Chapter 8

Scattering Theory

I ask you to look both ways. For the road to a knowledge of the stars leads through the atom; and important knowledge of the atom has been reached through the stars.
-Sir Arthur Eddington (1882 - 1944)

Most of our knowledge about microscopic physics originates from scattering experiments. In these experiments the interactions between atomic or sub-atomic particles can be measured. This is done by letting them collide with a fixed target or with each other. In this chapter we present the basic concepts for the analysis of scattering experiments.

We will first analyze the asymptotic behavior of scattering solutions to the Schrödinger equation and define the differential cross section. With the method of partial waves the scattering amplitudes are then obtained from the phase shifts for spherically symmetric potentials. The Lippmann–Schwinger equation and its formal solution, the Born series, provides a perturbative approximation technique which we apply to the Coulomb potential. Eventually we define the scattering matrix and the transition matrix and relate them to the scattering amplitude.

8.1 The central potential

The physical situation that we have in mind is an incident beam of particles that scatters at some localized potential $V(\vec{x})$ which can represent a nucleus in some solid target or a particle in a colliding beam. For fixed targets we can usually focus on the interaction with a single nucleus. In beam-beam collisions it is more difficult to produce sufficient luminosity, but this has to be dealt with in the ultrarelativistic scattering experiments of particle physics for kinematic reasons.[1] We will mostly confine our interest to elastic scattering where the particles are not excited and there is no particle production. It is easiest to work in the center of mass frame, where a spherically symmetric potential has the form $V(r)$ with $r = |\vec{x}|$. For a fixed target experiment the scattering amplitude can then easily be converted to the laboratory frame for comparison with the experimental data. Because of the quantum mechanical uncertainty we can only predict the *probability* of scattering into a certain direction, in contrast to the deterministic scattering angle in classical mechanics. With particle beams that contain a sufficiently large number of particles we can, however, measure the probability distribution (or differntial cross section) with arbitrary precision.

8.1.1 Differential cross section and frames of reference

Imagine a beam of monoenergetic particles being scattered by a target located at $\vec{x} = 0$. Let the detector cover a solid angle $d\Omega$ in direction (θ, φ) from the scattering center. We choose a coordinate system

$$\vec{x} = (r\sin\theta\cos\varphi, r\sin\theta\sin\varphi, r\cos\theta), \qquad \vec{k}_{in} = \frac{\sqrt{2mE}}{\hbar}\,\vec{e}_3 \tag{8.2}$$

so that the incoming beam travels along the z-axis. The number of particles per unit time entering the detector is then given by $N d\Omega$. The flux of particles F in the incident beam is defined as the number of particles per unit time, crossing a unit area placed normal to the direction of incidence. To characterize the collisions we use the *differential scattering cross-section*

$$\frac{d\sigma}{d\Omega} = \frac{N}{F}, \tag{8.3}$$

which is defined as the ratio of the number of particles scattered into the direction (θ, φ) per unit time, per unit solid angle, divided by the incident flux. The *total scattering cross-section*

$$\sigma_{tot} = \int \left(\frac{d\sigma}{d\Omega}\right) d\Omega = \int_0^{2\pi} d\varphi \int_0^{\pi} d\theta \sin\theta \frac{d\sigma}{d\Omega} \tag{8.4}$$

is defined as the integral of the differential scattering cross-section over all solid angles. Both the differential and the total scattering cross-sections have the dimension of an area.

Center-of-Mass System. As shown in fig. 8.1 we denote by $\vec{p}_1$ and $\vec{p}_2$ the momenta of the incoming particles and of the target, respectively. The center of mass momentum is $\vec{p}_g = \vec{p}_1 + \vec{p}_2 = \vec{p}_{1L}$ with the target at rest $\vec{p}_{2L} = 0$ in the laboratory frame. As we derived

[1] Using the notation of figure 8.1 below with an incident particle of energy $E_1 = E_{\text{in}} = \sqrt{c^2\vec{p}_{1L}^{\,2} + m_1^2c^4}$ hitting a target with mass m_2 at rest in the laboratory system the total energy

$$E^2 = c^2(p_{1L} + p_{2L})^2 = (E_1 + m_2c^2)^2 - c^2\vec{p}_{1L}^{\,2} = m_1^2c^4 + m_1^2c^4 + 2E_{\text{in}}m_2c^2 \tag{8.1}$$

available for particle production in the center of mass system is only $E \approx \sqrt{2E_{in}m_2c^2}$ for $E_{\text{in}} \gg m_1c^2, m_2c^2$.

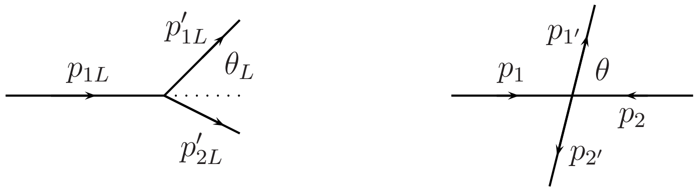

Figure 8.1: Scattering angle for fixed target and in the center of mass frame.

in section 4, the kinematics of the reduced 1-body problem is given by the reduced mass $\mu = m_1 m_2/(m_1 + m_2)$ and the momentum

$$\vec{p} = \frac{\vec{p}_1 m_2 - \vec{p}_2 m_1}{m_1 + m_2}. \tag{8.5}$$

Obviously $\varphi = \varphi_L$, while the relation between θ in the center of mass frame and the angle θ_L in the fixed target (laboratory) frame can be obtained by comparing the momenta $\vec{p}_1'$ of the scattered particles. With $p_i = |\vec{p}_i|$ the transversal momentum is

$$p'_{1L} \sin\theta_L = p'_1 \sin\theta. \tag{8.6}$$

The longitudinal momentum is $\vec{p}_1' \cos\theta$ in the center of mass frame. In the laboratory frame we have to add the momentum due to the center of mass motion with velocity $\vec{v}_g$, where

$$\vec{p}_{1L} = \vec{p}_1 + m_1\vec{v}_g = \vec{p}_g = (m_1 + m_2)\vec{v}_g \qquad \Rightarrow \qquad m_2\vec{v}_g = \vec{p}_1. \tag{8.7}$$

Restricting to elastic scattering where $|\vec{p}_1{}'| = |\vec{p}_1|$ we find for the longitudinal motion

$$p'_{1L}\cos\theta_L = p'_1\cos\theta + m_1 v_g \overset{el.}{=} p'_1(\cos\theta + \frac{m_1}{m_2}) \tag{8.8}$$

We hence find the formula

$$\tan\theta_L^{elastic} = \frac{\sin\theta}{\cos\theta + \tau} \qquad \text{with} \qquad \tau = \frac{m_1}{m_2} = \frac{m_{in}}{m_{target}} \tag{8.9}$$

for the scattering angle in the laboratory frame for elastic scattering. According to the change of the measure of the angular integration the differential cross section also changes by a factor

$$\left(\frac{d\sigma}{d\Omega}\right)_L (\theta_L(\theta)) = \left|\frac{d(\cos\theta)}{d(\cos\theta_L)}\right| \frac{d\sigma}{d\Omega}(\theta) = \frac{(1 + 2\tau\cos\theta + \tau^2)^{3/2}}{|1 + \tau\cos\theta|} \frac{d\sigma}{d\Omega}(\theta) \tag{8.10}$$

where we used $\cos\theta_L = 1/\sqrt{1 + \tan^2\theta} = (\cos\theta + \tau)/\sqrt{1 + 2\tau\cos\theta + \tau^2}$.

8.1.2 Asymptotic expansion and scattering amplitude

We now consider the scattering of a beam of particles by a fixed center of force and let m denote the reduced mass and $\vec{x}$ the relative coordinate. If the beam of particles is switched on for a long time compared to the time one particle needs to cross the interaction area, steady-state conditions apply and we can focus on stationary solutions of the time-independent Schrödinger equation

$$\left[-\frac{\hbar^2}{2m}\Delta + V(\vec{x})\right] u(\vec{x}) = Eu(\vec{x}), \qquad \psi(\vec{x},t) = e^{-i\omega t}u(\vec{x}). \tag{8.11}$$

The energy eigenvalues E is related by

$$E = \frac{1}{2}m\vec{v}^2 = \frac{\vec{p}^2}{2m} = \frac{\hbar^2\vec{k}^2}{2m} \tag{8.12}$$

to the incident momentum $\vec{p}$, the incident wave vector $\vec{k}$ and the incident velocity $\vec{v}$. For convenience we introduce the reduced potential

$$U(\vec{x}) = 2m/\hbar^2 \cdot V(\vec{x}) \tag{8.13}$$

so that we can write the Schrödinger equation as

$$[\nabla^2 + k^2 - U(\vec{x})]u(\vec{x}) = 0. \tag{8.14}$$

For potentials that asymptotically decrease faster then r^{-1}

$$|V_{as}(r)| \le c/r^\alpha \qquad \text{for} \quad r \to \infty \qquad \text{with} \quad \alpha > 1, \tag{8.15}$$

we can neglect $U(\vec{x})$ for large r and the Schrödinger equation reduces to the Helmholtz equation of a free particle

$$[\Delta + k^2]u_{as}(\vec{x}) = 0. \tag{8.16}$$

Potentials satisfying (8.15) are called *finite range*. (The important case of the Coulomb potential is, unfortunately, of infinite range, but we will be able to treat it as the limit $\alpha \to 0$ of the finite range Yukawa potential $e^{-\alpha r}/r$.) For large r we can decompose the wave function into a part u_{in} describing the incident beam and a part u_{sc} for the scattered particles

$$u(\vec{x}) \;\to\; u_{in}(\vec{x}) + u_{sc}(\vec{x}) \qquad \text{for} \qquad r \to \infty. \tag{8.17}$$

Since we took the z-axis as the direction of incidence and since the particles have all the same momentum $p = \hbar k$ the incident wave function can be written as

$$u_{in}(\vec{x}) = e^{i\vec{k}\cdot\vec{x}} = e^{ikz}, \tag{8.18}$$

where we were free to normalize the amplitude of u_{in} since all equations are linear.

