) with respect to spherical waves. With

$$\begin{aligned} e^{ipz} &= \sum_{\ell=0}^{\infty} i^{\ell}\ (2\ell+1)\ j_{\ell}(pr)\ P_{\ell}(\cos\theta) \\ f_E(\theta) &= \sum_{\ell=0}^{\infty} (2\ell+1)\ f_{\ell}(p)\ P_{\ell}(\cos\theta) \end{aligned} \tag{11.65}$$

we can write (11.30) as

$$\begin{aligned} \psi_{\vec{p}}(\vec{r}) &\rightsquigarrow \sum_{\ell=0}^{\infty} (2\ell+1)\ \left[i^{\ell}\ \frac{\sin\left(pr - \frac{\ell\pi}{2}\right)}{pr}\ +\ f_{\ell}(p)\ \frac{e^{ipr}}{r}\right]\ P_{\ell}(\cos\theta) \\ &= \sum_{\ell=0}^{\infty} (2\ell+1)\ \left[\frac{e^{ipr}}{2ipr}\ -(-1)^{\ell}\ \frac{e^{-ipr}}{2ipr}\ +\ f_{\ell}(p)\ \frac{e^{ipr}}{r}\right]\ P_{\ell}(\cos\theta) \\ &= \sum_{\ell=0}^{\infty} \left[(-1)^{\ell+1}\ \frac{(2\ell+1)}{2ip}\ \frac{e^{-ipr}}{r}\ +\ (2\ell+1)\left(\frac{1}{2ip}\ +\ f_{\ell}(p)\right)\ \frac{e^{ipr}}{r}\right]\ P_{\ell}(\cos\theta)\ . \end{aligned} \tag{11.66}$$

Here we used that $i^{\ell} = e^{i\ell\frac{\pi}{2}}$ and $\frac{1}{pr}\sin\left(pr - \frac{\ell\pi}{2}\right) = \frac{1}{2ipr}\ \left\{e^{i\left(pr-\frac{\ell\pi}{2}\right)}\ -\ e^{-i\left(pr-\frac{\ell\pi}{2}\right)}\right\}$. In (11.64) the asymptotic form of the scattering solution was given. If one does not use this form, the original wave function reads in terms of 'standing waves'

$$\psi_{\vec{p}}(\vec{r})\ =\ \sum_{\ell=0}^{\infty}\ a_{\ell}(p)\ \left[\cos\delta_{\ell}(p)\ j_{\ell}(pr)\ -\ \sin\delta_{\ell}(p)\ n_{\ell}(pr)\right]\ P_{\ell}(\cos\theta)\ , \tag{11.67}$$

or in terms of in and out-going waves

$$\begin{aligned} \psi_{\vec{p}}(\vec{r}) &= \sum_{\ell=0}^{\infty}\ a_{\ell}(p)\ \frac{1}{2ipr}\left[e^{i(pr-\frac{\ell\pi}{2}+\delta_{\ell})} - e^{-i(pr-\frac{\ell\pi}{2}+\delta_{\ell})}\right] P_{\ell}(\cos\theta) \\ &= \sum_{\ell=0}^{\infty}\left[-\frac{a_{\ell}}{2ip} i^{\ell} e^{-i\delta_{\ell}}\frac{-e^{ipr}}{r} + \frac{a_{\ell}}{2ip} i^{-\ell} e^{-i\delta_{\ell}}\frac{e^{ipr}}{r}\right] P_{\ell}(\cos\theta) \end{aligned} \tag{11.68}$$

Comparing with the coefficients of (11.66) leads to the determination of $a_{\ell}(p)$ and $f_{\ell}(p)$. From

$$-\frac{a_{\ell}}{2ip} i^{\ell} e^{-i\delta_{\ell}} = (i^2)^{(\ell+1)}\frac{(2\ell+1)}{2ip} = i^{2\ell}(-1)\frac{(2\ell+1)}{2ip}$$

follows

$$a_\ell(p) = (2\ell+1)\; i^\ell\; e^{i\delta_\ell(p)} \tag{11.69}$$

and from

$$(2\ell+1) i^\ell e^{i\delta_\ell(p)} \frac{1}{2ip} i^{-\ell} e^{i\delta_\ell(p)} = \frac{2\ell+1}{2ip} e^{i\delta_\ell(p)}$$

follows

$$e^{2i\delta_\ell(p)} = 1 \;+\; 2ip\; f_\ell(p) \tag{11.70}$$

from which follows

$$f_\ell(p) \;=\; \frac{1}{2ip}\; [e^{2i\delta_\ell(p)} \;-1] \tag{11.71}$$

or

$$f_\ell(p) \;=\; \frac{1}{p}\; e^{i\delta_\ell(p)} \sin\delta_\ell(p) \;=:\; \frac{1}{p}\; t_\ell(p)\;, \tag{11.72}$$

where $t_\ell(p)$ is called the **partial wave amplitude**.

