

Chapter 11

Scattering Off Potentials

Most two-particle interaction potentials $V(\mathbf{x}_1 - \mathbf{x}_2)$ assume a finite value V_∞ if $|\mathbf{x}_1 - \mathbf{x}_2| \rightarrow \infty$. If the relative motion of the two-particle system has an energy $E > V_\infty$ the particles can have arbitrary large distance. In particular, we can imagine a situation where the two particles approach each other from an initially large separation and after reaching some minimal distance move away from each other. The force between the two particles will influence the trajectories of the two particles, and this influence will be strongest when the particles are close together. The deflection of particle trajectories due to interaction forces is denoted as scattering. This is denoted as potential scattering if the interaction forces between the particles can be expressed through a potential. We have seen in Section 7.1 that the motion of two particles with an interaction potential of the form $V(\mathbf{r}) = V(\mathbf{x}_1 - \mathbf{x}_2)$ can be separated into center of mass motion and relative motion, $\Psi(\mathbf{x}_1, \mathbf{x}_2) = \psi(\mathbf{r}) \exp(i\mathbf{K} \cdot \mathbf{R}) / \sqrt{2\pi^3}$, where the factor $\psi(\mathbf{r})$ for relative motion of the two particles satisfies

$$E\psi(\mathbf{r}) = -\frac{\hbar^2}{2m} \Delta\psi(\mathbf{r}) + V(\mathbf{r})\psi(\mathbf{r}). \quad (11.1)$$

E is the contribution from relative motion to the total energy (7.9) of the two-particle system, and I wrote m for the reduced mass of the two-particle system.

Equation (11.1) with $E > V_\infty$ does not only describe two-particle scattering, but also scattering of a particle of mass m off a potential with fixed center $r = 0$, e.g. because the source of the potential is fixed by forces which do not affect the scattered particle.

Scattering is an important technique for the determination of properties of a physical system. Within the framework of potential scattering, observations of deflections of particle trajectories in a potential can be used to determine the strength and functional dependence $V(\mathbf{r})$ of a scattering potential.

Suppose that we wish to determine a scattering potential $V(\mathbf{r})$ through scattering of non-relativistic particles of momentum $\hbar\mathbf{k}$ off the potential. The deflected particles will have momenta $\mathbf{k}' \neq \mathbf{k}$, and one observable that we should certainly be able to measure is the number $dn(\Omega)/dt$ of particles per time which are deflected into a small solid angle $d\Omega = d\vartheta d\varphi \sin\vartheta$ in the direction $\hat{\mathbf{x}} = (\sin\vartheta \cos\varphi, \sin\vartheta \sin\varphi, \cos\vartheta)$. According to the definition of particle current densities j , this number will be given by

$$\frac{dn(\Omega)}{dt} = \lim_{r \rightarrow \infty} j_{out}(\mathbf{k}') r^2 d\Omega,$$

where $j_{out}(\mathbf{k}')$ is the number of deflected particles per area and per time which are moving in the direction $\hat{\mathbf{k}}' = \hat{\mathbf{x}}$ with momentum $\hbar\mathbf{k}'$. We are taking the limit $r \rightarrow \infty$ because we are interested in measuring $dn(\Omega)/dt$ far from the scattering center (or for large separation of particles in particle-particle scattering), to make sure that the scattering potential does not deflect the scattered particles any further.

The number of particles $dn(\Omega)/dt$ which are scattered into the direction $\hat{\mathbf{k}}'$ is of course proportional to the number $j_{in}(\mathbf{k})$ of particles per area and per time which are incident on the scattering center, and it is also proportional to the width $d\Omega$ of the solid angle over which we sum the scattered particles. Therefore we expect that the observable which may really tell us something about the scattering potential is gotten by dividing out the trivial dependence on j_{in} and $d\Omega$, i.e. we define

$$\frac{d\sigma}{d\Omega} = \frac{1}{j_{in}(\mathbf{k})} \frac{dn(\Omega)}{d\Omega dt} = \lim_{r \rightarrow \infty} r^2 \frac{j_{out}(\mathbf{k}')}{j_{in}(\mathbf{k})}. \quad (11.2)$$

The quantity $d\sigma(\Omega) = (dn(\Omega)/dt)/j_{in}$ has the dimension of an area and is therefore known as a *differential scattering cross section*. Differential scattering cross sections are the observables of primary interest in potential scattering.

If we integrate over all possible scattering directions, we get the *scattering cross section*

$$\sigma = \int d\sigma = \frac{1}{j_{in}(\mathbf{k})} \int d\Omega \frac{dn(\Omega)}{dt} = \frac{1}{j_{in}(\mathbf{k})} \frac{dn}{dt},$$

i.e. the scattering cross section is the total number of scattered particles per time, dn/dt , divided by the current density of incident particles.

For an explanation of the name *cross section* we also remark that the calculation of scattering of particles off a hard sphere of radius R in *classical mechanics* yields a scattering cross section $\sigma = \pi R^2$ which equals the cross section of the sphere. We will see below in Section 11.3 that quantum mechanics actually yields a larger scattering cross section of a sphere, e.g. $\sigma = 4\pi R^2$ for scattering of very low energetic particles. Scattering of low energy particles off a sphere could be considered as a most basic illustration of measuring properties of a scattering center. Measuring the number dn/dt of low energy particles per time which are

scattered off the sphere and dividing by the incident particle current density provides a measurement of the radius $R = \sqrt{\sigma/4\pi} = \sqrt{(dn/dt)/4\pi j_{in}}$ of the scattering center.

The particle current density of particles described by a wave function $\psi(\mathbf{x}, t)$ will be proportional to the corresponding probability current density

$$\mathbf{j} = \frac{\hbar}{2im} (\psi^+ \cdot \nabla \psi - \nabla \psi^+ \cdot \psi),$$

and therefore we can use probability current densities in the calculation of the ratio in (11.2).

11.1 The free energy-dependent Green's function

Many applications of quantum mechanics require the calculation of the inverse (or resolvent) $\mathcal{G}(E)$ of the operator $E - H_0 = E - (\mathbf{p}^2/2m)$,

$$(E - H_0)\mathcal{G}(E) = 1. \quad (11.3)$$

E.g. if we consider a time-independent potential V , the time-independent Schrödinger equation

$$(E - H_0)|\psi(E)\rangle = V|\psi(E)\rangle \quad (11.4)$$

is satisfied if the energy eigenstate $|\psi(E)\rangle$ satisfies a *Lippmann-Schwinger equation*¹

$$|\psi(E)\rangle = |\psi_0(E)\rangle + \mathcal{G}(E)V|\psi(E)\rangle, \quad (11.5)$$

where $|\psi_0(E)\rangle$ satisfies the condition $(E - H_0)|\psi_0(E)\rangle = 0$. Iteration of (11.5) for $|\psi_0(E)\rangle \neq 0$ then yields the perturbation series

$$|\psi(E)\rangle = \sum_{n=0}^{\infty} [\mathcal{G}(E)V]^n |\psi_0(E)\rangle. \quad (11.6)$$

Equations (11.5, 11.6) with $|\psi_0(E)\rangle \neq 0$ are also sometimes written as

$$|\psi(E)\rangle = \frac{1}{1 - \mathcal{G}(E)V} |\psi_0(E)\rangle. \quad (11.7)$$

¹B.A. Lippmann, J. Schwinger, Phys. Rev. 79, 469 (1950).