Far from the scattering center the scattered wave function represents an outward radial flow of particles. We can parametrize it in terms of the *scattering amplitude* $f(k,\theta,\varphi)$ as

$$u_{sc}(\vec{x}) = f(k,\theta,\varphi)\frac{e^{ikr}}{r} + \mathcal{O}(\frac{1}{r^\alpha}), \tag{8.19}$$

where (r, θ, φ) are the polar coordinates of the position vector $\vec{x}$ of the scattered particle. The asymptotic form u_{as} of the scattering solution thus becomes

$$u_{as} = (e^{i\vec{k}\cdot\vec{x}})_{as} + f(k,\theta,\varphi)\frac{e^{ikr}}{r}. \tag{8.20}$$

The scattering amplitude can now be related to the differential cross-section. From chapter 2 we know the probability current density for the stationary state

$$\vec{j}(\vec{x}) = \frac{\hbar}{2im}(\psi^*\vec{\nabla}\psi - \psi\vec{\nabla}\psi^*) = \frac{\hbar}{m}\,\mathrm{Re}\,(u^*\vec{\nabla}u) \tag{8.21}$$

with the gradient operator in spherical polar coordinates (r, θ, φ) reading

$$\vec{\nabla} = \vec{e}_r\,\frac{\partial}{\partial r} + \vec{e}_\theta\,\frac{1}{r}\frac{\partial}{\partial\theta} + \vec{e}_\varphi\,\frac{1}{r\sin\theta}\frac{\partial}{\partial\varphi}. \tag{8.22}$$

For large r the scattered particle current flows in radial direction with

$$j_r = \frac{\hbar k}{mr^2}|f(k,\theta,\varphi)|^2 + \mathcal{O}(\frac{1}{r^3}). \tag{8.23}$$

Since the area of the detector is $r^2 d\Omega$ the number of particles $Nd\Omega$ entering the detector per unit time is

$$Nd\Omega = \frac{\hbar k}{m}|f(k,\theta,\varphi)|^2 d\Omega. \tag{8.24}$$

For $|\psi_{in}(\vec{x})|^2 = 1$ the incoming flux $F = \hbar k/m = v$ is given by the particle velocity. We thus obtain the differential cross-section

$$\boxed{\frac{d\sigma}{d\Omega} = |f(k,\theta,\varphi)|^2} \tag{8.25}$$

as the modulus squared of the scattering amplitude.

8.2 Partial wave expansion

For a spherically symmetric central potential $V(\vec{x}) = V(r)$ we can use rotation invariance to simplify the computation of the scattering amplitude by an expansion of the angular dependence in spherical harmonics. Since the system is completely symmetric under rotations about the direction of incident beam (chosen along the z-axis), the wave function and the scattering amplitude do not depend on φ. Thus we can expand both $u_{\vec{k}}(r,\theta)$ and $f(k,\theta)$ into a series of Legendre polynomials, which form a complete set of functions for the interval $-1 \leqslant \cos\theta \leqslant +1$,

$$u_{\vec{k}}(r,\theta) = \sum_{l=0}^{\infty} R_l(k,r)P_l(\cos\theta), \tag{8.26}$$

$$f(k,\theta) = \sum_{l=0}^{\infty}(2l+1)f_l(k)P_l(\cos\theta), \tag{8.27}$$

where the factor $(2l+1)$ in the definition of the *partial wave amplitudes* $f_l(k)$ corresponds to the degeneracy of the magnetic quantum number. (Some authors use different conventions, like either dropping the factor $(2l+1)$ or including an additional factor $1/k$ in the definition of f_l.) The terms in the series (8.26) are known as a *partial waves*, which are simultaneous eigenfunctions of the operators $\mathcal{L}^2$ and $\mathcal{L}_z$ with eigenvalues $l(l+1)\hbar^2$ and 0, respectively. Our aim is now to determine the amplitudes f_l in terms of the radial functions $R_l(k,r)$ for solutions (8.27) to the Schrödinger equation.

The radial equation. We recall the formula for the Laplacian in spherical coordinates

$$\Delta = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) - \frac{\mathcal{L}^2}{\hbar^2 r^2} \qquad \text{with} \qquad -\frac{\mathcal{L}}{\hbar^2} = \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2} \tag{8.28}$$

With the separation ansatz

$$u_{Elm}(\vec{x}) = R_{El}(r)Y_{lm}(\theta,\varphi) \tag{8.29}$$

for the time-independent Schrödinger equation with central potential in spherical coordinates

$$\left\{-\frac{\hbar^2}{2m}\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) - \frac{\mathcal{L}^2}{\hbar^2 r^2}\right] + V(r)\right\}u(\vec{x}) = Eu(\vec{x}), \tag{8.30}$$

and $\mathcal{L}^2 Y_{lm}(\theta,\varphi) = l(l+1)\hbar^2 Y_{lm}(\theta,\varphi)$ we find the *radial equation*

$$\left(-\frac{\hbar^2}{2m}\left(\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr}\right) + \frac{l(l+1)\hbar^2}{2mr^2} + V(r)\right)R_{El}(r) = ER_{El}(r). \tag{8.31}$$

and its reduced form

$$\boxed{\left(\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr} - \frac{l(l+1)}{r^2} - U(r) + k^2\right)R_l(k,r) = 0} \tag{8.32}$$

with $k = \sqrt{2mE/\hbar^2}$ and the reduced potential $U(r) = (2m/\hbar^2)V(r)$.

Behavior near the center. For potentials less singular than r^{-2} at the origin the behavior of $R_l(k,r)$ at $r=0$ can be determined by expanding R_l into a power series

$$R_l(k,r) = r^s\sum_{n=0}^{\infty} a_n r^n. \tag{8.33}$$

Substitution into the radial equation (8.32) leads to the quadratic indicial equation with the two solutions $s=l$ and $s=-(l+1)$. Only the first one leads to a non-singular wave function $u(r,\theta)$ at the origin $r=0$.

Introducing a new radial function $\tilde{R}_{El}(r) = rR_{El}(r)$ and substituting into (8.31) leads to the equation

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dr^2} + V_{eff}(r)\right)\tilde{R}_{El}(r) = E\tilde{R}_{El}(r) \tag{8.34}$$

which is similar to the one-dimensional Schrödinger equation but with $r \geq 0$ and an effective potential

$$V_{eff} = V(r) + \frac{l(l+1)\hbar^2}{2mr^2} \tag{8.35}$$

containing the repulsive *centrifugal barrier* term $l(l+1)\hbar^2/2mr^2$ in addition to the interaction potential $V(r)$.

Free particles and asymptotic behavior. We now solve the radial equation for $V(r) = 0$ so that our solutions can later be used either for the representation of the wave function of a free particle at any radius $0 \leq r < \infty$ or for the asymptotic form as $r \to \infty$ of scattering solutions for finite range potentials. Introducing the dimensionless variable $\rho = kr$ with $R_l(\rho) = R_{El}(r)$ for $U(r) = 0$ the radial equation (8.31) turns into the *spherical Bessel differential equation*

$$\left[\frac{d^2}{d\rho^2} + \frac{2}{\rho}\frac{d}{d\rho} + \left(1 - \frac{l(l+1)}{\rho^2}\right)\right] R_l(\rho) = 0, \tag{8.36}$$

whose independent solutions are the *spherical Bessel functions*

$$j_l(\rho) = (-\rho)^l \left(\frac{1}{\rho}\frac{d}{d\rho}\right)^l \frac{\sin\rho}{\rho} \tag{8.37}$$

and the *spherical Neumann functions*

$$n_l(\rho) = -(-\rho)^l \left(\frac{1}{\rho}\frac{d}{d\rho}\right)^l \frac{\cos\rho}{\rho}. \tag{8.38}$$

Their leading behavior at $\rho = 0$,

$$\lim_{\rho\to 0} j_l(\rho) \quad \to \quad \frac{\rho^l}{1\cdot 3\cdot 5\cdot \ldots \cdot (2l+1)}, \tag{8.39}$$

$$\lim_{\rho\to 0} n_l(\rho) \quad \to \quad -\frac{1\cdot 3\cdot 5\cdot \ldots \cdot (2l-1)}{\rho^{l+1}} \tag{8.40}$$

can be obtained by expanding $\rho^{-1}\sin\rho$ and $\rho^{-1}\cos\rho$ into a power series in ρ. In accord with our previous result for the ansatz (8.33) the spherical Neumann function $n_l(\rho)$ has a pole of order $l+1$ at the origin and is therefore an *irregular* solution, whereas the spherical Bessel function $j_l(\rho)$ is the *regular* solution with a zero of order l at the origin. The radial part of the wave function of a free particle can hence only contain spherical bessel functions $R_{El}^{free}(r) \propto j_l(kr)$.