Note: If the potentials is absorptive, then $\delta_\ell(p) \to \delta_{\ell,R}(p) + i\delta_{\ell,I}(p)$. Then (11.71) reads

$$f_\ell(p) \;=\; \frac{1}{2ip}\; [e^{2i\delta_{\ell,R}(p)} e^{-2\delta_{\ell,I}(p)} \;-1],$$

where one usually defines $\eta_\ell \equiv e^{-2\delta_{\ell,I}}$ as absoption factor.
End note

Thus, the solution of the Schrödinger equation for positive energies is given by

$$\psi^{(+)}_{\vec{p}}(\vec{r}) \;=\; \sum_{\ell=0}^{\infty} (2\ell+1)\; i^\ell\; e^{i\delta_\ell(p)}\; \frac{u_{\ell,p}(r)}{r}\; P_\ell\;(\cos\theta) \tag{11.73}$$

and

$$\begin{aligned} f_E(\theta) \;&=\; \frac{1}{p} \sum_{\ell=0}^{\infty} (2\ell+1)\; e^{i\delta_\ell(p)} \sin\delta_\ell(p)\; P_\ell(\cos\theta) \\ &=\; \frac{1}{p} \sum_{\ell=0}^{\infty} (2\ell+1)\; t_\ell(p)\; P_\ell(\cos\theta)\;. \end{aligned} \tag{11.74}$$

The differential cross section is then given by

$$\begin{aligned}\frac{d\sigma}{d\Omega} \;&=\; \mid f_E(\theta) \mid^2 = \; \frac{1}{p^2} \; \sum_{\ell\ell'} \, (2\ell+1)(2\ell'+1) \\ &\qquad e^{i(\delta_\ell - \delta_{\ell'})} \sin\delta_\ell \sin\delta_{\ell'} \; P_\ell(\cos\theta) \; P_{\ell'}(\cos\theta)\end{aligned} \tag{11.75}$$

and the total cross section by

$$\begin{aligned}\sigma_{tot} \;&=\; \int_0^{2\pi} \, d\varphi \, \int_{-1}^{1} \, d\cos\theta \, \frac{d\sigma}{d\Omega} \\ &=\; \frac{2\pi}{p^2} \, \sum_{\ell=0}^{\infty} \, \frac{2}{2\ell+1} \, (2\ell+1)^2 \sin^2\delta_\ell(p) \\ &=\; \frac{4\pi}{p^2} \, \sum_{\ell=0}^{\infty} \, (2\ell+1)\sin^2\delta_\ell(p)\end{aligned} \tag{11.76}$$

where us used $\int \, d\theta \; P_\ell \; P'_\ell \;=\; \frac{2}{2\ell+1)} \; \delta_{\ell'\ell}$. If we define a "partial wave" cross section as

$$\begin{aligned}\sigma_{p,\ell} \;&:=\; \frac{4\pi}{p^2} \, (2\ell+1)\sin^2\delta_\ell \\ \sigma_{tot} \;&=\; \sum_{\ell=0}^{\infty} \, \sigma_{p,\ell}\end{aligned} \tag{11.77}$$

then we see that for each $\ell, \sigma_{p,\ell}^{max} \;=\; \frac{4\pi}{p^2} \, (2\ell+1)$ is the upper bound for $\sigma_{p,\ell}$.

The expressions (11.75) and (11.76) for the differential and total cross sections are only practically useful if only a few partial waves contribute, i.e., are different from zero. This is the case for short-ranged potentials and small energies, as we will see later. If too many ℓ's have to be taken into account, the use of a partial wave expansion becomes questionable.

Insert: Different view on boundary conditions:

Consider the free solution of the radial Schrödinger equation

$$\begin{aligned} u_{l,p}(r) &= A_{l,p}\left[\cos\delta_l r j_l(pr) - \sin\delta_l r n_l(pr)\right] \\ &\equiv e^{i\delta_l}\left[\sin\delta_l G_l(pr) + \cos\delta_l F_l(pr)\right] \end{aligned} \tag{11.78}$$

with

$$\begin{aligned} F_l(pr) &= prj_l(pr) \\ G_l(pr) &= -prn_l(pr). \end{aligned} \tag{11.79}$$

Then

$$\tan\delta_l = -\frac{-F_l'(pr) - F_l(pr)\gamma(R)}{-G_l'(pr) - G_l(pr)\gamma(R)} \tag{11.80}$$

and

$$\gamma(R) = \frac{1}{u_{l,p}}\frac{du_{l,p}}{dr}\bigg|_{r=R} \tag{11.81}$$

Here one can establish a connection to bound states. A bound state is characterized by a square integrable solution,

$$\begin{aligned} \int_0^\infty dr u_l^2(r) &= 1 \\ \lim_{r\to\infty} u_l(r) &\to 0. \end{aligned} \tag{11.82}$$

For scattering states one has the asymptotic behavior

$$u_l(r) \sim e^{\pm i(pr - l\frac{\pi}{2})}, \tag{11.83}$$

with $E_p = p^2/2\mu$. With $p \equiv i\kappa$ this becomes $E_p = -\kappa^2/2\mu$ and

$$e^{\pm i(pr - l\frac{\pi}{2})} = e^{\mp\kappa r} i^l, \tag{11.84}$$

where only $p = i\kappa$ gives a normalizable wave function. Then the logarithmic derivative is given by

$$\gamma = -\kappa. \tag{11.85}$$

This gives an extra condition to the wave function which makes our artificial bound state problem into an eigenvalue problem.

End insert

The most simplest case occurs if only the lowest partial wave has to be considered ($\ell = 0$), i.e., if we have s-wave scattering. Then

$$\frac{d\sigma}{d\Omega} \;=\; \frac{\sin^2\delta_0}{p^2} \;, \tag{11.86}$$

which is independent of the scattering angle θ. Thus, for s-wave scattering, the differential cross section is isotropic.