Contrary to equation (11.5), the equations (11.6, 11.7) assume that E is an eigenvalue of *both* H and H_0 . A necessary condition for equations (11.6, 11.7) is therefore $E \geq 0$ because we use $H_0 = \mathbf{p}^2/2m$. We also assume that the series on the right hand side of (11.6) converges in a suitable sense (e.g. such that we can integrate it with square integrable functions).

Equation (11.5) is more general than equations (11.6, 11.7) because if E is not an eigenvalue of H_0 we have $|\psi_0(E)\rangle = 0$ and equation (11.5) simply states that the solutions of (11.4) are eigenstates of $\mathcal{G}(E)V$ with eigenvalue 1, whereas equations (11.6, 11.7) become singular if $\mathcal{G}(E)V$ has eigenvalue 1.

For potential scattering theory it is customary to rescale $\mathcal{G}(E)$ by a factor $-\hbar^2/2m$, such that the zero energy Green's function $G(0)$ is the inverse of the negative Laplace operator. The equation

$$\mathcal{G}(E) = -\frac{2m}{\hbar^2}G(E) = \frac{1}{E - H_0 + i\epsilon}, \quad \epsilon \rightarrow +0, \quad (11.8)$$

is then in k -representation

$$\langle \mathbf{k} | G(E) | \mathbf{k}' \rangle = \frac{\delta(\mathbf{k} - \mathbf{k}')}{\mathbf{k}^2 - (2mE/\hbar^2) - i\epsilon} = G(E, \mathbf{k})\delta(\mathbf{k} - \mathbf{k}'). \quad (11.9)$$

The condition (11.3) for the energy-dependent Green's function in \mathbf{x} -representation

$$\begin{aligned} \langle \mathbf{x} | G(E) | \mathbf{x}' \rangle &= \int d^3\mathbf{k} \int d^3\mathbf{k}' \langle \mathbf{x} | \mathbf{k} \rangle \langle \mathbf{k} | G(E) | \mathbf{k}' \rangle \langle \mathbf{k}' | \mathbf{x}' \rangle \\ &= \frac{1}{(2\pi)^3} \int d^3\mathbf{k} \exp[i\mathbf{k} \cdot (\mathbf{x} - \mathbf{x}')] G(E, \mathbf{k}) \\ &= G(E, \mathbf{x} - \mathbf{x}') \end{aligned} \quad (11.10)$$

is

$$\Delta G(E, \mathbf{x} - \mathbf{x}') + \frac{2m}{\hbar^2}EG(E, \mathbf{x} - \mathbf{x}') = -\delta(\mathbf{x} - \mathbf{x}'). \quad (11.11)$$

The shift $i\epsilon \rightarrow +i0$ in equation (11.8) defines the *retarded Green's function* for the Schrödinger equation. The reason for this terminology is that the corresponding Green's function in the time domain (cf. (5.11)),

$$\mathcal{G}(t) = \frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} dE \mathcal{G}(E) \exp\left(-\frac{i}{\hbar}Et\right) = \frac{\Theta(t)}{i\hbar} \exp\left(-\frac{i}{\hbar}H_0t\right), \quad (11.12)$$

satisfies the conditions

$$i\hbar \frac{\partial \mathcal{G}(t)}{\partial t} - H_0 \mathcal{G}(t) = \delta(t), \quad \mathcal{G}(t) \Big|_{t < 0} = 0.$$

This implies that \mathcal{G} propagates time-dependent perturbations

$$i\hbar \frac{\partial}{\partial t} |\psi(t)\rangle - H_0 |\psi(t)\rangle = V(t) |\psi(t)\rangle$$

forward in time,

$$\begin{aligned}
 |\psi(t)\rangle &= |\psi_0(t)\rangle + \int_{-\infty}^{\infty} dt' \mathcal{G}(t-t')V(t')|\psi(t')\rangle \\
 &= |\psi_0(t)\rangle - \frac{i}{\hbar} \int_{-\infty}^t dt' \exp\left(-\frac{i}{\hbar}H_0(t-t')\right)V(t')|\psi(t')\rangle. \quad (11.13)
 \end{aligned}$$

We will revisit time-dependent perturbations in Chapter 13 and focus on scattering due to time-independent perturbations (11.4–11.6) for now.

We first calculate the Green's function $G(E, \mathbf{x})$ for $E > 0$. The equations (11.9) and (11.10) yield

$$\begin{aligned}
 G(E, \mathbf{x}) &= \frac{1}{(2\pi)^3} \int d^3\mathbf{k} \frac{\exp(i\mathbf{k} \cdot \mathbf{x})}{k^2 - (2mE/\hbar^2) - i\epsilon} \\
 &= \frac{1}{(2\pi)^2} \int_0^{\infty} dk \int_{-1}^1 d\xi k^2 \frac{\exp(ikr\xi)}{k^2 - (2mE/\hbar^2) - i\epsilon} \\
 &= \frac{1}{(2\pi)^2 i r} \int_0^{\infty} dk k \frac{\exp(ikr) - \exp(-ikr)}{k^2 - (2mE/\hbar^2) - i\epsilon} \\
 &= \frac{1}{(2\pi)^2 i r} \int_{-\infty}^{\infty} dk k \frac{\exp(ikr)}{k^2 - (2mE/\hbar^2) - i\epsilon}. \quad (11.14)
 \end{aligned}$$

Due to $r > 0$ we can add a semi-circle with radius $|k| \rightarrow \infty$ in the upper half of the complex k plane to the integration contour, see Figure 11.1. This additional