8.2.1 Expansion of a plane wave in spherical harmonics

In order to use the spherical symmetry of a potential $V(r)$ we need to expand the plane wave representing the incident particle beam in terms of spherical harmonics. Since $e^{i\vec{k}\cdot\vec{x}}$ is a regular solution to the free Schrödinger equation we can make the ansatz

$$e^{i\vec{k}\cdot\vec{x}} = \sum_{l=0}^{\infty}\sum_{m=-l}^{+l} c_{lm} j_l(kr) Y_{lm}(\theta,\varphi), \tag{8.41}$$

where the radial part is given by the spherical Bessel functions with constants c_{lm} that have to be determined. Choosing $\vec{k}$ in the direction of the z-axis the wave function $\exp(i\vec{k}\cdot\vec{r}) = \exp(ikr\cos\theta)$ is independent of φ so that only the Y_{lm} with $m = 0$, which are proportional to the Legendre polynomials $P_l(\theta)$, can contribute to the expansion

$$e^{ikr\cos\theta} = \sum_{l=0}^{\infty} a_l j_l(kr) P_l(\cos\theta). \tag{8.42}$$

With $\rho = kr$ and $u = \cos\theta$ this becomes

$$e^{i\rho u} = \sum_{l=0}^{\infty} a_l j_l(\rho) P_l(u). \tag{8.43}$$

One way of determining the coefficients a_l is to differentiate this ansatz with respect to ρ,

$$iue^{i\rho u} = \sum_l a_l \frac{dj_l}{d\rho} P_l. \tag{8.44}$$

The left hand side of (8.44) can now be evaluated by inserting the series (8.43) and using the recursion relation

$$(2l+1)uP_l^m = (l+1-m)P_{l+1}^m + (l+m)P_{l-1}^m \tag{8.45}$$

of the Legendre polynomials for $m = 0$. This yields

$$i\sum_{l=0}^{\infty} a_l j_l \left(\frac{l+1}{2l+1}P_{l+1} + \frac{l}{2l+1}P_{l-1}\right) = \sum_{l=0}^{\infty} a_l j_l' P_l \tag{8.46}$$

and, since the Legendre polynomials are linearly independent, for the coefficient of P_l

$$a_l j_l' = i\left(\frac{l}{2l-1}a_{l-1}j_{l-1} + \frac{l+1}{2l+3}a_{l+1}j_{l+1}\right). \tag{8.47}$$

The derivative j_l' can now be expressed in terms of $j_{l\pm1}$ by using the recursion relations

$$j_{l-1} = \left(\frac{d}{d\rho} + \frac{l+1}{\rho}\right) j_l = \frac{1}{\rho^{l+1}}\frac{d}{d\rho}(\rho^{l+1}j_l) \tag{8.48}$$

and

$$(2l+1)j_l = \rho[j_{l+1} + j_{l-1}], \tag{8.49}$$

which imply

$$j_l' = j_{l-1} - \frac{l+1}{\rho}j_l = j_{l-1} - \frac{l+1}{2l+1}(j_{l+1} + j_{l-1}) = \frac{l}{2l+1}j_{l-1} - \frac{l+1}{2l+1}j_{l+1} \tag{8.50}$$

[the equations (8.48-8.50) also holds for the spherical Neumann functions n_l]. Substituting this expression for j_l' into eq. (8.47) we obtain the two equivalent recursion relations

$$\frac{a_l}{2l+1} = i\frac{a_{l-1}}{2l-1} \qquad \text{and} \qquad \frac{a_l}{2l+1} = -i\frac{a_{l+1}}{2l+3} \tag{8.51}$$

as coefficients of the independent functions $j_{l-1}(\rho)$ and $j_{l+1}(\rho)$, respectively. These relations have the solution $a_l = (2l+1)i^l a_0$. The coefficient a_0 is obtained by evaluating our ansatz at $\rho = 0$: Since $j_l(0) = \delta_{l0}$ and $P_0(u) = 1$ eq. (8.43) implies $a_0 = 1$, so that the expansion of a plane wave in spherical harmonics becomes

$$\boxed{e^{ikr\cos\theta} = \sum_{l=0}^{\infty}(2l+1)i^l j_l(kr)P_l(\cos\theta).} \tag{8.52}$$

Using the addition theorem of spherical harmonics

$$\frac{2l+1}{4\pi}P_l(\cos\alpha) = \sum_{m=-l}^{+l} Y^*_{lm}(\theta_1,\varphi_1)Y_{lm}(\theta_2,\varphi_2) \tag{8.53}$$

with α being the angle between the directions (θ_1,φ_1) and (θ_2,φ_2) this result can be generalized to the expansion of the plane wave in any polar coordinate system

$$e^{i\vec{k}\cdot\vec{x}} = 4\pi\sum_{l=0}^{\infty}\sum_{m=-l}^{+l} i^l j_l(kr)Y^*_{lm}(\theta_{\vec{k}},\varphi_{\vec{k}})Y_{lm}(\theta_{\vec{x}},\varphi_{\vec{x}}), \tag{8.54}$$

where the arguments of Y^*_{lm} and Y_{lm} are the angular coordinates of $\vec{k}$ and $\vec{x}$, respectively.

8.2.2 Scattering amplitude and phase shift

The computation of the scattering data for a given potential requires the construction of the regular solution of the radial equation. In the next section we will solve this problem for the example of the square well, but first we analyse the asymptotic form of the partial waves in order to find out how to extract and interpret the relevant data.

For large r we can neglect the potential $U(r)$ and it is common to write the asymptotic form of the radial solutions as a linear combination of the spherical Bessel and Neumann functions

$$R_l(k,r) = B_l(k)j_l(kr) + C_l(k)n_l(kr) + \mathcal{O}(r^{-\alpha}) \tag{8.55}$$

with coefficients $B_l(k)$ and $C_l(k)$ that depend on the incident momentum k. Inserting the asymptotic forms

$$j_l(kr) = \frac{1}{kr}\sin\left(kr - \frac{l\pi}{2}\right) + \mathcal{O}(\frac{1}{r^2}), \tag{8.56}$$

$$n_l(kr) = -\frac{1}{kr}\cos\left(kr - \frac{l\pi}{2}\right) + \mathcal{O}(\frac{1}{r^2}), \tag{8.57}$$

we can write

$$R_l^{as}(k,r) = \frac{1}{kr}\left[B_l(k)\sin\left(kr - \frac{l\pi}{2}\right) - C_l(k)\cos\left(kr - \frac{l\pi}{2}\right)\right] \tag{8.58}$$

$$= A_l(k)\frac{1}{kr}\sin\left(kr - \frac{l\pi}{2} + \delta_l(k)\right) \tag{8.59}$$

where

$$A_l(k) = [B_l^2(k) + C_l^2(k)]^{1/2} \tag{8.60}$$

and

$$\delta_l(k) = -\tan^{-1}[C_l(k)/B_l(k)]. \tag{8.61}$$

The $\delta_l(k)$ are called *phase shifts*. We will see that they are real functions of k and completely characterize the strength of the scattering of the lth partial wave by the potential $U(r)$ at the energy $E = \hbar^2 k^2/2m$. In order to relate the phase shifts to the scattering amplitude we now insert the asymptotic form of the expansion (8.52) of the plane wave

$$e^{i\vec{k}\vec{x}} = \sum_{l=0}^{\infty}(2l+1)i^l j_l(kr)P_l(\cos\theta). \tag{8.62}$$

$$\to \sum_{l=0}^{\infty}(2l+1)i^l (kr)^{-1}\sin\left(kr - \frac{l\pi}{2}\right)P_l(\cos\theta). \tag{8.63}$$

into the scattering ansatz (8.20)

$$u_{\vec{k}}^{as}(r,\theta) \to e^{i\vec{k}\vec{x}} + f(k,\theta)\frac{e^{ikr}}{r}. \tag{8.64}$$

With $\sin x = (e^{ix} - e^{-ix})/(2i)$ and the partial wave expansions (8.26)–(8.27) of $u(\vec{x})$ and $f(\theta,\varphi)$ we can write the radial function $R_l(k,r)$, i.e. the coefficient of $P_l(\cos\theta)$, asymptotically as

$$R_l^{as}(k,r) = (2l+1)i^l(kr)^{-1}\sin\left(kr - \frac{l\pi}{2}\right) + \frac{2l+1}{r}e^{ikr}f_l(k) \tag{8.65}$$

$$= \frac{2l+1}{2ikr}\left(i^l\left(\frac{e^{ikr}}{i^l} - \frac{e^{-ikr}}{(-i)^l}\right) + 2ike^{ikr}f_l\right) \tag{8.66}$$

Rewriting (8.59) in terms of exponentials

$$R_l^{as}(k,r) = \frac{A_l}{2ikr}\left(\frac{e^{i(kr+\delta_l)}}{i^l} - \frac{e^{-i(kr+\delta_l)}}{(-i)^l}\right) \tag{8.67}$$

comparison of the coefficients of e^{-ikr} implies

$$A_l(k) = (2l+1)i^l e^{i\delta_l(k)}. \tag{8.68}$$

The coefficients of $e^{ikr}/(2ikr)$ are $(2l+1)(1+2ikf_l)$ and $A_l e^{i\delta_l}/i^l$, respectively. Hence

$$f_l(k) = \frac{e^{2i\delta_l(k)} - 1}{2ik} = \frac{1}{k}e^{i\delta_l}\sin\delta_l. \tag{8.69}$$