A different expression for the phase shift can be obtained in the following way. We consider the differential equations for the free solution

$$(r\; j_\ell(pr))'' \;+\; \left[p^2 - \;\frac{\ell(\ell+1)}{r^2}\right] (r\; j_\ell(pr)) \;=\; 0 \tag{11.87}$$

and for the full solution

$$u''_{\ell,p}(r) \;+\; \left[p^2 - \;\frac{\ell(\ell+1)}{r} \;-\; \frac{2m}{\hbar^2}\, V(r)\right]\; u_{\ell,p}(r) \;=\; 0\;. \tag{11.88}$$

Multiplying (11.87) with $u_{\ell,p}(r)$ and (11.88) with $r\; j_\ell(pr)$ and subtracting both equations leads to

$$\frac{d}{dr}\left[(r\; j_\ell(pr))'\; u_{\ell,p}(r) \;-\; (r\; j_\ell(pr))\; u'_{\ell,p}(r)\right] \;=\; -j_\ell(pr)\;\frac{2m}{\hbar^2}\; V(r) r\; u_{\ell,p}(r)\;. \tag{11.89}$$

Integrating over r and taking into account the boundary condition $u_{s,p}(0) = j_\ell(0) = 0$ as well as asymptotic forms

$$\begin{aligned}
r\; j_\ell(pr) \;&\overset{r\to\infty}{\longrightarrow}\; \frac{1}{p}\sin\left(pr - \;\frac{\ell\pi}{2}\right)\\
u_{\ell,p}(r) \;&\overset{r\to\infty}{\longrightarrow}\; \frac{1}{p}\sin\left(pr - \;\frac{\ell\pi}{2} \;+\; \delta_\ell(p)\right)\\
(r\; j_\ell(pr))' \;&\overset{r\to\infty}{\longrightarrow}\; \cos\left(pr - \;\frac{\ell\pi}{2}\right)
\end{aligned} \tag{11.90}$$

leads to

$$\sin\delta_\ell(p) \;=\; -\,\frac{2m}{\hbar^2}\int_0^\infty dr\; pr\; j_\ell(pr)\; V(r)\; u_{\ell,p}(r) \tag{11.91}$$

where

$$\cos\left(pr - \frac{\ell\pi}{2}\right)\;\frac{1}{p}\;\sin\left(pr - \frac{\ell\pi}{2} + \delta_\ell(p)\right) \;-\; \frac{1}{p}\sin\left(pr - \frac{\ell\pi}{2}\right)$$
$$\cos\left(pr - \;\frac{\ell\pi}{2} \;+\; \delta_\ell(p)\right) \;=\; \frac{1}{p}\sin\delta_\ell(p)$$

has been used. The expression (11.91) is no simplification with respect to the form (11.62). Though no asymptotic conditions enter, the integral of (11.91) has to be solved for all values of r to give the exact solution for $\sin\delta_\ell(p)$. In addition, (11.91) requires the calculation of the scattering solution $u_{\ell,p}(r)$. However, if one uses the approximation

$$u_{\ell,p}(r) \;\approx\; pr\; j_\ell(pr) \;, \tag{11.92}$$

one obtained the so-called **Born approximation for the phase shift**

$$\sin\delta_\ell(p) \;\approx\; -\frac{2m}{\hbar^2}\,\frac{1}{p}\int_0^\infty dr\; V(r)\;[pr\; j_\ell(pr)]^2 \;. \tag{11.93}$$

The question is under which conditions can (11.93) provide a good approximation for the phase shift. This should be expected if the right-hand side of (11.96) is small compared to $\mathbf{1}$, or more precisely, if the function $j_\ell(pr)$ is small in the domain of $V(r)$. For small incident energies, one can argue as follows: The function $\rho\; j_\ell(\rho)$ increases close to the origin ($\rho = 0$) from zero as $\rho^{\ell+1}$. It has a turning point at $\rho = \sqrt{\ell(\ell+1)}$. Thus, we can assume that $pr\; j_\ell(pr)$ stays small up to $r = \frac{1}{p}\sqrt{\ell(\ell+1)}$ and that, therefore, the approximation (11.93) is good if the range of the potential fulfills

$$R \;\leq\; \frac{1}{p}\sqrt{\ell(\ell+1)} \;. \tag{11.94}$$

Formulated in a different way: If the range R and the incident particle energy (given p) are fixed, the phase shifts θ_ℓ are small for all ℓ values which fulfill (11.94) and then (11.93) is a good approximation. This result can also be understood semi-classically. The length

$$b_\ell \;=\; \frac{\sqrt{\ell(\ell+1)}}{p} \;=\; \frac{\hbar\sqrt{\ell(\ell+1)}}{\hbar p} \;=\; \frac{\text{angular momentum}}{\text{momentum}}$$

is the impact parameter of the particles incident with a specific angular momentum. From classical mechanics, we know that there is no scattering if the impact parameter becomes larger than the range. For large energies, we use that the function $\xi\; j_\ell(\xi)$ is bounded for all values of the argument. Then the right-hand side of (11.93) will be small if p is so large that

$$\frac{2m}{\hbar^2 p}\int_0^\infty \mid V(r)\mid\; dr \;\ll\; \mathbf{1} \;.$$

(This estimate is, of course, only valid if the integral over $\mid V(r)\mid$ exists.) Thus, for high energies the Born approximation (11.93) should be valid for all values of ℓ. However, at high energies one should calculate relativistically.

A final remark:
If we had started with a radial wave function normalized such that

$$u_{\ell,p}(r) \;\longrightarrow\; j_\ell(pr) \;+\; \tan\delta_\ell\; n_\ell(pr) \;, \tag{11.95}$$

then (11.91) becomes

$$\tan\delta_\ell \;=\; -\frac{2m}{\hbar^2}\,\frac{1}{p}\int_0^\infty dr\; j_\ell(pr)\; V(r)\; u_{\ell,p}(r)\;. \tag{11.96}$$

From the Born approximation for the phase-shift (11.93) we can draw some conclusions about the relation of the sign of the phase-shift δ_ℓ and the behavior of $V(r)$, since all other terms under the integral are positive.