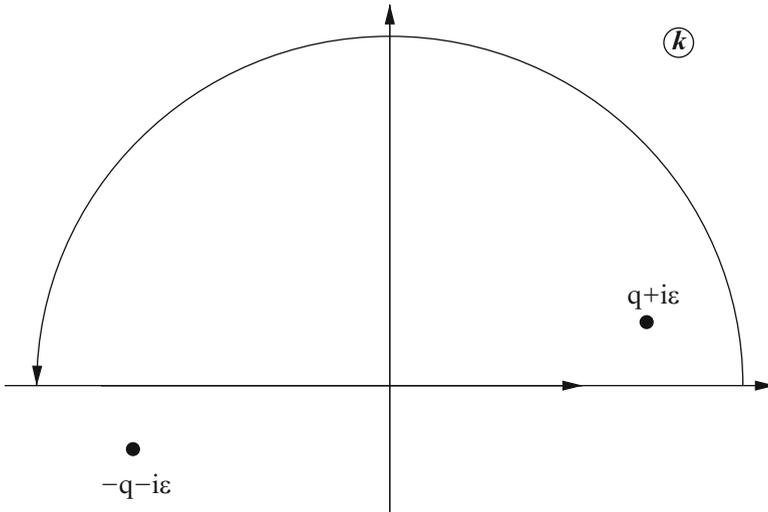


Fig. 11.1 Location of the poles and integration contour in the complex k plane. Here $q \equiv \sqrt{2mE/\hbar^2}$

path segment \cap will not change the integral in (11.14) because we have with $k = |k| \exp(i\phi)$

$$\begin{aligned} & \lim_{|k| \rightarrow \infty} \int_{\cap} dk k \frac{\exp(ikr)}{k^2 - (2mE/\hbar^2) - i\epsilon} \\ &= \lim_{|k| \rightarrow \infty} \int_0^\pi d\phi \frac{i|k|^2 \exp(2i\phi) \exp[i|k|r \cos(\phi)]}{|k|^2 \exp(2i\phi) - (2mE/\hbar^2)} \exp[-|k|r \sin(\phi)] = 0. \end{aligned}$$

However, adding the semi-circle to the integration contour allows us to use the residue theorem. Decomposing the denominator into its simple poles

$$\frac{1}{k^2 - (2mE/\hbar^2) - i\epsilon} = \frac{1}{[k - (\sqrt{2mE/\hbar}) - i\epsilon][k + (\sqrt{2mE/\hbar}) + i\epsilon]}$$

then yields

$$\begin{aligned} G(E, \mathbf{x}) &= \frac{1}{2\pi r} \frac{k \exp(ikr)}{k + (\sqrt{2mE/\hbar})} \Big|_{k=\sqrt{2mE/\hbar}} \\ &= \frac{1}{4\pi r} \exp(i\sqrt{2mE}r/\hbar), \end{aligned} \quad (11.15)$$

i.e. the retardation requirement $\mathcal{G}(t) \propto \Theta(t)$ yields only outgoing spherical waves for positive energy.

If we perform the same calculation for $E < 0$ we find a denominator

$$\frac{1}{k^2 - (2mE/\hbar^2)} = \frac{1}{[k - i(\sqrt{-2mE/\hbar})][k + i(\sqrt{-2mE/\hbar})]},$$

and integration yields

$$G(E, \mathbf{x}) = \frac{1}{4\pi r} \exp(-\sqrt{-2mE}r/\hbar). \quad (11.16)$$

We can combine the results for positive and negative energy into

$$G(E, \mathbf{x}) = \frac{\Theta(E)}{4\pi r} \exp(i\sqrt{2mE}r/\hbar) + \frac{\Theta(-E)}{4\pi r} \exp(-\sqrt{-2mE}r/\hbar). \quad (11.17)$$

This is the energy-dependent Green's function for the free non-relativistic particle.

11.2 Potential scattering in the Born approximation

We consider a particle of energy $E = \hbar^2 k^2/2m$ in a static potential $V(\mathbf{x})$ of finite range. The time-independent Schrödinger equation

$$(\Delta + k^2)\psi(\mathbf{x}) = \frac{2m}{\hbar^2} V(\mathbf{x})\psi(\mathbf{x}) \quad (11.18)$$

can be converted into an integral equation using the Green's function (11.15),

$$\psi(\mathbf{x}) = \frac{\exp(i\mathbf{k} \cdot \mathbf{x})}{(2\pi)^{3/2}} - \frac{m}{2\pi\hbar^2} \int d^3\mathbf{x}' \frac{\exp(ik|\mathbf{x} - \mathbf{x}'|)}{|\mathbf{x} - \mathbf{x}'|} V(\mathbf{x}') \psi(\mathbf{x}'). \quad (11.19)$$

Note that the Lippmann-Schwinger equation (11.5) is the representation free operator version of this equation for static potential and plane waves as unperturbed states.

First order iteration of (11.19) and neglect of the irrelevant normalization factor $(2\pi)^{-3/2}$ yields

$$\psi(\mathbf{x}) \approx \exp(i\mathbf{k} \cdot \mathbf{x}) - \frac{m}{2\pi\hbar^2} \int d^3\mathbf{x}' \frac{V(\mathbf{x}')}{|\mathbf{x} - \mathbf{x}'|} \exp(ik|\mathbf{x} - \mathbf{x}'| + i\mathbf{k} \cdot \mathbf{x}'), \quad (11.20)$$

The overall normalization is irrelevant, because finally we are only interested in the ratio of the different parts of the wave function.

For $r \gg r'$ we have

$$|\mathbf{x} - \mathbf{x}'| \approx \sqrt{r^2 - 2rr' \cos \theta} \approx r - r' \cos \theta = r - \frac{1}{r} \mathbf{x} \cdot \mathbf{x}' = r - \hat{\mathbf{x}} \cdot \mathbf{x}'.$$

We need the expansion to this order in the exponent of the Green's function in equation (11.20). However, for the denominator the expansion

$$\frac{1}{|\mathbf{x} - \mathbf{x}'|} \approx \frac{1}{r}$$

will suffice, because the subleading term $(r'/r^2) \cos \theta$ will not contribute to the differential scattering cross section (11.2) due to the limit $\lim_{r \rightarrow \infty} r^2 j_{out}$.

Substitution of the approximations yields the *Born approximation*

$$\begin{aligned} \psi(\mathbf{x}) &= \exp(i\mathbf{k} \cdot \mathbf{x}) - \frac{m}{2\pi\hbar^2} \frac{1}{r} \exp(ikr) \int d^3\mathbf{x}' \exp[i(\mathbf{k} - k\hat{\mathbf{x}}) \cdot \mathbf{x}'] V(\mathbf{x}') \\ &= \exp(i\mathbf{k} \cdot \mathbf{x}) + f(k\hat{\mathbf{x}} - \mathbf{k}) \frac{1}{r} \exp(ikr) = \psi^{(in)}(\mathbf{x}) + \psi^{(out)}(\mathbf{x}), \end{aligned} \quad (11.21)$$

with the *scattering amplitude*

$$f(\Delta\mathbf{k}) = -\frac{m}{2\pi\hbar^2} \int d^3\mathbf{x} \exp(-i\Delta\mathbf{k} \cdot \mathbf{x}) V(\mathbf{x}). \quad (11.22)$$

Note that $\hbar\Delta\mathbf{k} \equiv \hbar(k\hat{\mathbf{x}} - \mathbf{k}) = \hbar\mathbf{k}' - \hbar\mathbf{k}$ is the momentum transfer imparted on the particle which is detected in the direction $\hat{\mathbf{x}}$, i.e. the scattering amplitude is up to a factor the Fourier transformed scattering potential evaluated at the momentum transfer. For later reference, we note that $f(\Delta\mathbf{k})$ can also be written as a transition matrix element of the operator $V(\mathbf{x})$,

$$f(\Delta\mathbf{k}) = -(2\pi)^2 \frac{m}{\hbar^2} \langle \mathbf{k}' | V | \mathbf{k} \rangle. \quad (11.23)$$