The scattering amplitude

$$f(k,\theta) = \sum_{l=0}^{\infty}(2l+1)f_l(k)P_l(\cos\theta) = \frac{1}{2ik}\sum_{l=0}^{\infty}(2l+1)(e^{2i\delta_l} - 1)P_l(\cos\theta) \tag{8.70}$$

hence *depends only on the phase shifts* $\delta_l(k)$ and the asymptotic form of $R_l(k,r)$ takes the form

$$R_l^{as}(k,r) = -\frac{1}{2ik}A_l(k)e^{-i\delta_l(k)}\left[\frac{e^{-i(kr-l\pi/2)}}{r} - S_l(k)\frac{e^{i(kr-l\pi/2)}}{r}\right] \tag{8.71}$$

where we defined

$$S_l(k) = e^{2i\delta_l(k)}. \tag{8.72}$$

S_l is the partial wave contribution to the *S-matrix*, which we will introduce in the last section of this chapter. Reality of the phase shift $|S_l| = 1$ expresses equality of the incoming and outgoing particle currents, i.e. conservation of particle number or unitarity of the S matrix. For inelastic scattering we could write the radial wave fuction as (8.71) with $S_l = s_l e^{i\delta_l}$ for $s_l \leq 1$ describing the loss of part of the incoming current into inelastic processes like energy transfer of particle production. (The complete scattering matrix, including the contribution of inelastic channels, would however still be unitary as a consequence of the conservation of probability.)

The optical theorem. The total cross section for scattering by a central potential can be written as

$$\sigma_{\text{tot}} = \int |f(k,\theta)|^2 d\Omega = 2\pi \int_{-1}^{+1} d(\cos\theta) f^*(k,\theta) f(k,\theta). \tag{8.73}$$

Using (8.70) and the orthogonality property of the Legendre polynomials

$$\int_{-1}^{+1} d(\cos\theta) P_l(\cos\theta) P_{l'}(\cos\theta) = \frac{2}{2l+1}\delta_{ll'} \tag{8.74}$$

we find

$$\sigma_{\text{tot}} = \sum_{l=0}^{\infty} 4\pi(2l+1)|f_l(k)|^2 = \sum_{l=0}^{\infty}\sigma_l \qquad \text{with} \qquad \sigma_l = \frac{4\pi}{k^2}(2l+1)\sin^2\delta_l. \tag{8.75}$$

Since (8.69) implies $\operatorname{Im} f_l = k|f_l|^2$ we can set $\theta = 0$ in (8.70) and use the fact that $P_l(1) = 1$ to obtain the *optical theorem*

$$\boxed{\sigma_{\text{tot}} = \frac{4\pi}{k}\text{Im} f(k,\theta = 0),} \tag{8.76}$$

The optical theorem can be shown to hold also for inelastic scattering with $\sigma_{tot} = \sigma_{el} + \sigma_{inel}$. The proof relates the total cross section to the interference of the incoming with the forward-scattered amplitude so that (8.76) is a consequence of the unitarity of the S-matrix [Hittmair].

8.2.3 Example: Scattering by a square well

The centrally symmetric square well is a potential for which the phase shifts can be calculated by analytical methods. Starting with the radial equation (8.32) and the reduced potential

$$U(r) = \begin{cases} -U_0, & r < a \quad (U_0 > 0) \\ 0, & r > a, \end{cases} \tag{8.77}$$

we can write the radial equation inside the well as

$$\left[\frac{d^2}{dr^2}+\frac{2}{r}\frac{d}{dr}-\frac{l(l+1)}{r^2}+K^2\right]R_l(k,r)=0 \qquad \text{for} \quad r<a \tag{8.78}$$

with $K^2=k^2+U_0$. Inside the well the regular solution is thus

$$R_l^{in}(K,r)=N_l\,j_l(Kr), \qquad r<a \tag{8.79}$$

where N_l is related to the exact solution in the exterior region

$$R_l^{ext}(k,r)=B_l(k)[j_l(kr)-\tan\delta_l(k)n_l(kr)], \qquad r>a \tag{8.80}$$

by the matching condition at $r=a$. Continuity of R and R' at $r=a$ hence implies

$$N_l\,j_l(Ka) = B_l(j_l(ka)-\tan\delta_l\,n_l(ka)), \tag{8.81}$$

$$KN_l\,j_l'(Ka) = kB_l\left(j_l'(ka)-\tan\delta_l\,n_l'(ka)\right). \tag{8.82}$$

The ratio of these two equations yields an equation for $\tan\delta_l(k)$ whose solution is

$$\tan\delta_l(k)=\frac{kj_l'(ka)j_l(Ka)-Kj_l(ka)j_l'(Ka)}{kn_l'(ka)j_l(Ka)-Kn_l(ka)j_l'(Ka)} \tag{8.83}$$

with $K=\sqrt{k^2+U_0}$.

In the low energy limit $k=\sqrt{2mE}/\hbar\to 0$ we can insert the leading behavior $j_l(\rho)\propto\rho^l$ and $n_l(\rho)\propto\rho^{-l-1}$, and thus for the derivatives $j_l'(\rho)\propto\rho^{l-1}$ and $n_l'(\rho)\propto\rho^{-l-2}$, to conclude that $\tan\delta_l(k)$ goes to zero like a constant times $k^l/k^{-l-1}=k^{2l+1}$. In this limit the cross section,

$$\boxed{\sigma_l\propto k^{4l},} \tag{8.84}$$

is dominated by $l=0$ so that the scattering probability approximately goes to a θ-independent constant. With

$$j_0(\rho)=\tfrac{\sin\rho}{\rho},\quad n_0(\rho)=-\tfrac{\cos\rho}{\rho},\qquad j_0'(\rho)=\tfrac{\rho\cos\rho-\sin\rho}{\rho^2},\quad n_0'(\rho)=\tfrac{\rho\sin\rho+\cos\rho}{\rho^2} \tag{8.85}$$

and the abbreviations $x=ka$, $X=Ka$ we find

$$\tan\delta_0=\tfrac{((x\cos x-\sin x)\sin X-\sin x(X\cos X-\sin X))/(xX)}{(x\sin x+\cos x)\sin X+\cos x(X\cos X-\sin X))/(xX)}=\tfrac{x\cos x\sin X-X\sin x\cos X}{x\sin x\sin X+X\cos x\cos X}. \tag{8.86}$$

Dividing numerator and denominator by $\cos x\cos X$ we obtain the result

$$\tan\delta_0(k)=\frac{k\tan(Ka)-K\tan(ka)}{K+k\tan(ka)\tan(Ka)}. \tag{8.87}$$

For $k\to 0$ we observe that $\tan\delta_0$ becomes proportial to k. The limit

$$\boxed{a_s=-\lim_{k\to 0}\frac{\tan\delta_0(k)}{k}} \tag{8.88}$$

is called *scattering length* and it determines the limit of the partial cross section

$$\sigma_0 = \frac{4\pi}{k^2}\sin^2\delta_0 = \frac{4\pi}{k^2}\frac{1}{1+\cot^2\delta_0(k)} \quad \overset{k\to 0}{\longrightarrow} \quad 4\pi a_s^2. \tag{8.89}$$

For the square well we find

$$a_s = \left(1 - \frac{\tan(a\sqrt{U_0})}{a\sqrt{U_0}}\right) a, \tag{8.90}$$

The coefficient of the next term of the expansion

$$k\cot\delta_0(k) = -\frac{1}{a_s} + \frac{1}{2}r_0k^2 + \cdots \tag{8.91}$$

defines the *effective range* r_0. This definition of the scattering length a_s and the effective range r_0 can be used for all short-range potentials.

Another exactly solvable potential is the hard-sphere potential

$$U(r) = \begin{cases} +\infty, & r < a, \\ 0, & r > a, \end{cases} \tag{8.92}$$

for which the total cross section can be shown to obey

$$\sigma(k) \quad \to \quad \begin{cases} 4\pi a^2, & k \to 0, \\ 2\pi a^2, & k \gg 1/a. \end{cases} \tag{8.93}$$

For $k \to 0$ the scattering length a_s hence coincides with a and the cross section is 4 times the classical value. For $ka \gg 1$ the wave lengths of the scattered particles goes to 0 and one might naively expect to observe the classical area $a^2\pi$. The fact that quantum mechanics yield twice that value is in accord with refraction phenomena in optics and can be attributed to interference between the incoming and the scattered beam close to the forward direction. This effect is hence called refraction scattering, or shadow scattering.

8.2.4 Interpretation of the phase shift

For a weak and slowly varying potential we may think of the phase shift as arising from the change in the effective wavelength $k \sim \sqrt{2m(E - V(x))}/\hbar$ due to the presence of the potential. For an attractive potential we hence expect an advanced oscillation and a positive phase shift $\delta_l > 0$, while a repulsive potential should lead to retarded oscillation and a negative phase shift $\delta_l < 0$. Comparing this expectation with the result (8.90) for the square well and using $\tan x \approx x + \frac{1}{3}x^3$ for small U_0 we find $a_s \approx -\frac{1}{3}a^3U_0$ so that indeed the scattering length (8.88) becomes negative and the phase shift δ_0 positive for an attractive potential $U_0 > 0$. It can also be shown quite generally that small angular momenta dominate the scattering at low energies and that the partial cross sections σ_l are negligible for $l > ka$ where a is the range of the potential.