- If $\delta_\ell < 0$, then $V(r) > 0$, i.e. repulsive.
- If $\delta_\ell > 0$, then $V(r) < 0$, i.e. attractive.

Example: Hard Sphere Scattering

Imagine a hard sphere of radius R, i.e. a potential that is infinitely repulsive for $r < R$ and zero outside the sphere. Since the wave function does not penetrate inside the sphere, the wave function must vanish for $r < R$. That is we obtain

$$u_0(kr) = \begin{cases} 0, & r < R \\ \sin(kr - kR), & r > R \end{cases} \tag{11.97}$$

A comparison with the free solution

$$u_l(kr) \sim e^{i\delta_l}\sin(kr - l\frac{\pi}{2} + \delta_l) \tag{11.98}$$

gives for the phase shift obtained for scattering from a hard sphere

$$\delta_0(E) = -kR. \tag{11.99}$$

Here we see that a negative phase shift usually arises from repulsive potentials. Note also, that even a very simple potentials produce energy dependent phase shifts.

11.6 The Low Energy Limit

Here the behavior of the phase shift at low energies will be considered. For potentials that can be assumed to vanish beyond $r = R$, the earlier expressions for $\tan\delta_\ell$, (11.62) and (11.96) can be used to explore the low energy behavior of the phase shift. When the external kinetic energy E is small compared to the depth of the potential, the wave function inside the potential will not depend sensitively on E. The total kinetic energy at any radius is $E+ \mid V(r) \mid$, which is for small E nearly equal to $\mid V(r) \mid$. Thus, we can to first approximation consider the logarithmic derivative γ (11.63) to be independent of energy.

If we introduce the low energy behavior of $j_\ell(pr)$ and $n_\ell(pr)$ as

$$\begin{aligned} pr\ j_\ell(pr) &\stackrel{pr<<\ell}{\longrightarrow} \frac{(pr)^{\ell+1}}{1\cdot 3\cdot 5\cdots(2\ell+1)} \\ -pr\ n_\ell(pr) &\stackrel{pr<<\ell}{\longrightarrow} \frac{1\cdot 3\cdot 5\cdots(2\ell-1)}{(pr)^\ell} \end{aligned} \tag{11.100}$$

then we obtain from (11.62) after multiplying numerator and denominator with pR

$$\tan\delta_\ell \stackrel{p\to 0}{\longrightarrow} \frac{(\ell+1) - R\ \gamma_0(R)}{\ell + R\ \gamma_0(R)} \frac{(pR)^{2\ell+1}}{[1\cdot 3\cdot 5\cdots(2\ell-1)]^2\ (2\ell+1)} \tag{11.101}$$

where $\gamma_0(R)$ is the zero energy logarithmic derivative. Thus, as the energy approaches zero, the tangent of the phase shift also approaches zero as

$$\tan\delta_\ell \ \approx\ a_\ell\ p^{2\ell+1}\ . \tag{11.102}$$

For $\ell = 0$ (s-waves) (11.101) yields

$$\tan\delta_0 \stackrel{p\to 0}{\longrightarrow} \frac{1 - R\ \gamma_0(R)}{\gamma_0(R)}\ p \ =\ -pa_0\ . \tag{11.103}$$

The quantity a_0 is usually called the **zero energy scattering length**, or simply the **scattering length** and is defined by

$$a_0 \ =\ \frac{R\ \gamma_0(R) - 1}{\gamma_0(R)}\ . \tag{11.104}$$

If the wave function is small at $r = R$, the quantity $R\gamma_0(R)$ will be large at $\left(\frac{a_0}{R}\right) \simeq 1$; if, instead, $u'_{\ell,p}(R)$ is nearly zero, $R\gamma_0(R)$ will be small and $a \simeq\ -\frac{1}{\gamma_0(R)}$. The scattering length a_0 has a simple geometric interpretation. In the low energy limit, the wave function

$$u_0(r) \overset{r\geq R}{=} e^{i\delta_0}\sin(pr+\delta_0) \xrightarrow{p\to 0} p(r-a_0) \ , \tag{11.105}$$

where $\sin\alpha \approx \tan\alpha \approx \alpha$ was used.

Thus a_0 is the point nearest to the origin at which the external wave function, or its extrapolation toward the origin, vanishes. Considering the radial Schrödinger equation for $p \to 0, \ell = 0$, i.e.,

$$\left[\frac{d^2}{dr^2} - U(r)\right] u_0(r) = 0$$

we can deduce

1. For a repulsive potential ($U > 0$), the curvature of $u_0(r)$ is always away from the r axis so that $a_0 > 0$.

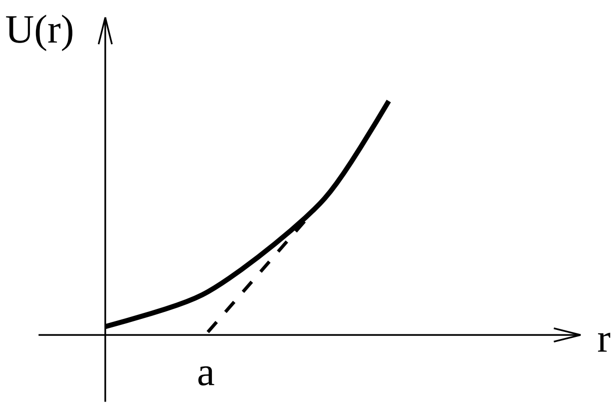

Fig. 11.2

Illustration of the geometrical meaning of the scattering length a_0.