Like in the prototype one-dimensional scattering event described in Section 3.1, the monochromatic asymptotic wave function (11.21) describes both the incident and the scattered particles simultaneously, for the same reasons as in Section 3.1. The current density j_{out} of scattered particles is therefore calculated from the outgoing spherical wave component $\psi^{(out)}$ (\mathbf{x}) in the wave function (11.21), and we only need the leading term for $r \rightarrow \infty$,

$$\begin{aligned} \mathbf{j}_{out} &= \frac{\hbar}{2im} \left(\psi^{(out)+} \nabla \psi^{(out)} - \nabla \psi^{(out)+} \cdot \psi^{(out)} \right) \Big|_{\text{leading term for } r \rightarrow \infty} \\ &= \frac{\hbar k}{m} \frac{\hat{\mathbf{x}}}{r^2} |f(k\hat{\mathbf{x}} - \mathbf{k})|^2. \end{aligned} \quad (11.24)$$

The incoming current density j_{in} is calculated from the incoming plane wave component $\psi^{(in)}$ (\mathbf{x}),

$$\mathbf{j}_{in} = \frac{\hbar \mathbf{k}}{m}. \quad (11.25)$$

Both j_{in} and j_{out} come in units of cm/s instead of the expected cm^{-2}/s for particle or probability current densities. The reason for this is the use of plane or spherical wave states in \mathbf{k} space which are dimensionless in \mathbf{x} representation, see Section 5.3. Therefore the current densities (11.24) and (11.25) are actually current densities per \mathbf{k} space volume². The normalization to \mathbf{k} space volume cancels in the ratio j_{out}/j_{in} , and substitution of equations (11.24, 11.25) into (11.2) yields

$$\frac{d\sigma_k}{d\Omega} = |f(k\hat{\mathbf{x}} - \mathbf{k})|^2. \quad (11.27)$$

The scattering amplitude (11.22) for a spherically symmetric potential is

$$f(\Delta \mathbf{k}) \equiv f_k(\theta) = -\frac{2m}{\hbar^2 \Delta k} \int_0^\infty dr r \sin(\Delta k r) V(r), \quad (11.28)$$

where $\Delta k = 2k \sin(\theta/2)$ and θ is the scattering angle, see Figure 11.2.

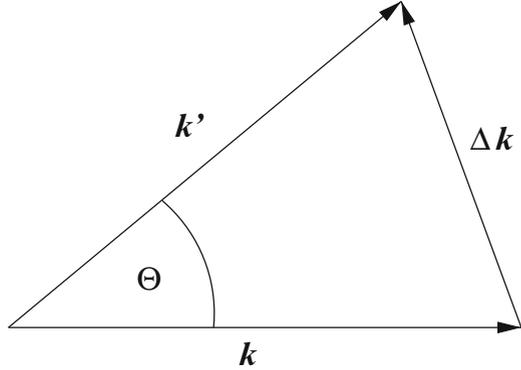
In agreement with the observation that the energy-dependent wave function describes both the incoming and the scattered particles, we have split the wave function $\psi(\mathbf{r})$ into the components $\psi^{(in)}$ (\mathbf{r}) and $\psi^{(out)}$ (\mathbf{r}), and then calculated separate current densities \mathbf{j}_{in} and \mathbf{j}_{out} from both contributions rather than calculate a total current density \mathbf{j} for $\psi(\mathbf{r})$. On the other hand, probability conservation implies for stationary states $\nabla \cdot \mathbf{j} = 0$, but only for the full current density including the

²We could more appropriately write $d\mathbf{j}(\mathbf{k})/d^3\mathbf{k} = \hbar \mathbf{k}/m$, and the current density from a volume \tilde{V} in \mathbf{k} space is

$$\mathbf{j}(\tilde{V}) = \int_{\tilde{V}} d^3\mathbf{k} \frac{\hbar \mathbf{k}}{m}. \quad (11.26)$$

Note that this has the correct units cm^{-2}/s for a current density.

Fig. 11.2 Energy conservation implies $k \equiv |\mathbf{k}| = |\mathbf{k}'|$. Δk is therefore related to k and the scattering angle θ according to $\Delta k = 2k \sin(\theta/2)$



interference terms $\mathbf{j} - \mathbf{j}_{in} - \mathbf{j}_{out}$ between the incoming and scattered parts of the wave function. Therefore the interference terms will describe reduction of the current of incoming particles due to scattering.

When we discuss this effect on the basis of the wave function (11.21), we have to keep in mind that this is only a large distance approximation which was justified by the observation that we are interested in the large distance limit of $r^2 j_{out}$. Furthermore, the wave function (11.21) will only yield components j_r and j_θ in spherical coordinates, and only j_r will be relevant for the detailed balance between incoming and scattered particles. The radial current density from (11.21) in the large distance approximation, i.e. for $kr \gg 1$ and under neglect of terms which drop off faster than r^{-2} , is

$$\frac{m}{\hbar} j_r = \Im \left(\psi^+ \frac{\partial}{\partial r} \psi \right) \simeq k \cos \theta + k \frac{|f_k(\theta)|^2}{r^2} + \frac{k}{r} \times \Re [f_k(\theta) \exp[ikr(1 - \cos \theta)] + f_k^+(\theta) \cos \theta \exp[-ikr(1 - \cos \theta)]] .$$

Conservation of particles requires $\int d\Omega r^2 j_r = 0$. The first term $k \cos \theta$ yields null after integration over the sphere. The remaining terms yield with $u = 1 - \cos \theta$, $F_k(u) = f_k(\theta)$,

$$k\sigma_k + 2\pi k r \int_0^2 du \Re [F_k(u) \exp(ikru) + F_k^+(u)(1 - u) \exp(-ikru)] = 0. \quad (11.29)$$

Here $\sigma_k \equiv \int d\Omega d\sigma_k/d\Omega$ is the total scattering cross section.

Two-fold integration by parts yields

$$kr \int_0^2 du F_k(u) \exp(ikru) = iF_k(0) - iF_k(2) \exp(2ikr) - \frac{1}{kr} F_k'(0) + \frac{1}{kr} F_k'(2) \exp(2ikr) - \frac{1}{kr} \int_0^2 du F_k''(u) \exp(ikru) .$$

The last three terms vanish for $kr \rightarrow \infty$. For the term $F_k(2) \exp(2ikr)$ we observe that averaging over a very small momentum uncertainty $\Delta k/k = \pi/kr \ll 1$ also yields a null result because it corresponds to an integration in k space over a range $-\pi/r \leq k \leq \pi/r$. This can be understood physically as destructive interference between states with a minute variation in momentum. Therefore we find for $kr \rightarrow \infty$

$$kr \int_0^2 du F_k(u) \exp(ikru) \rightarrow if_k(0).$$

In the same way one finds

$$kr \int_0^2 du F_k^+(u)(1-u) \exp(-ikru) \rightarrow -if_k^+(0),$$

and equation (11.29) yields in the large kr limit the *optical theorem*

$$\sigma_k = \frac{4\pi}{k} \Im f_k(0) \quad (11.30)$$

between the total scattering cross section and the imaginary part of the scattering amplitude in forward direction.