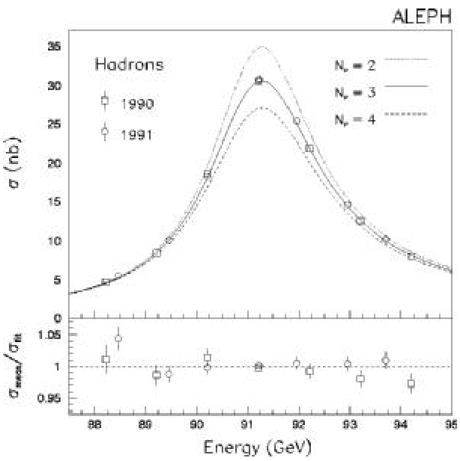

Figure 8.2: Z boson resonance in e^+e^- scattering at LEP and light neutrin number.

As we increase the energy the phase shift varies and the partial cross sections

$$\sigma_l(E) = \frac{4\pi}{k^2}(2l+1)\sin^2\delta_l = \frac{4\pi}{k^2}(2l+1)\frac{1}{1+\cot^2\delta_l} \tag{8.94}$$

go through maxima and zeros as the phase shift δ_l goes through odd and even multiples of π, respectively. For small energies the single cross section σ_0 dominates so that we can get minima where the target becomes almost transparent. This is called *Ramsauer-Townsend effect*.

A rapid move of the phase shift through an odd multiple of π, i.e.

$$\cot\delta_l \approx \big((n+\tfrac{1}{2})\pi - \delta_l\big) \approx \frac{E_R - E}{\Gamma(E)/2} + \mathcal{O}(E_R - E)^2 \qquad \text{for} \qquad \delta_l \approx (n+\tfrac{1}{2})\pi \tag{8.95}$$

with $\Gamma(E_R)$ small at the resonance energy E_R, leads to a sharp peak in the cross section with an angular distibution characteristic for the angular momentum chanel l. This is called *resonance scattering* and described by the *Breit-Wigner resonance formula*

$$\sigma_l(E) = \frac{4\pi}{k^2}(2l+1)\frac{\Gamma^2/4}{(E-E_R)^2+\Gamma^2/4}. \tag{8.96}$$

A resonance can be thought of as a metastable bound state with positive energy whose lifetime is $\hbar/\Gamma$. For a sharp resonance the inverse width Γ^{-1} is indeed related to the dwelling time of the scattered particles in the interaction region. Note that σ_{max} at a resonance is determined by the momentum k of the scattered particles and not by properties of the target. A striking example of a resonance in particle physics is the peak in electron-positron scattering at the Z-boson mass which was analyzed by the LEP-experiment ALEPH as shown in fig. 8.2. Since the Z boson has no electric charge but couples to the weakly interacting particles its lifetime is very sensitive to the number of light neutrinos, which are otherwise extremely hard to observe. This experiment confirmed with great precision the number $N_\nu = 3$ of such species, which is also required for nucleosynthesis, about one second after the big bang, to produce the right amount of helium and other light elements as observed in the interstellar gas clouds.

Resonances can be interpreted as poles in the scattering amplitudes that are close to the real axis (with the imaginary part related to the lifetime). Poles on the positive imaginary axis, on the other hand, correspond to bound states for the potential $V(x)$. The information of the number of such bound states is also contained in the phase shift. For the precise statement we fix the ambiguity modulo 2π in the definition (8.61) of δ_l by requiring continuity. The *Levinson theorem* then states that

$$\delta_l(0) - \delta_l(\infty) = n_l\,\pi \qquad \text{for} \qquad l > 0, \tag{8.97}$$

where n_l denotes the number of bound states with angular momentum l [Chadan-Sabatier]. The theorem also holds for $l = 0$ except for a shift $n_l \to n_l + \frac{1}{2}$ in the formula (8.97) if there is a so-called bound state a zero energy with $l = 0$. While we consider in this chapter the problem of determining the scattering data from the potential, in inverse problem of obtaining information on the potential from the scattering data is physically equally important, but mathematically quite a bit more complicated. *Inverse scattering theory* has been a very active field of research in the last decades with a number of interesting interrelations to other fields like integrable systems [Chadan-Sabatier].

8.3 The Lippmann-Schwinger equation

We can use the method of *Green's functions* to solve the stationary Schrödinger equation (8.14)

$$(\nabla^2 + k^2)u(\vec{x}) = U(\vec{x})u(\vec{x}). \tag{8.98}$$

Using the defining equation of the Green's function for the Helmholtz equation

$$(\nabla^2 + k^2)G_0(k, \vec{x}, \vec{x}') = \delta(\vec{x} - \vec{x}') \tag{8.99}$$

we can write down the general solution of equation (8.98) as a convolution integral

$$u(\vec{x}) = u_{hom}(\vec{x}) + \int G_0(k, \vec{x}, \vec{x}')U(\vec{x}')u(\vec{x}')\; d^3x' \tag{8.100}$$

where u_{hom} is a solution of the homogenous Schrödinger equation

$$(\nabla^2 + k^2)u_{hom}(\vec{x}) = 0. \tag{8.101}$$

We will see that the scattering boundary condition (8.20) is equivalent to taking $u_{hom}(\vec{x})$ to be an incident plane wave

$$u_{hom}(\vec{x}) = \phi_{\vec{k}}(\vec{x}) \equiv e^{i\vec{k}\vec{x}} \tag{8.102}$$

if $G_0 = G_0^{ret}$ is the retarded Green's function. The existence of solutions to the homogeneous equation is of course related to the ambiguity of G_0, as we will see explicitly in the following computation.

Since (8.99) is a linear differential equation with constant coefficients we can determine the Green's function by Fourier transformation. Because of translation invariance

$$G_0(k,\vec{x},\vec{x}') = G_0(k,\vec{R}) \qquad \text{with} \qquad \vec{R} = \vec{x}-\vec{x}', \tag{8.103}$$

hence

$$G_0(k,\vec{x}-\vec{x}') = \frac{1}{(2\pi)^3}\int e^{i\vec{K}\cdot\vec{R}}\,\tilde{g}_0(k,\vec{K})d\vec{K} \tag{8.104}$$

$$\delta(\vec{x}-\vec{x}') = \frac{1}{(2\pi)^3}\int e^{i\vec{K}\cdot\vec{R}}d\vec{K}. \tag{8.105}$$

Substituting the Fourier representations into the defining equation of the Green's function (8.99) we find that

$$\tilde{g}_0(k,\vec{K}) = \frac{1}{k^2-K^2}. \tag{8.106}$$

Since $\tilde{g}_0$ has a pole on the real axis we give a small imaginary part to k and define

$$G_0^{\pm}(k,\vec{x},\vec{x}') = \frac{1}{(2\pi)^3}\int \frac{e^{i\vec{K}\cdot(\vec{x}-\vec{x}')}}{k^2-K^2\pm i\varepsilon}d\vec{K}. \tag{8.107}$$

Let (K,Θ,Φ) be the spherical coordinates of $\vec{K}$ and let the z-axis be along $\vec{R}=\vec{x}-\vec{x}'$. Then

$$G_0^{\pm}(k,\vec{R}) = \frac{1}{(2\pi)^3}\int_0^\infty dK K^2\int_0^\pi \mathrm{d}\Theta\sin\Theta\int_0^{2\pi}\mathrm{d}\Phi\frac{e^{iKR\cos\Theta}}{k^2-K^2\pm i\varepsilon}. \tag{8.108}$$

Performing the angular integrations and observing that the integrand is an even function of K we can extend the integral from $-\infty$ to $+\infty$ and obtain

$$G_0^{\pm}(k,\vec{R}) = \frac{1}{8\pi^2 iR}\int_{-\infty}^{+\infty}\frac{K(e^{iKR}-e^{-iKR}))}{k^2-K^2\pm i\varepsilon}dK. \tag{8.109}$$

With the partial fraction decomposition $\frac{1}{k^2-K^2} = -\frac{1}{2K}\left(\frac{1}{K-k}+\frac{1}{K+k}\right)$ we can split the integral into two parts

$$G_0(k,R) = \frac{i}{16\pi^2 R}(I_1-I_2), \tag{8.110}$$

with

$$I_1 = \int_{-\infty}^{+\infty} e^{iKR}\left(\frac{1}{K-k}+\frac{1}{K+k}\right)\mathrm{d}K \tag{8.111}$$

$$I_2 = \int_{-\infty}^{+\infty} e^{-iKR}\left(\frac{1}{K-k}+\frac{1}{K+k}\right)\mathrm{d}K \tag{8.112}$$

The integrals can now be evaluated using the Cauchy integral formula if we close the integration path with a half-circle in the upper or lower complex half-plane, respectively, so that the contribution from the arcs at infinity vanish. The ambiguity of the Green's function arises from different choices of the integration about the poles of the integrand on the real axis, and different pole prescriptions obviously differ by terms localized at $K^2 = k^2$ and hence by a