2. For an attractive potential
    1. incapable of producing an s-wave bound state: $a_0 < 0$ (Fig. 11.3.a)
    2. capable of producing an s-wave virtual state or "zero energy resonance": $a_0 = \infty$ (Fig. 11.3.b)
    3. capable of producing one s-wave bound state: $a_0 > 0$ (Fig. 11.3.c)

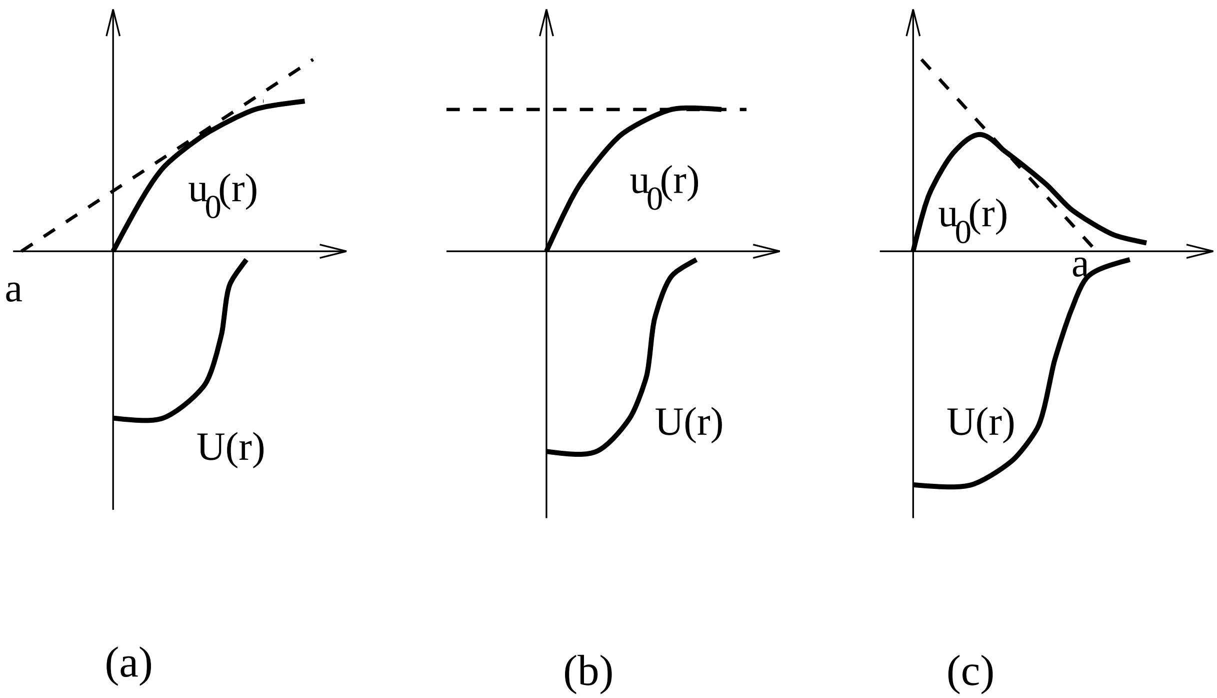

Fig. 11.3

Illustration of the scattering length a_0 for various attractive potentials $U(r)$.

The scattering length also has an important physical significance. In the low energy limit, only the s-wave makes a non-zero contribution to the cross section (11.102) so that the angular distribution of the scattering is spherically symmetric and the total cross section is

$$\sigma_{tot} \;=\; \frac{4\pi}{p^2}\sin^2\;\delta_0 \;\xrightarrow{p\to 0}\; 4\pi a_0^2\;. \tag{11.106}$$

This is similar to the result one obtains for the low energy scattering of a hard sphere of radius a. Thus, the scattering length is the "effective radius" of the target at zero energy. **However**, there is a factor of 4 between the quantum mechanical cross section at low energies and the classical cross section for scattering from a hard sphere ($\sigma_{classical} = \pi a^2$). This can be explained by the fact that in quantum mechanics one considers probabilities, i.e. the square of wave functions. At low energies the wave length is considerably larger than the size of the target, thus the scattering can be viewed as scattering by on the entire surface of the sphere, not only the cross section area of the sphere.

11.6.1 Effective Range Expansion

Here we only consider the very low energy regime, and thus we only need to take $l = 0$ into account. For the scattering amplitude we have

$$\begin{aligned} f_0(k) &= \frac{1}{k} e^{i\delta_0} \sin\delta_0 \\ &= \frac{1}{k}\frac{\sin\delta_0}{e^{-i\delta_0}} = \frac{1}{k}\frac{\sin\delta_0}{\cos\delta_0 - i\sin\delta_0} \\ &= \frac{1}{k}\frac{\tan\delta_0}{1 - i\tan\delta_0} = \frac{1}{k}\frac{1}{\cot\delta_0 - i} \\ &= \frac{1}{k\cot\delta_0 - ik}. \end{aligned} \tag{11.107}$$

Using the definition of the scattering length, $k\cot\delta_0 = -1/a_0$, we can rewrite the scattering amplitude as

$$\begin{aligned} f_0(k) &= \frac{1}{-\frac{1}{a_0} - ik} = \frac{a_0}{-(1 + ia_0 k)} \\ &= \frac{-a_0 + ia_0^2 k}{1 + a_0^2 k^2}. \end{aligned} \tag{11.108}$$

For the different pieces of the scattering amplitude we thus get

$$\begin{aligned} \Re e f_0(k) &\stackrel{k\to 0}{\longrightarrow} \sim a_0 \\ \Im m f_0(k) &\stackrel{k\to 0}{\longrightarrow} \sim a_0^2 k. \end{aligned} \tag{11.109}$$

From Eq. (11.106) we saw that the elastic cross section in the low energy limit is given by $\sigma = 4\pi a_0^2$. Thus in the low energy limit the optical theorem

$$\sigma = \frac{4\pi}{k}\Im m f_0(k) \tag{11.110}$$

is fulfilled.