11.3 Scattering off a hard sphere

The hard sphere of radius R corresponds to the $V_0 \rightarrow \infty$ limit of a potential $V(r) = V_0 \Theta(R-r)$. This reduces to the solution of the free Schrödinger equation for $r > R$ and a boundary condition on the surface of the sphere,

$$\psi(r) \Big|_{r=R} = 0. \quad (11.31)$$

We recall that the radial Schrödinger equation for a free particle with fixed angular momentum M_z , M^2 and energy $E = \hbar^2 k^2 / 2m$ yields the radial equation (7.43),

$$\left(\frac{d^2}{dr^2} - \frac{\ell(\ell+1)}{r^2} + k^2 \right) r\psi(r) = 0. \quad (11.32)$$

We have seen in Section 7.7 that the regular solutions for arbitrary ℓ can be gotten through repeated application of $r^{-1}d/dr$ on the regular solution for $\ell = 0$,

$$\psi_{\ell,k}^{(\text{in})}(r) \propto j_\ell(kr), \quad j_\ell(x) = (-x)^\ell \left(\frac{1}{x} \frac{d}{dx} \right)^\ell j_0(x), \quad j_0(x) = \frac{\sin x}{x}.$$

We denote the regular solutions $j_\ell(kr)$ as $\psi_{\ell,k}^{(\text{in})}(r)$, because we can superimpose those functions according to equation (7.51) to form an incoming plane wave.

However, equation (11.32) also has an outgoing radial wave as a solution for $\ell = 0$,

$$\psi_{0,k}^{(\text{out})}(r) \propto \frac{\exp(ikr)}{kr} = -ih_0^{(1)}(kr).$$

The reasoning leading to equations (7.46, 7.47) also implies that repeated application of $r^{-1}d/dr$ on the outgoing radial wave solution leads to solutions for higher ℓ ,

$$\psi_{\ell,k}^{(\text{out})}(r) \propto -ih_\ell^{(1)}(kr), \quad h_\ell^{(1)}(x) = (-x)^\ell \left(\frac{1}{x} \frac{d}{dx} \right)^\ell h_0^{(1)}(x).$$

In leading order in $1/r$, these are again outgoing radial waves,

$$h_\ell^{(1)}(kr) \simeq (-)^\ell \frac{\exp(ikr)}{ikr}. \quad (11.33)$$

The functions $h_\ell^{(1)}(x)$ are known as spherical Hankel functions of the first kind.

We can use the spherical Bessel and Hankel functions to form solutions of equation (11.32) which satisfy the condition (11.31) and contain an outgoing spherical wave in the asymptotic limit,

$$\psi_{\ell,k}(r) = \psi_{\ell,k}^{(\text{in})}(r) + \psi_{\ell,k}^{(\text{out})}(r) \propto j_\ell(kr) - h_\ell^{(1)}(kr) \frac{j_\ell(kR)}{h_\ell^{(1)}(kR)}.$$

However, equation (7.51) then tells us how to write down a solution to the free Schrödinger equation for energy $E = \hbar^2 k^2 / 2m$ outside of the hard sphere, which satisfies the boundary condition (11.31) and contains both a plane wave and an outgoing spherical wave,

$$\begin{aligned} \psi_k(\mathbf{r}) &= \sum_{\ell=0}^{\infty} (2\ell + 1) i^\ell \left(j_\ell(kr) - h_\ell^{(1)}(kr) \frac{j_\ell(kR)}{h_\ell^{(1)}(kR)} \right) P_\ell(\cos \theta) \\ &= \exp(ikz) - \sum_{\ell=0}^{\infty} (2\ell + 1) i^\ell h_\ell^{(1)}(kr) \frac{j_\ell(kR)}{h_\ell^{(1)}(kR)} P_\ell(\cos \theta) \\ &= \psi^{(\text{in})}(\mathbf{r}) + \psi^{(\text{out})}(\mathbf{r}). \end{aligned} \quad (11.34)$$

From our previous experience in Sections 3.1 and 11.2 we already anticipated that the monochromatic wave function will describe both incoming and scattered particles. According to equation (11.33), the asymptotic expansion of the wave function for large r is

$$\begin{aligned} \psi_k(\mathbf{r}) &\simeq \exp(ikz) + f_k(\theta) \frac{\exp(ikr)}{r}, \\ f_k(\theta) &= -\frac{1}{k} \sum_{\ell=0}^{\infty} (2\ell + 1) (-i)^{\ell+1} P_\ell(\cos \theta) \frac{j_\ell(kR)}{h_\ell^{(1)}(kR)}. \end{aligned}$$

The resulting expression for the differential scattering cross section of the hard sphere is a little unwieldy,

$$\begin{aligned} \frac{d\sigma_k}{d\Omega} = |f_k(\theta)|^2 &= \frac{1}{k^2} \sum_{\ell, \ell'=0}^{\infty} (2\ell + 1)(2\ell' + 1) i^{\ell - \ell'} P_{\ell}(\cos \theta) P_{\ell'}(\cos \theta) \\ &\times \frac{j_{\ell}^+(kR) j_{\ell'}(kR)}{h_{\ell}^{(1)+}(kR) h_{\ell'}^{(1)}(kR)}. \end{aligned} \quad (11.35)$$

However, for the scattering cross section the orthogonality property of Legendre polynomials

$$\int_0^{\pi} d\theta \sin \theta P_{\ell}(\cos \theta) P_{\ell'}(\cos \theta) = \frac{2}{2\ell + 1} \delta_{\ell, \ell'}$$

yields a much simpler result,

$$\sigma_k = \frac{4\pi}{k^2} \sum_{\ell=0}^{\infty} (2\ell + 1) \left| \frac{j_{\ell}(kR)}{h_{\ell}^{(1)}(kR)} \right|^2. \quad (11.36)$$