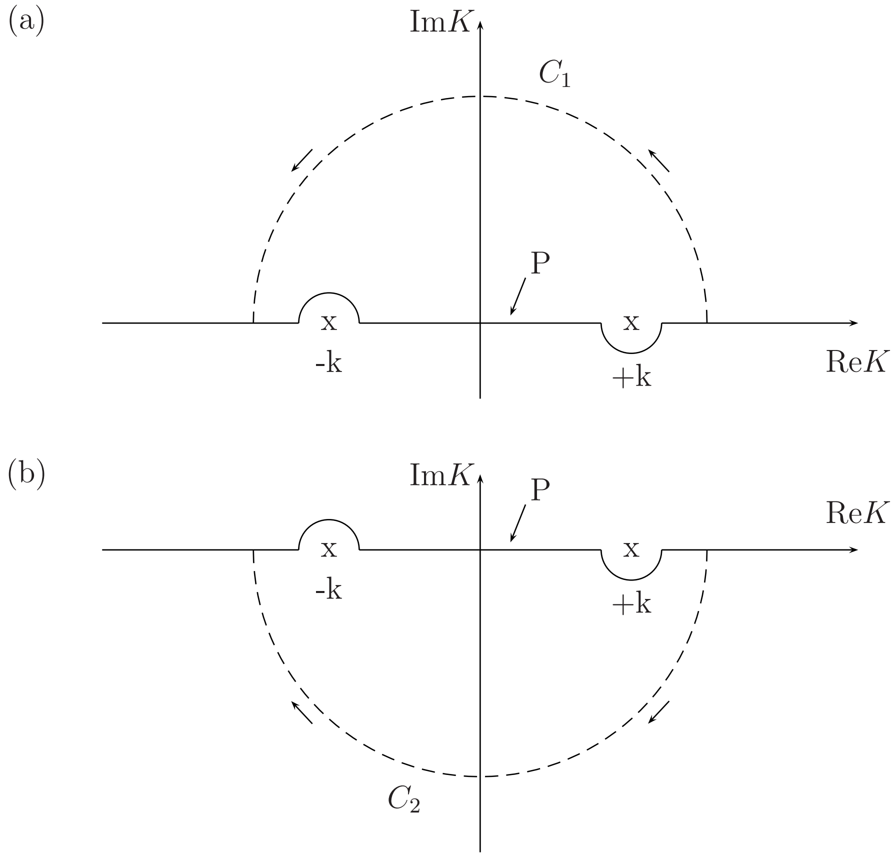

Figure 8.3: (a) The contour (P+C_1) for calculating the integral I_1 by avoiding the poles $K = \pm k$ and closing via a semi-circle in infinity. (b) the contour for calculating the integral I_2.

superposition of plane wave solutions to the homogeneous equation. The integration contour in the complex K-plane shown in fig. 8.3 corresponds to a small positive imaginary part of k and hence to G_0^+. Since e^{iKR} vanishes on C_1 and e^{-iKR} vanishes on C_2 we find

$$I_1 = 2\pi i e^{ikR} \tag{8.113}$$

$$I_2 = -2\pi i e^{ikR} \tag{8.114}$$

With a similar calculation for $k \to k - i\varepsilon$ the Green's function in the original variables $\vec{x}$ and $\vec{x}'$ becomes

$$G_0^{\pm}(k, \vec{x}, \vec{x}') = -\frac{1}{4\pi}\frac{\pm e^{ik|\vec{x}-\vec{x}'|}}{|\vec{x}-\vec{x}'|}. \tag{8.115}$$

so that $G_0^+ = G_0^{ret}$ corresponds to retarded boundary conditions. With $U = \frac{2m}{\hbar^2}V$ we can now write the integral equation for the wave function as

$$\boxed{u_{\vec{k}}(\vec{x}) = e^{i\vec{k}\cdot\vec{x}} - \frac{m}{2\pi\hbar^2}\int \frac{e^{ik|\vec{x}-\vec{x}'|}}{|\vec{x}-\vec{x}'|}V(\vec{x}')u_{\vec{k}}(\vec{x}')\mathrm{d}\vec{x}'.} \tag{8.116}$$

This integral equation is known as the *Lippmann-Schwinger equation* for potential scattering. It is equivalent to the Schrödinger equation *plus* the scattering boundary condition (8.20).

We can now relate this integral representation to the scattering amplitude by considering the situation where the distance of the detector $r \to \infty$ is much larger than the range of the potential to which the integration variable $\vec{x}'$ is essentially confined so that $r' \ll r$. Hence

$$|\vec{x} - \vec{x}'| = \sqrt{r^2 - 2\vec{x}\vec{x}' + r'^2} = r - \frac{\vec{x}\vec{x}'}{r} + \mathcal{O}(\frac{1}{r}). \tag{8.117}$$

Since $\vec{x}$ points in the same direction (θ, φ) as the wave vector $\vec{k}'$ of the scattered particles we have $\vec{k}' = k\vec{x}/r$ for elastic scattering and hence

$$\frac{e^{ik|\vec{x}-\vec{x}'|}}{|\vec{x} - \vec{x}'|} \xrightarrow[r\to\infty]{} \frac{e^{ikr}}{r} e^{-i\vec{k}'\cdot\vec{x}'} + \cdots , \tag{8.118}$$

where terms of order in $1/r^2$ have been neglected. Substituting this expansion into the Lippmann-Schwinger equation we find

$$u_{\vec{k}}(\vec{x}) \xrightarrow[r\to\infty]{} e^{i\vec{k}\cdot\vec{x}} - \frac{1}{4\pi}\frac{e^{ikr}}{r} \int e^{-i\vec{k}'\cdot\vec{x}'} U(\vec{x}')u_{\vec{k}}(\vec{x}')\mathrm{d}\vec{x}'. \tag{8.119}$$

Comparing with the ansatz (8.20) we thus obtain the integral representation

$$\begin{aligned} f(k, \theta, \phi) &= -\frac{1}{4\pi} \int e^{-i\vec{k}'\cdot\vec{x}} U(\vec{x})u_{\vec{k}}(\vec{x})\mathrm{d}\vec{x} \\ &= -\frac{1}{4\pi}\langle\phi_{\vec{k}'}|U|u_{\vec{k}}\rangle = -\frac{m}{2\pi\hbar^2}\langle\phi_{\vec{k}'}|V|u_{\vec{k}}\rangle \end{aligned} \tag{8.120}$$

for the scattering amplitude, where $\langle\phi_{\vec{k}'}| = e^{-i\vec{k}'\cdot\vec{x}}$ and $|\phi_{\vec{k}'}\rangle = e^{i\vec{k}'\cdot\vec{x}} = (2\pi)^{3/2}|k'\rangle$.

8.4 The Born series

The *Born series* is the iterative solution of the Lippmann-Schwinger equation by the ansatz

$$u(\vec{x}) = \sum_{n=0}^{\infty} u_n(\vec{x}) \qquad \text{for} \qquad u_0(\vec{x}) = \phi_{\vec{k}}(\vec{x}) = e^{i\vec{k}\cdot\vec{x}}, \tag{8.121}$$

which yields

$$u_1(\vec{x}) = \int G_0^+(k, \vec{x}, \vec{x}')U(\vec{x}')u_0(\vec{x}')\, d\vec{x}', \tag{8.122}$$

$$\vdots$$

$$u_n(\vec{x}) = \int G_0^+(k, \vec{x}, \vec{x}')U(\vec{x}')u_{n-1}(\vec{x}')\mathrm{d}\vec{x}', \tag{8.123}$$

so that the n^{th} term u_n is formally of order $\mathcal{O}(V^n)$. It usually converges well for weak potentials or at high energies. Insertion of the Born series into of the formula (8.120) yields

$$f = -\frac{1}{4\pi}\langle\phi_{\vec{k}'}|U + UG_0^+U + UG_0^+UG_0^+U + \cdots|\phi_{\vec{k}}\rangle \tag{8.124}$$

and keeping only the first term we obtain the (first) *Born approximation*

$$f^B = -\frac{1}{4\pi}\langle\phi_{\vec{k}'}|U|\phi_{\vec{k}}\rangle. \tag{8.125}$$

to the scattering amplitude.

Phase shift in Born approximation. The Lippmann Schwinger equation (8.116) can also be analysed using partial waves. We assume that our potential is centrally symmetric and expand the scattering wave function $u_{\vec{k}}$ in Legendre polynomials (see equation (8.26)). With the normalisation

$$R_l(k,r) \underset{r\to\infty}{\longrightarrow} j_l(kr) - \tan\delta_l(k) n_l(kr) \tag{8.126}$$

$$\underset{r\to\infty}{\longrightarrow} \frac{1}{kr}\left[\sin\left(kr - \frac{l\pi}{2}\right) + \tan\delta_l(k)\cos\left(kr - \frac{l\pi}{2}\right)\right], \tag{8.127}$$

we find that each radial function satisfies the radial integral equation

$$R_l(k,r) = j_l(kr) + \int_0^\infty G_l(k,r,r')U(r')R_l(k,r')r'^2\mathrm{d}r', \tag{8.128}$$

where

$$G_l = kj_l(kr_<)n_l(kr_>) \qquad \text{with} \qquad r_< \equiv \min(r,r') \quad \text{and} \quad r_> \equiv \max(r,r') \tag{8.129}$$

is the partial wave contribution to the Green's function

$$\frac{e^{ik|\vec{x}-\vec{x}'|}}{|\vec{x}-\vec{x}'|} = ik\sum_{l=0}^{\infty}(2l+1)\, j_l(kr_<)\Big(j_l(kr_>) + in_l(kr_>)\Big)P_l(\cos\theta). \tag{8.130}$$

We solve this equation by iteration, starting with $R_l^{(0)}(k,r) = j_l(kr)$. When we analyse equation (8.128) for $r \to \infty$ we obtain the integral representation

$$\tan\delta_l(k) = -k\int_0^\infty j_l(kr)U(r)R_l(k,r)r^2\mathrm{d}r. \tag{8.131}$$

Substituting the iteration for R_l into the integral equation yields a Born series whose first term

$$\boxed{\tan\delta_l^B(k) = -k\int_0^\infty [j_l(kr)]^2U(r)r^2\mathrm{d}r.} \tag{8.132}$$

is the *first Born approximation to* $\tan\delta_l$.