Important consequence: A single, real number, a_0, completely parameterizes **all** low energy scattering. This is an advantage for e.g. experiments that use low energy neutron scattering to study solids. It is a disadvantage for deduction of specific properties of the projectile-target interaction.

Consider the s-wave wave function

$$\begin{aligned} u_0(r) &\equiv e^{i\delta_0}\left[\sin\delta_0 G_0(kr) + \cos\delta_0 F_0(kr)\right] \\ &\stackrel{k\to 0}{\longrightarrow} kr + \tan\delta_0 \end{aligned}$$

$$\sim \quad (r + a_0)k \tag{11.111}$$

This shows that outside of the range of the potential the wave function for in the low energy limit is proportional to $a_0 + r$, and thus intercepts the axis at $r = -a_0$.

Let's go back to Eq. (11.107) and insert the effective range expansion to the next order, i.e.

$$k \cot \delta_0 = -\frac{1}{a_0} + \frac{1}{2}k^2 r_0. \tag{11.112}$$

This leads to the scattering amplitude

$$\begin{aligned} f_0(k) &= \frac{1}{-\frac{1}{a_0} - ik + \frac{1}{2}k^2 r_0} \\ &= -\frac{a_0}{1 + ia_0 k - \frac{1}{2}a_0 k^2 r_0} \end{aligned} \tag{11.113}$$

Again, this expression for the scattering amplitude fulfills the optical theorem:

$$\frac{4\pi}{k}\Im m f_0(k) = \frac{4\pi}{k}\frac{a_0^2 k}{(1 - \frac{1}{2}a_0 k^2 r_0)^2 + a_0^2 k^2} = \frac{4\pi a_0^2}{(1 - \frac{1}{2}a_0 k^2 r_0)^2 + a_0^2 k^2} \tag{11.114}$$

and

$$\sigma = \int \frac{d\sigma}{d\Omega} = 4\pi \left| f_0(k) \right|^2 = \frac{4\pi a_0^2}{(1 - \frac{1}{2}a_0 k^2 r_0)^2 + a_0^2 k^2} \tag{11.115}$$

11.6.2 Relation to Bound States

Consider the scattering amplitude

$$f_{l=0} \simeq \frac{1}{k}e^{i\delta_0} \sin \delta_0 = \frac{1}{k}\frac{\tan \delta_0}{1 - i \tan \delta_0} \approx \frac{-a_0}{1 + ia_0 k}. \tag{11.116}$$

f is an analytic function and has a pole at $\tan \delta_0 = 1/i$. Here this means that $k = i/a_0$. Considering the energy we have

$$E = \frac{k^2}{2m} = \frac{-1}{2ma_0^2} \equiv -E_B. \tag{11.117}$$

Thus, the knowledge of the scattering length seems equivalent to the knowledge of the scattering amplitude. If there is a bound state (with a small binding energy), it determines the low energy scattering:

$$\sigma \approx |f_0|^2 \approx \frac{1}{2m(E + E_B)}. \tag{11.118}$$

Conversely, knowledge of the scattering length determines the bound state energy. E.g. from the knowledge of the deuteron binding energy one determines the triplet nucleon-nucleon scattering length to be

$$a_0^t \approx \frac{1}{\sqrt{E_B 2m}} = +4.32 fm \tag{11.119}$$

Experimentally a value $a_0^t = 5.42 fm$ is extracted. The difference comes from the fact that the bound state is not truly at zero energy and some higher order terms are needed.

Note: While the scattering length approximation does not hold if the energy gets far from zero, the relation of the poles of the scattering amplitude to bound states is general.

11.7 Levinson's Theorem

The scattering length a_0 is not simply a measure of the potential size or strength. If $U(r)$ becomes stronger, then more than one bound state can exist, and the cycle going from negative to positive scattering length can repeat. This is consistent with $\tan\delta_0 = pa_0$, where tan is a multi-valued function.

$\tan\delta_0$ varies periodically and discontinuously from $-\infty$ to $+\infty$. If the potential is strong enough to have a bound state at $k = 0$, we must be on the second branch of the tan function, and the zero energy phase shift is π rather than zero.

The general result of this consideration is **Levinson's Theorem**

$$\delta(k = 0) - \delta(k \equiv \infty) = n_B \pi \tag{11.120}$$

where n_B is the number of bound states supported by the specific potential $U(r)$. Levinson's theorem relates the phase shift as zero and infinite energy to the number of bound states n_B.

11.8 Breit-Wigner Resonances

Negative energy state (bound states) are stationary states and obey the stationary Schrödinger equation. States with positive energy, confined in a positive potential well are confined, but will eventually through the potential barrier. Those state are called quasi-bound states or resonances.