This is shown in Figure 11.3. The asymptotic behavior for small arguments kR , $j_{\ell}(kR) \simeq (kR)^{\ell} / (2\ell + 1)!!$ and $h_{\ell}^{(1)}(kR) \simeq -i(2\ell - 1)!! (kR)^{-\ell - 1}$, imply for the low energy or long wavelength limit $\lambda \gg R$ that only the $\ell = 0$ contribution survives with

$$\lim_{kR \rightarrow 0} \sigma_k = 4\pi R^2.$$

The quantum mechanical scattering cross section drops continuously from $\lim_{kR \rightarrow 0} \sigma_k = 4\pi R^2$ to $\lim_{kR \rightarrow \infty} \sigma_k = 2\pi R^2$, i.e. it always exceeds the classical value $\sigma_{cl} = \pi R^2$ by more than a factor of 2. In terms of the variables k and R , σ_k seems to be independent of \hbar and one might naively expect that this is the reason for absence of a classical limit for scattering off a hard sphere, but this is wrong for two reasons. If one compares with classical results one should use the same variables as in classical mechanics, and if in terms of the classical variables the quantum mechanical result is independent of \hbar , we rather expect to find the same result as in classical mechanics. Furthermore, when one calculates classical scattering cross sections, one uses the momentum $p = \hbar k$ for the incident particles as a variable besides the radius R of the sphere, i.e. in terms of classical variables the cross section σ_k does depend on \hbar , and the classical limit should correspond to $pR \gg \hbar$, $kR \gg 1$. However, the classical limit fails because there is an important difference between the classical calculation and quantum mechanical scattering. The classical calculation requires particles to hit the hard sphere with an impact parameter $b = |\mathbf{M}|/|p|$ which is limited by the requirement that all scattered particles must actually hit the sphere, $b \leq R$. This corresponds to a classical angular momentum cutoff $|\mathbf{M}| \leq pR$. However, quantum mechanically, particles with arbitrary high angular momentum still feel the presence of the hard sphere

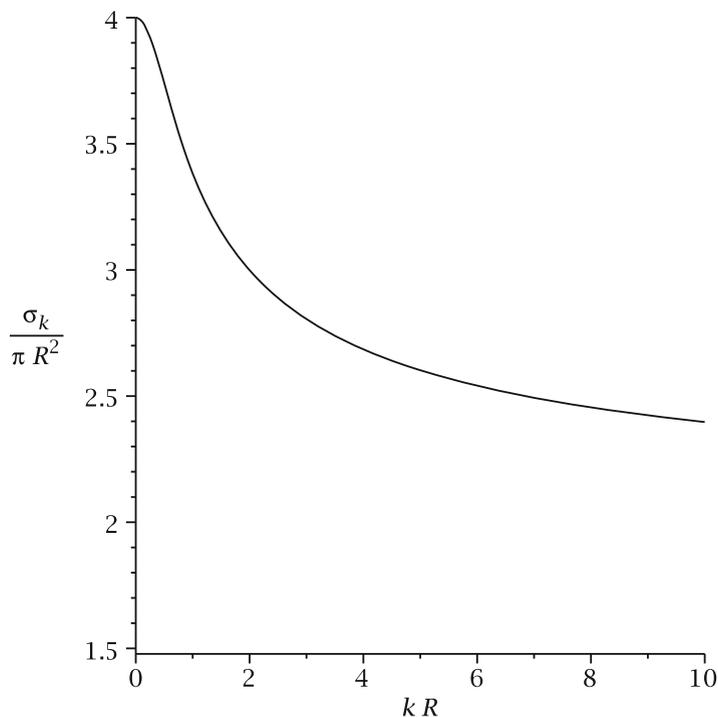


Fig. 11.3 The scattering cross section of a hard sphere normalized to the classical scattering cross section $\sigma_{classical} = \pi R^2$

and can be scattered similar to classical wave diffraction. This regime of deviation between the classical and quantum picture concerns large angular momenta and small deflection angles, i.e. the forward scattering region. In the classical picture the forward scattered particles are considered as missing the sphere and therefore ignored in the classical scattering cross section. Therefore the classical cross section is always smaller than the quantum mechanical cross section, even in the classical limit $kR \gg 1$. The increasing concentration of scattering in forward direction with increasing kR is demonstrated in Figures 11.4 and 11.5.

An approximate evaluation of the θ dependence of the extra “non-classical” part of the differential cross section for $kR \gg 1$ in terms of shadow forming waves is given in [29]. However, the Figures 11.4 and 11.5 use the exact result (11.35). Either way, the ultimate reason for the discrepancy between the quantum result and the classical result in the classical limit $kR \gg 1$ is different accounting of scattered versus unscattered particles in the forward scattering region.

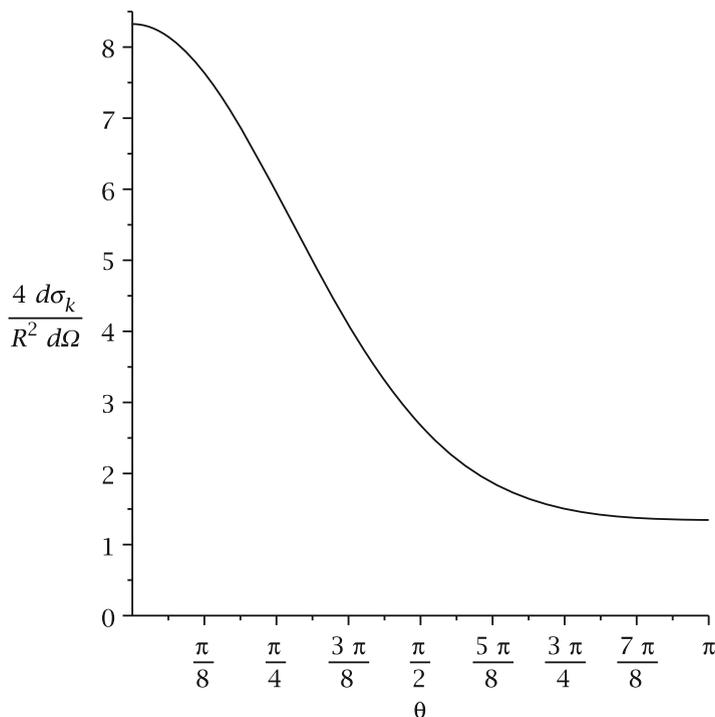


Fig. 11.4 The differential scattering cross section $d\sigma_k/d\Omega$ of a hard sphere of radius R normalized to the classical differential scattering cross section $(d\sigma_k/d\Omega)_{classical} = R^2/4$ for $kR = 1$

11.4 Rutherford scattering

Axial symmetry often plays a role in atoms which interact with their surroundings. External fields will often have axial symmetry, and this motivated Schrödinger to solve the hydrogen problem in parabolic coordinates for his perturbative analysis of the Stark effect³. Furthermore, if a hydrogen atom is formed through electron-proton recombination, the initial plane wave state describing the mutual approach of the electron and the proton will also break the rotational symmetry to axial symmetry and the calculation of recombination cross sections can be performed in terms of parabolic coordinates [3]. Maybe the best known application of parabolic coordinates concerns the calculation of Rutherford scattering. The incident plane wave $\psi^{(in)} \sim \exp(ikz)$ breaks the rotational symmetry of the problem down to an axial symmetry, but we still expect an outgoing spherical wave $\psi^{(out)} \sim \exp(ikr)/r$. The reconciliation of axial symmetry with the use of r makes parabolic coordinates more useful than cylinder coordinates for the study of scattering in rotationally

³E. Schrödinger, *Annalen Phys.* 385, 437 (1926).