Total scattering cross section in first Born approximation. With the *wave vector transfer*

$$\vec{q} = \vec{k} - \vec{k}' \tag{8.133}$$

the first Born approximation of the scattering amplitude can be written as the Fourier transform

$$f^B = -\frac{1}{4\pi}\int e^{i\vec{q}\cdot\vec{x}}U(\vec{x})\mathrm{d}\vec{x} \tag{8.134}$$

of the potential. For elastic scattering with $k = k'$ and $\vec{k}\cdot\vec{k}' = k^2\cos\theta$ we find

$$q = 2k\sin\frac{\theta}{2}, \tag{8.135}$$

with θ being the scattering angle. For a central potential it is now useful to introduce polar coordinates with angles (α, β) such that $\vec{q}$ is the polar axis. We thus find that

$$\begin{aligned} f^B(q) &= -\frac{1}{4\pi}\int_0^\infty \mathrm{d}r r^2 U(r)\int_0^\pi \mathrm{d}\alpha\sin\alpha\int_0^{2\pi}\mathrm{d}\beta e^{iqr\cos\alpha} \\ &= -\frac{1}{2}\int_0^\infty \mathrm{d}r r^2 U(r)\int_{-1}^{+1}\mathrm{d}(\cos\alpha)e^{iqr\cos\alpha} \\ &= -\frac{1}{q}\int_0^\infty r\sin(qr)U(r)\mathrm{d}r \end{aligned} \tag{8.136}$$

only depends on $q(k,\theta)$. The total cross-section in the first Born approximation hence becomes

$$\boxed{\sigma^B_{\text{tot}}(k) = 2\pi\int_0^\pi |f^B(q)|^2\sin\theta\mathrm{d}\theta = \frac{2\pi}{k^2}\int_0^{2k}|f^B(q)|^2 q\mathrm{d}q} \tag{8.137}$$

where we used the differential $dq = k\cos\frac{\theta}{2}d\theta$ of (8.135) and $\sin\theta\, d\theta = 2\sin\frac{\theta}{2}\,\cos\frac{\theta}{2}\,d\theta = \frac{q}{k}\frac{dq}{k}$.

8.4.1 Application: Coulomb scattering and the Yukawa potential

Since the Coulomb potential has infinite range we apply the Born approximation to the *Yukawa potential*

$$U(r) = C\frac{e^{-\alpha r}}{r} = C\frac{e^{-r/a}}{r} \qquad \text{with} \qquad a = \alpha^{-1}, \tag{8.138}$$

which can be regarded as a screened Colomb potential. At the end of the calculation we can then try to send the screening length $a \to \infty$. For the Born approximation (8.136) we obtain

$$f^B = -\frac{1}{q}\int_0^\infty r\sin(qr)\,\frac{C}{r}e^{-\alpha r}dr = -\frac{C}{q}\,\mathrm{Im}\int_0^\infty e^{iqr-\alpha r}dr = -\frac{C}{q}\,\mathrm{Im}\,\frac{1}{\alpha - iq} = -\frac{C}{\alpha^2+q^2} \tag{8.139}$$

and the corresponding differential cross section

$$\frac{\mathrm{d}\sigma^B}{\mathrm{d}\Omega} = \frac{C^2}{(\alpha^2+q^2)^2} \tag{8.140}$$

of the Yukawa potential.

The Coulomb potential. The electrostatic force between charges Q_A and Q_B corresponds to the potential

$$V_{Coulomb}(r) = \frac{Q_A Q_B}{4\pi\varepsilon_0}\frac{1}{r} \tag{8.141}$$

which corresponds to

$$C = \frac{2m}{\hbar^2}\frac{Q_A Q_B}{4\pi\varepsilon_0} \tag{8.142}$$

but obviously violates the finite range condition. Nevertheless, there is a finite limit $\alpha \to 0$ for which we obtain the scattering amplitude $f^B = -C/q^2$ and the differential cross-section in first Born approximation as

$$\frac{\mathrm{d}\sigma_c^B}{\mathrm{d}\Omega} = \frac{C^2}{q^4} = \left(\frac{\gamma}{2k}\right)^2 \frac{1}{\sin^4(\theta/2)} = \left(\frac{Q_A Q_B}{4\pi\varepsilon_0}\right)^2 \frac{1}{16E^2\sin^4(\theta/2)} \tag{8.143}$$

where

$$\gamma = \frac{Q_A Q_B}{(4\pi\varepsilon_0)\hbar v} = \frac{C}{2k} \tag{8.144}$$

is a dimensionless quantity.

- This result for the differential cross-section for scattering by a Coulomb potential is identical with the formula that *Rutherford* obtained 1911 by using classical mechanics.
- The *exact* quantum mechanical treatment of the Coulomb potential yields the same result for the differential cross-section. The scattering amplitude f_c however differs by a phase factor. It can be shown that

$$f_c = -\frac{\gamma}{2k\sin^2(\theta/2)}\frac{\Gamma(1+i\gamma)}{\Gamma(1-i\gamma)}e^{-i\gamma\log[\sin^2(\theta/2)]} \tag{8.145}$$

  where Γ denotes the Gamma-function [Hittmair].
- The Rutherford differential cross-section scales with the energy E at all angles by the factor $(Q_A Q_B/16\pi\varepsilon_0 E)^2$ so that the angular distribution is independent of the energy.
- The phase correction in (8.145) becomes observable in the scattering of identical particles due to interference terms. This will be discussed in chapter 10.

8.5 Wave operator, transition operator and S-matrix

In this section we introduce the scattering matrix S and relate it to the scattering amplitude via the transition matrix T. We start with the observation that the Greens function $G_0^\pm$ can be interpreted as the inverse of $E - H_0 \pm i\varepsilon$ up to a factor $\frac{2m}{\hbar^2}$. Indeed, with $k = \sqrt{\frac{2mE}{\hbar^2}}$ and the free Hamiltonian $H_0 = -\frac{\hbar^2}{2m}\Delta$ we find for a momentum eigenstate with $\vec{p}|K\rangle = \hbar\vec{K}|K\rangle$ that

$$(E - H_0)|K\rangle = \frac{\hbar^2}{2m}(k^2 - K^2)|K\rangle \tag{8.146}$$

so that

$$\lim_{\varepsilon\to 0}\frac{1}{E - H_0 \pm i\varepsilon} = \frac{2m}{\hbar^2}G_0^\pm \tag{8.147}$$

follows by Fourier transformation and regularization with a small imaginary part of the energy. More explicitly, the matrix elements of the operator $(E - H_0 \pm i\varepsilon)^{-1}$ in position space are

$$\langle x|\frac{1}{E - H_0 \pm i\varepsilon}|x'\rangle = \langle x|\frac{1}{E - H_0 \pm i\varepsilon}\int d^3K|K\rangle\langle K|x'\rangle \tag{8.148}$$

$$= \int d^3K\ \langle x|\frac{1}{\frac{\hbar^2}{2m}(k^2 - K^2) \pm i\varepsilon}|K\rangle\ \frac{e^{-i\vec{K}\vec{x}'}}{(2\pi)^{3/2}} \tag{8.149}$$

$$= \frac{2m}{\hbar^2}\int \frac{d^3K}{(2\pi)^3}\frac{e^{i\vec{K}(\vec{x}-\vec{x}')}}{k^2 - K^2 \pm i\varepsilon} = \frac{2m}{\hbar^2}G_0^{\pm}(\vec{x} - \vec{x}'). \tag{8.150}$$

With $z = E \pm i\varepsilon$ this is proportional to the resolvent $R_z(H_0) = (H_0 - z)^{-1}$ of H_0, which is a bounded operator for $\varepsilon > 0$. The Lippmann–Schwinger equation can now be written as

$$|u_\pm\rangle = |u_0\rangle + \frac{1}{E - H_0 \pm i\varepsilon}V|u_\pm\rangle \tag{8.151}$$

where $|u_+\rangle$ corresponds to the scattering solution with retarded boundary conditions.