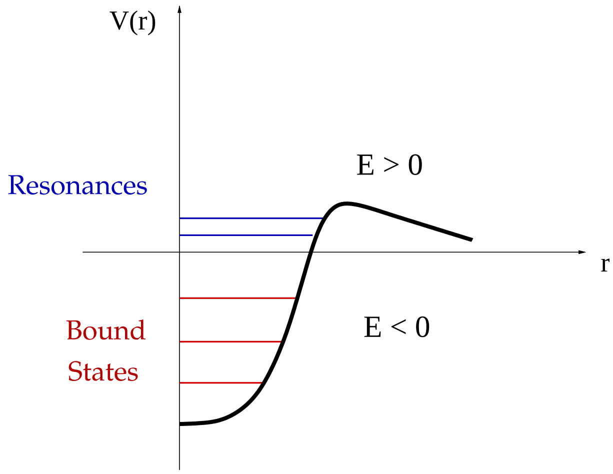

Fig. 11.6

Sketch of a potential supporting bound states and resonance states.

Consider the expansion of the phase shift $\tan\delta_\ell$ for $p \to 0$ as given in Eq. (11.101),

$$\tan\delta_\ell \ \xrightarrow{p\to 0}\ \frac{(\ell+1) - R\,\gamma_\ell(R)}{\ell + R\,\gamma_\ell(R)}\ \frac{(pR)^{2\ell+1}}{[1\cdot 3\cdot 5\cdots(2\ell-1)]^2\ (2\ell+1)} \tag{11.121}$$

The denominator vanishes for $R\,\gamma_\ell(R) = -\ell$. Thus $\tan\delta_\ell \to \infty$, i.e. $\delta_\ell = \frac{\pi}{2} + \mathrm{n}\pi$, This condition occurs for a specific momentum p_R at a specific energy $E_R = p_R/2\mu$.

Expanding $\gamma(R)$ around E_R gives

$$\gamma_\ell(R)R \approx -l + (E - E_R)\frac{d(\gamma_\ell R)}{dE}\,|_{E=E_R} \tag{11.122}$$

Substitution of Eq. (11.122) into Eq. (11.121) and neglecting the term $(E - E_R)$ in the numerator for $E \to E_R$ leads to

$$\begin{aligned}\tan\delta_\ell &\approx \frac{1}{E-E_R}\,\frac{1}{2}\,\frac{2(pR)^{2\ell+1}}{[(2\ell-1)!!]^2\frac{d(\gamma R)}{dE}}\\ &= \frac{1}{E_R-E}\,\frac{\Gamma_l}{2}\end{aligned} \tag{11.123}$$

with

$$\Gamma_l = \frac{-2(pR)^{2\ell+1}}{[(2\ell-1)!!]^2\frac{d(\gamma R)}{dE}}. \tag{11.124}$$

This leads to the **Breit-Wigner** resonance form of the amplitude

$$f_\ell = e^{i\delta_\ell}\sin\delta_\ell = \frac{\Gamma_l/2}{E_R - E - i\Gamma_l/2} \tag{11.125}$$

and the famous **Breit-Wigner cross section** in a specific partial wave partial wave ℓ.

$$\sigma_\ell^{tot} = \frac{4\pi(2\ell+1)}{p^2}\frac{\Gamma_l^2/4}{(E-E_R)^2+\Gamma_l^2/4} \tag{11.126}$$

where Γ_l is called the width of the resonance. From the derivation it is apparent that $\Gamma_l \sim (d\gamma_\ell(R)/dE)^{-1}$. Thus, if Γ_l is small, $\gamma_\ell(R)$ (and thus δ_ℓ) varies rapidly near E_R. If this is the case, the resonance will be **sharp**, and the total cross section σ^{tot} will have a sharp peak.
However, unless the resonance is **very** narrow, then the $1/k^2$ factor in σ^{tot} will distort the shape of the cross section and may shift the peak from E_R to a lower energy.

Physically, a sharp peak in the energy dependence of the cross section indicates a dynamical origin, such as a strong attraction at that energy. If the phase shift passes rapidly through $\pi/2$ (modulo π), this probably means a resonance, i.e. beam and target particle binding temporarily and then breaking up again.

Resonances are poles in $f_\ell(E)$ at $E = E_R - i\Gamma_l/2$. This means

$$\begin{aligned} p = \sqrt{2\mu E} &= \sqrt{2\mu E_r - i\mu\Gamma_l} = \sqrt{2\mu E}\,\sqrt{1-i\Gamma_l/2E_r} \\ &\approx p_r - i\frac{\mu\Gamma_l/2}{p_r}\ (\text{for small}\,\Gamma_l) \end{aligned} \tag{11.127}$$

If Γ_l is small, the pole is right below the real positive p-axis. When taking $E = p^2/2\mu$, bound state poles map to the first Riemann sheet, resonance poles move into the lower half of the second (unphysical) Riemann energy sheet.

The smaller Γ_l, the sharper σ^{tot} peaks, the longer lived the resonance is, and the closer the pole is to the real axis.

11.9 The Classical Limit

Let us now examine the scattering amplitude (11.71, 11.74) in the classical limit, that is, at a sufficiently high energy that the particle may be localized. At these energies, many partial waves will contribute so that the partial wave expansion for $f_\ell(\theta)$ may be approximated by an integral. In addition, most of the scattering will result from high partial waves so that we can assume that the phase shift for "normal" potentials will behave as shown in Fig. 11.4.