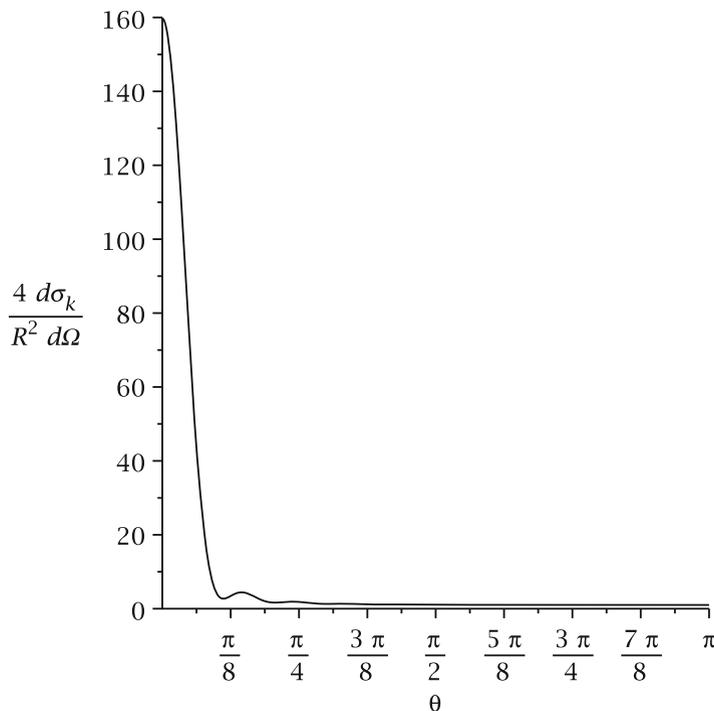


Fig. 11.5 The differential scattering cross section $d\sigma_k/d\Omega$ of a hard sphere of radius R normalized to the classical differential scattering cross section $(d\sigma_k/d\Omega)_{classical} = R^2/4$ for $kR = 10$

symmetric potentials beyond the Born approximation, and can occasionally render them also more useful than spherical coordinates. The separability of the Coulomb problem in parabolic coordinates makes them particularly useful for the study of Rutherford scattering.

We define parabolic coordinates through the following relations⁴,

$$\begin{aligned}
 x &= 2\sqrt{\xi\eta} \cos \varphi, & y &= 2\sqrt{\xi\eta} \sin \varphi, & z &= \xi - \eta, \\
 2\xi &= r + z, & 2\eta &= r - z, & \varphi &= \arctan \frac{y}{x}.
 \end{aligned}
 \tag{11.37}$$

Using the methods developed in Section 5.4, one finds the Schrödinger equation for motion of a particle of energy $E = \hbar^2 k^2 / 2\mu$ in the Coulomb potential $V = q_1 q_2 / 4\pi\epsilon_0 r = \hbar^2 K / 2\mu(\xi + \eta)$ in parabolic coordinates,s

$$\frac{1}{\xi + \eta} \left[\frac{\partial}{\partial \xi} \left(\xi \frac{\partial}{\partial \xi} \right) + \frac{\partial}{\partial \eta} \left(\eta \frac{\partial}{\partial \eta} \right) \right] \psi + \frac{1}{4\xi\eta} \frac{\partial^2 \psi}{\partial^2 \varphi} + k^2 \psi - \frac{K}{\xi + \eta} \psi = 0. \tag{11.38}$$

⁴ Please note that the definition used here differs by factors of 2 from the definition used by Schrödinger, $\lambda_1 \equiv \xi_S = 2\xi$, $\lambda_2 \equiv \eta_S = 2\eta$.

The arguments in Section 5.5, in particular concerning Hamiltonians of the form (5.36), imply that the solutions of this equation must have the form

$$\psi(\xi, \eta, \varphi) = f(\xi)g(\eta) \exp(im\varphi),$$

with the remaining separated equations

$$\left(\xi \frac{d}{d\xi}\right)^2 f + \left(k^2 \xi^2 - K_1 \xi - \frac{m^2}{4}\right) f = 0, \quad (11.39)$$

$$\left(\eta \frac{d}{d\eta}\right)^2 g + \left(k^2 \eta^2 - K_2 \eta - \frac{m^2}{4}\right) g = 0, \quad (11.40)$$

with $K_1 + K_2 = K$. We want $\psi^{(\text{in})} \sim \exp(ikz) = \exp(ik\xi) \exp(-ik\eta)$ to be the dominant term in the solution near the half-axis $z < 0$, i.e. for $\xi \rightarrow 0$. This requirement complies with equation (11.39) if we choose $m = 0$ and $K_1 = ik$. If we then substitute $f(\xi) = F(\xi) \exp(ik\xi)$ into equation (11.39) to find the second solution, we find $F(\xi) = A + BE_i(-2ik\xi)$, which implies a singularity of the second solution near the half-axis $z < 0$. Therefore we conclude that the solution to our scattering problem must have the form $\psi(\xi, \eta) = g(\eta) \exp(ik\xi)$ with the remaining condition

$$\eta \frac{d^2 g}{d\eta^2} + \frac{dg}{d\eta} + (k^2 \eta - K + ik) g = 0. \quad (11.41)$$

Comparison with equation (11.39) for $m = 0$ and $K_1 = ik$ tells us that $g(\eta) = \exp(-ik\eta)$ is the regular solution of equation (11.41) if $K = 0$. This is also clear from the physical point of view. If there is no scattering potential, the plane wave $\exp(ikz) = \exp(ik\xi) \exp(-ik\eta)$ that we imposed near the half-axis $z < 0$ must persist everywhere. This motivates a substitution $g(\eta) = h(\eta) \exp(-ik\eta)$ in (11.41),

$$\eta \frac{d^2 h}{d\eta^2} + (1 - 2ik\eta) \frac{dh}{d\eta} - Kh = 0. \quad (11.42)$$

Substitution of $h(\eta) = \sum_{n \geq 0} c_n \eta^n$ yields

$$c_{n+1} = \frac{K + 2ikn}{(n+1)^2} c_n$$

and therefore

$$\begin{aligned} h(\eta) &= c_0 \sum_{n=0}^{\infty} \frac{K(K+2ik) \dots (K+2ik(n-1))}{n!} \frac{\eta^n}{n!} \\ &= c_0 {}_1F_1(-iK/2k; 1; 2ik\eta) = c_0 \exp(2ik\eta) {}_1F_1(1 + iK/2k; 1; 2ik\eta). \end{aligned}$$

The wave function for our scattering problem is therefore up to normalization⁵

$$\begin{aligned}\psi(\mathbf{r}) &= \exp[ik(\xi - \eta)] {}_1F_1(-iK/2k; 1; 2ik\eta) \\ &= \exp(ikz) {}_1F_1(-iK/2k; 1; ik(r-z)) \\ &= \exp(ikr) {}_1F_1(1 + iK/2k; 1; ik(r-z)).\end{aligned}\quad (11.43)$$

The normalization factor c_0 is irrelevant because it cancels in the calculation of the cross section.