Wave operator and transition matrix. The Born series for the solutions of (8.151) is

$$|u_\pm\rangle = |u_0\rangle + \sum_{n=1}^{\infty}(\frac{1}{E - H_0 \pm i\varepsilon}V)^n|u_0\rangle \tag{8.152}$$

In order to sum up the geometric operator series we use the matrix formula

$$1 + \tfrac{1}{A}V + (\tfrac{1}{A}V)^2 + \ldots = (1 - \tfrac{1}{A}V)^{-1} = (\tfrac{1}{A}(A - V))^{-1} = (A - V)^{-1}A$$
$$= \tfrac{1}{A-V}(A - V + V) = 1 + \tfrac{1}{A-V}V \tag{8.153}$$

for $A = E - H_0 \pm i\varepsilon$. Since $A - V = E - H \pm i\varepsilon$ with $H = H_0 + V$ the Born series can thus be summed up in terms of the resolvent of the full Hamiltonian

$$|u_\pm\rangle = |u_0\rangle + \frac{1}{E - H \pm i\varepsilon}V|u_0\rangle = \Omega_\pm|u_0\rangle, \tag{8.154}$$

where we introduced the *wave operator* or *Møller operator*

$$\Omega_\pm = 1 + \frac{1}{E - H \pm i\varepsilon}V \tag{8.155}$$

which maps plane waves $|u_0\rangle$ to exact stationary scattering solution $|u_0\rangle \to |u_\pm\rangle = \Omega_\pm|u_0\rangle$. If we insert this representation for the scattering solution into the formula (8.120) we need to be careful about the normalization of the wave function. In the present section we prefer to work with momentum eigenstates normalized as $\langle\vec{k}'|\vec{k}\rangle = \delta^3(\vec{k}' - \vec{k})$ which yield a factor $(2\pi)^3$ as compared to the plane waves $e^{\pm ikx}$ with normalized amplitude $|\phi_k(x)| = 1$. We hence obtain

$$f = -2\pi^2\langle\vec{k}'|U|u_+\rangle = -4\pi^2\frac{m}{\hbar^2}\ \langle\vec{k}'|V\Omega_+|k\rangle \tag{8.156}$$

for the scattering amplitude, which suggests to define the transition operator T as

$$T := V\Omega_+ = V(1 + \tfrac{1}{E-H+i\varepsilon}V) = (1 + V\tfrac{1}{E-H+i\varepsilon})V = \Omega_-^\dagger V \tag{8.157}$$

so that

$$f(k,\theta,\varphi) = -4\pi^2 \frac{m}{\hbar^2} \langle k'|T|k\rangle \tag{8.158}$$

with (θ,φ) corresponding to the direction of $\vec{k}'$.

The S–matrix. The idea behind the definition of the scattering matrix in terms of the wave operator is that the incoming scattering state $\Omega_+|k\rangle$ is reduced by the measurement in the detector to a state that is a plane wave in the asymptotic future and hence, as an exact solution to the Schrödinger equation, corresponds to advanced boundary conditions $\Omega_-|k'\rangle$. Since $(\Omega_-|k'\rangle)^\dagger = \langle k'|\Omega_-^\dagger$ the scattering amplitude should correspond to the matrix element $\langle k'|S|k\rangle$ in the momentum eigenstate basis. Hence we define

$$\langle k'|S|k\rangle = \langle k'|\Omega_-^\dagger\Omega_+|k\rangle \qquad \Rightarrow \qquad S = \Omega_-^\dagger\Omega_+. \tag{8.159}$$

It can be shown that this definition of the S-matrix agrees with the limit

$$S = \lim_{\substack{t_1\to+\infty \\ t_0\to-\infty}} U_I(t_1,t_0) \tag{8.160}$$

of the time evolution operator in the interaction picture [Hittmair], which implies unitarity.

Unitarity of the S-matrix. We first prove that $\Omega_\pm$ are isometries, i.e. that the wave operators preserve scalar products. It will then be easy to directly show that $SS^\dagger = S^\dagger S = \mathbb{1}$. For this we introduce a more abstract notation with a complete orthonormal basis $\langle u_i^0|u_j^0\rangle = \delta_{ij}$ of free energy eigenstates $|u_i^0\rangle$ with $H_0|u_i^0\rangle = E_i|u_i^0\rangle$ and the corresponding exact solutions

$$|u_i^\pm\rangle = \Omega_\pm|u_i^0\rangle, \qquad H|u_i^\pm\rangle = E_i|u_i^\pm\rangle, \tag{8.161}$$

for which we compute

$$\langle u_i^+|u_j^+\rangle = \langle u_i^+|u_j^0\rangle + \langle u_i^+|\frac{1}{E_j - H + i\varepsilon}V|u_j^0\rangle \tag{8.162}$$

$$= \langle u_i^+|u_j^0\rangle + \frac{1}{E_j - E_i + i\varepsilon}\langle u_i^+|V|u_j^0\rangle. \tag{8.163}$$

Hermitian conjugation of the Lippmann–Schwinger equation implies, on the other hand,

$$\langle u_i^+|u_j^0\rangle = \langle u_i^0|u_j^0\rangle + \langle u_i^+|V\frac{1}{E_i - H_0 - i\varepsilon}|u_j^0\rangle \tag{8.164}$$

$$= \langle u_i^0|u_j^0\rangle + \frac{1}{E_i - E_j - i\varepsilon}\langle u_i^+|V|u_j^0\rangle \tag{8.165}$$

Hence $\langle u_i^+|u_j^+\rangle = \langle u_i^0|u_j^0\rangle = \delta_{ij}$ and by complex conjugation $\langle u_i^-|u_j^-\rangle = \delta_{ij}$.

In contrast to the finite-dimensional situation the isometry property of $\Omega_\pm$ does not imply unitarity because an isometry in an infinite-dimensional Hilbert space does not need to be surjective. Indeed, the maps $\Omega_\pm$ send plane waves, which form a complete system, to scattering states, which are not complete if the potential V supports bound states. More explicitly, we can write

$$\Omega_\pm = \Omega_\pm \sum_i |u_i^0\rangle\langle u_i^0| = \sum_i |u_i^\pm\rangle\langle u_i^0|. \tag{8.166}$$

Hence

$$\Omega_\pm^\dagger \Omega_\pm = \sum_{ij} |u_i^0\rangle\langle u_i^\pm|u_j^\pm\rangle\langle u_j^0| = \sum_{ij} |u_i^0\rangle\delta_{ij}\langle u_j^0| = \mathbb{1} \tag{8.167}$$

$$\Omega_\pm \Omega_\pm^\dagger = \sum_{ij} |u_i^\pm\rangle\langle u_i^0|u_j^0\rangle\langle u_j^\pm| = \sum_{i} |u_i^\pm\rangle\langle u_i^\pm| = \mathbb{1} - P_{b.s.} \tag{8.168}$$

where $P_{b.s.}$ is the projector to the bound states. If the potential V has negative energy solutions these states cannot be produced in a scattering process and are hence missing from the completeness relation in the last sum. Combining these results unitarity of the S matrix

$$S^\dagger S = \Omega_+^\dagger \Omega_- \Omega_-^\dagger \Omega_+ = \Omega_+^\dagger (\mathbb{1} - P_{b.s.})\Omega_+ = \Omega_+^\dagger \Omega_+ = \mathbb{1} \tag{8.169}$$

$$S S^\dagger = \Omega_-^\dagger \Omega_+ \Omega_+^\dagger \Omega_- = \Omega_-^\dagger (\mathbb{1} - P_{b.s.})\Omega_- = \Omega_-^\dagger \Omega_- = \mathbb{1} \tag{8.170}$$

is established.

Relating the S-matrix to the transition matrix. In order to derive the relation between S and T we write the S-matrix elements S_{ij} as

$$S_{ij} = \langle u_i^-|u_j^+\rangle = \langle u_i^+|u_j^+\rangle + (\langle u_i^-| - \langle u_i^+|)\,|u_j^+\rangle. \tag{8.171}$$

With $\langle u_i^+|u_j^+\rangle = \delta_{ij}$ and

$$\langle u_i^-| = \langle u_i^0|\Omega_-^\dagger = \langle u_i^0|(1 + V\frac{1}{E_i - H + i\varepsilon}), \tag{8.172}$$

$$\langle u_i^+| = \langle u_i^0|\Omega_+^\dagger = \langle u_i^0|(1 + V\frac{1}{E_i - H - i\varepsilon}). \tag{8.173}$$

we obtain

$$S_{ij} = \delta_{ij} + \langle u_i^0|V(\frac{1}{E_i - H + i\varepsilon} - \frac{1}{E_i - H - i\varepsilon})|u_j^+\rangle. \tag{8.174}$$

Since $H|u_j^+\rangle = E_j|u_j^+\rangle$ and

$$\lim_{\varepsilon\to 0}(\frac{1}{z - i\varepsilon} - \frac{1}{z + i\varepsilon}) = 2\pi i\,\delta(z) \tag{8.175}$$

we conclude $S_{ij} = \delta_{ij} - 2\pi i\delta(E_i - E_j)\langle u_i^0|V|u_j^+\rangle$ and hence

$$\boxed{S_{ij} = \delta_{ij} - 2\pi i\delta(E_i - E_j)T_{ij}.} \tag{8.176}$$

The non-relativistic dispersion $E = (\hbar k)^2/2m$ implies $\delta(E_i - E_j) = \frac{m}{\hbar^2 k}\delta(k_i - k_j)$ so that

$$\langle k'|S|k\rangle = \delta^3(\vec{k} - \vec{k}') + \frac{i}{2\pi k}\delta(k - k')f(\vec{k}', \vec{k}). \tag{8.177}$$

Partial wave decomposition on the energy shell [Hittmair] then leads to $S_l = e^{2i\delta_l} = 1 - 2\pi i T_l$.