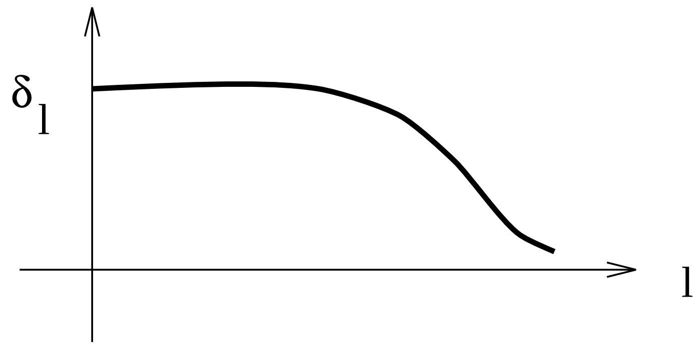

Fig. 11.4 The phase shift δ_ℓ as function of ℓ for high energies E.

Fig. 11.4 The phase shift δ_ℓ as function of ℓ for high energies E.

The region where δ_ℓ is relatively constant will make little contribution, as we will see below. As a result, we have from (11.74)

$$\begin{aligned} f_E(\theta) &= \sum_{\ell=0} (2\ell+1) \frac{e^{2i\delta_\ell}-1}{2ip} P_\ell(\cos\theta) \\ &\simeq \int_0^\infty d\ell\ \ell\ \frac{e^{2i\delta_\ell}-1}{ip} P_\ell(\cos\theta)\ . \end{aligned} \tag{11.128}$$

For large ℓ and small angles, the Legendre polynomial may be replaced by a Bessel function using the expansion

$$P_\ell(\cos\theta) \simeq j_0\left[2\left(\ell+\frac{1}{2}\right)\sin\frac{1}{2}\theta\right] + \frac{1}{4}\sin^2\frac{1}{2}\theta + \cdots\ . \tag{11.129}$$

This greatly simplifies the integration since it avoids integrating over the order of the Legendre polynomial. It is also convenient to use $b = \frac{\ell}{p}$ and to recognize that the momentum transferred to the scattered particle, which we shall denote by q, is

$$\begin{aligned} q = |\vec{p} - \vec{p}\,'| &= (p^2 + p'^2 - 2pp'\cos\theta)^{1/2} \\ &= p(2(1-\cos\theta))^{\frac{1}{2}} = 2p\sin\frac{\theta}{2} \end{aligned} \tag{11.130}$$

for elastic scattering, i.e., $|\vec{p}| = |\vec{p}\,'|$. Then (11.128) may be rewritten to obtain the semi classical approximation

$$f_E(\theta) = \frac{p}{i}\int_0^\infty db\ b\ (e^{2i\delta(b)}-1)\ j_0\ (qb)\ . \tag{11.131}$$

This formula is reminiscent of very similar formulas in the classical theory of diffraction. Its physical implications can be seen most strikingly by assuming that $\delta(b)$ has a limiting form as suggested by Fig. 11.4, namely that it is constant for $b < R$ and zero for $b > R$. In this simple case, the integral in (11.131) can be performed analytically giving

$$f_E(\theta) \;\approx\; \frac{j_0(qR)}{qR} \tag{11.132}$$

where $j_1(qR)$ is the first-order Bessel function. This result, familiar from the theory of Fraunhofer diffraction, gives a cross section as shown in Fig. 11.5.

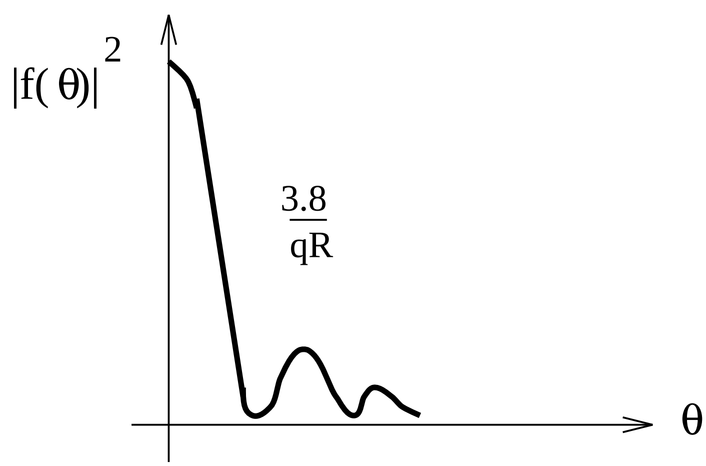

Fig. 11.5 Differential cross section is the classical limit.

As expected, the cross section is sharply peaked in the forward direction and is concentrated within the region having $\theta <\sim (\frac{1}{pR})$. At high energies, we can extract the physical content of (11.131) by using the method of "steepest descent." For large q the integrand will oscillate rapidly as b varies. Asymptotically, the Bessel function has the form

$$j_0(qb) \;\overset{qb\to\infty}{\longrightarrow}\; (2\pi qb)^{1/2} \;\left[exp\left(i\left(qb - \frac{\pi}{4}\right)\right) \;+\; exp\left(-i\left(qb - \frac{\pi}{4}\right)\right)\right] \tag{11.133}$$

so that the dominant contribution to the integral will come from those values of b for which $2\delta(b) \pm qb$ is nearly constant. The term in (11.131) that is independent of the phase shift does not contribute to the scattering away from the forward direction as can be seen by returning to (11.128) and noting that $\sum_{\ell=0}^{\infty} \left(\ell + \frac{1}{2}\right) P_\ell(\cos\theta) \;=\; \delta(1-\cos\theta)$. Thus, the important region of b is determined, for fixed θ, by the relation

$$\frac{d\delta(b)}{db} \;\pm\; \frac{1}{2}q \;=\; \pm p\sin\frac{\theta}{2}\;. \tag{11.134}$$

It may be seen from this, as pointed out earlier, that values of b, for which $\delta(b)$ is a constant, will not contribute to scattering out of the forward direction ($q > 0$).