Identification of the incoming and scattered components in the wave function requires asymptotic expansion for large values of the argument $2k\eta = k(r-z)$. The asymptotic expansion of confluent hypergeometric functions ${}_1F_1(a; b; \zeta)$ for large $|\zeta|$ [1] yields the leading order terms

$$\begin{aligned}{}_1F_1(-iK/2k; 1; ik(r-z)) &\simeq \exp\left(\frac{\pi K}{4k}\right) \left[\frac{2k}{iK} \Gamma^{-1}\left(\frac{iK}{2k}\right) \right. \\ &\times \exp\left(\frac{iK}{2k} \ln[k(r-z)]\right) \left(1 + \frac{K^2}{4ik^3(r-z)}\right) + \frac{\exp[ik(r-z)]}{ik(r-z)} \Gamma^{-1}\left(\frac{K}{2ik}\right) \\ &\left. \times \exp\left(-\frac{iK}{2k} \ln[k(r-z)]\right) \right].\end{aligned}$$

After neglecting another irrelevant overall factor we find the asymptotic form

$$\begin{aligned}\psi(\mathbf{r}) &\simeq \exp\left(ikz + \frac{iK}{2k} \ln[k(r-z)]\right) \left(1 + \frac{K^2}{4ik^3r(1-\cos\theta)}\right) \\ &\quad + \frac{\Gamma(iK/2k)}{\Gamma(-iK/2k)} \frac{K}{2k^2r(1-\cos\theta)} \exp\left(ikr - \frac{iK}{2k} \ln[k(r-z)]\right) \\ &= \psi^{(\text{in})}(\mathbf{r}) + \psi^{(\text{out})}(\mathbf{r}),\end{aligned}\quad (11.44)$$

where $\theta = \arccos(z/r)$ is the scattering angle.

This yields a differential scattering cross section

$$\frac{d\sigma}{d\Omega} = \lim_{r \rightarrow \infty} \frac{r^2 j_{\text{out}}}{j_{\text{in}}} = \left(\frac{K}{4k^2 \sin^2(\theta/2)}\right)^2 = \left(\frac{q_1 q_2}{16\pi\epsilon_0 E}\right)^2 \frac{1}{\sin^4(\theta/2)}, \quad (11.45)$$

which equals exactly the corresponding cross section calculated in classical mechanics and used by Rutherford in 1911 to infer the existence of a tiny positively charged nucleus in atoms. The cross section (11.45) is an example of a quantum mechanical result which is independent of \hbar when expressed in terms of classical variables, and therefore it must agree with the classical result.

⁵W. Gordon, Z. Phys. 48, 180 (1928).

Use of the asymptotic expansion of the hypergeometric function ${}_1F_1(a; b; \zeta)$ for large $|\zeta|$ in the present case implies the requirement $kr(1 - \cos \theta) = 2kr \sin^2(\theta/2) \gg 1$, i.e. the Rutherford formula is only applicable for scattering angles $\theta \gg \sqrt{2/kr} = \sqrt{\lambda/\pi r}$. This limitation is usually irrelevant, because the values of λ e.g. in the experiments of Geiger and Marsden were only a few femtometers.

11.5 Problems

11.1. Show that the Lippmann-Schwinger equations (11.6, 11.7) can also be written in the form

$$|\psi(E)\rangle = (E - H_0 + i\epsilon) \frac{1}{E - H + i\epsilon} |\psi_0(E)\rangle.$$

11.2. The free time-dependent retarded Green's function in \mathbf{x} representation has to satisfy the conditions

$$\left(i\hbar \frac{\partial}{\partial t} + \frac{\hbar^2}{2m} \Delta \right) \mathcal{G}(\mathbf{x}, t) = \delta(\mathbf{x})\delta(t), \quad \mathcal{G}(\mathbf{x}, t) \Big|_{t < 0} = 0.$$

Show that this function satisfies the following equations,

$$\begin{aligned} \mathcal{G}(\mathbf{x}, t) &= \frac{1}{(2\pi)^4 \hbar} \int d^3\mathbf{k} \int_{-\infty}^{\infty} d\omega \frac{\exp[i(\mathbf{k} \cdot \mathbf{x} - \omega t)]}{\omega - (\hbar k^2/2m) + i\epsilon} \\ &= -\frac{m}{\pi \hbar^3} \int_{-\infty}^{\infty} dE G(\mathbf{x}, E) \exp(-iEt/\hbar) \\ &= \frac{\Theta(t)}{(2\pi)^3 i\hbar} \int d^3\mathbf{k} \exp\left[i\left(\mathbf{k} \cdot \mathbf{x} - \frac{\hbar t}{2m} k^2 \right) \right] \\ &= \frac{\Theta(t)}{i\hbar} \sqrt{\frac{m}{2\pi i\hbar t}} \exp\left(i \frac{m\mathbf{x}^2}{2\hbar t} \right). \end{aligned} \quad (11.46)$$

This also corresponds to the relation

$$\mathcal{G}(\mathbf{x}, t) = \frac{\Theta(t)}{i\hbar} U(\mathbf{x}, t) = \frac{\Theta(t)}{i\hbar} \langle \mathbf{x} | \exp\left(-\frac{it}{2m} \mathbf{p}^2 \right) | \mathbf{0} \rangle$$

between the retarded Green's function and the propagator for the free Schrödinger equation.

11.3. Show that transformation of equation (11.13) into the frequency domain (5.12, 5.13) yields

$$|\psi(\omega)\rangle = |\psi_0(\omega)\rangle + \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} d\omega' \mathcal{G}(\hbar\omega) V(\omega - \omega') |\psi(\omega')\rangle. \quad (11.47)$$

Show also that this reduces to the Lippmann-Schwinger equation (11.5) if the perturbation V is time-independent.

11.4. Calculate the differential scattering cross sections for the following potentials in Born approximation.

11.4a. $V(r) = V_0 \Theta(R - r),$

11.4b. $V(r) = V_0 \exp(-r/R),$

11.4c. $V(r) = V_0 \exp(-r^2/R^2).$

11.5. Calculate the total cross sections for the potentials from Problem 11.4 in Born approximation.

11.6. Calculate the differential cross section for Rutherford scattering in Born approximation. Compare with the exact result.

11.7. Calculate the differential and total scattering cross sections for Rutherford scattering with screened electromagnetic interactions in Born approximation. Use the following models for the screened interactions,

11.7a. $V(r) = (qQ/4\pi\epsilon_0 r) \exp(-r/R),$

11.7b. $V(r) = (qQ/4\pi\epsilon_0 r) \exp(-r^2/R^2).$

11.8. Show that the scattering amplitude in Born approximation (11.22) satisfies $\Im f_k(0) = 0$. Why does this not contradict the optical theorem (11.30)?

Hint: Split the potential into parity even and odd parts, $V(\mathbf{x}) = V_+(\mathbf{x}) + V_-(\mathbf{x})$, $V_{\pm}(\mathbf{x}) = [V(\mathbf{x}) \pm V(-\mathbf{x})]/2$. Consider powers of V (or equivalently of coupling constants) in (11.30).