

► **Introduction** The three prototypes of spectra of self-adjoint operators, the *discrete spectrum*, with or without degeneracy, the *continuous spectrum*, and the *mixed spectrum*, as well as the corresponding wave functions, contain important information about the physical systems that they describe. Yet, from a physicist's point of view, the results obtained until now remain somewhat academic as long as we do not know how to render the information they contain visible by means of concrete experiments. For example, the static spectrum of the Hamiltonian describing the hydrogen atom and the spatial shape of its stationary wave functions, *a priori*, are not observable for us, the macroscopic observers, as long as the atom is not forced to change its state by interaction with external electromagnetic fields or by interaction with scattering beams of electrons. In other terms, the pure stationary systems that we studied so far, must be subject to nonstationary interactions in set-ups of realistic experiments which allow for preparation and detection, before we can decide whether or not these systems describe reality. As this question is of central importance I insert here a first chapter on the description of scattering processes in what is called *potential scattering*, before turning to the more formal framework of quantum theory.

2.1 Macroscopic and Microscopic Scales

In studying classical macroscopic systems our experience shows that it is always possible to perform observations without disturbing the system: In observing the swinging pendulum of an upright clock we measure its maximal elongation, its period, perhaps even the velocity at the moment of passage through the vertical, a stop-watch in our hand, by just “looking” at it and without interfering, to any sizable degree, with the motion of the pendulum. Even extremely precise measurements on satellites or on planets by means of radar signals and interferometry are done with practically no back-reaction on their state of motion. This familiar, almost obvious fact is paraphrased by the statement that the object, i.e. the isolated physical system

that one wishes to study, is separated from the observer and his measuring apparatus in the sense that back-reactions of the measuring procedure on the object are negligible. The perturbation of the system by the measurement either is negligibly small, or can be corrected for afterwards. In particular, the system is obviously not influenced by the mere fact of being observed.

There is a further aspect that we should realize: The length scales and the time scales of macroscopic processes are the typical scales of our familiar environment, or do not differ from them much, that is, do not go beyond the realm of what we can imagine based on our day-to-day experience. Examples are the milliseconds that matter in sportive competitions, or the very precise length measurements in micro mechanics.

Matters change when the object of investigation is a microscopic system such as a molecule, an atom, an atomic nucleus, or a single elementary particle:

1. Every measurement on a micro system is a more or less intrusive intervention that can strongly modify the system or even destroy it. As an example, think of an atom described by a wave function $\psi(t, \mathbf{x})$. If this atom is bombarded by a relatively “coarse” beam such as, e.g., an unpolarized light beam, one intuitively expects the subtle phase correlations that are responsible for the interference phenomena of the wave function, to be partially or completely destroyed. In fact, the impossibility of separating measuring device and object belongs to the most difficult aspects of quantum theory.
2. Furthermore, the spatial and temporal scales of typical quantum processes, in general, are small as compared to spatial distances or time intervals of experiments set up to detect them. An example may illustrate this: The size of a hydrogen atom is of the order of the Bohr radius (1.8), that is about 10^{-10} m. This is a very small quantity as compared to the distance of the hydrogen target from the source emitting the incoming beam that is used to investigate the atom, as well as from the detector designed to detect the scattered beam. A similar remark applies to the temporal conditions in atoms. Characteristic times of an atom are defined by the transition energies,

$$\tau(m \rightarrow n) = \frac{2\pi}{c} \frac{\hbar c}{E_m - E_n}.$$

For the example of the (2p $\rightarrow$ 1s)-transition in hydrogen this time is $\tau(2 \rightarrow 1) \approx 4 \times 10^{-16}$ s – a time interval which is very short as compared to the time scales in a typical experiment.

The general conclusion from these considerations is that in general we can only observe *asymptotic* states, realized long before or long after the process proper, and at large spatial distances from it. More concretely this means the following: We wish to investigate a quantum system which, when isolated, is a stationary one, by means of a beam of particles. The system is the *target*, the particles are the *projectiles* which are directed onto the target, or which are seen in a detector after the scattering has taken place. The interaction process of the beam and the system happens within a time interval Δt around, say, $t = 0$. It is localized within a volume V of space around the origin $\mathbf{x} = 0$ that is characterized by the radius R_0 . At time $t \rightarrow -\infty$

the beam is constructed in a controlled way at an asymptotically large distance from the target. The beam and the target in this configuration define what is called the *in*-state (abbreviation for “incoming state”). For $t \rightarrow +\infty$ the scattered particles, or more generally the reaction products of the scattering process, are identified in the detector which also has an asymptotically large distance from the target. The scattered particles, together with the target in its final state, are in what one calls the *out*-state (abbreviation for “outgoing state”).

Other situations where we actually can perform measurements are provided by systems which are stationary by themselves but which are unstable because of interactions with other systems. For example, the 2p-state of hydrogen is unstable because it decays to the 1s-state by emission of a photon, the typical time for the transition being on the order of 10^{-9} s. In this example the *in*-state is the atom in its excited 2p-state, the *out*-state consists of the outgoing photon and the atom in the stable ground state. In this example, too, our information on the (unstable) quantum system stems from an asymptotic measurement, the decay products being detected a long time after the decay process happened and very far in space.¹

As a general conclusion we note that experimental information on quantum mechanical systems is obtained from asymptotic, incoming or outgoing states. We cannot penetrate the interaction region proper and cannot interfere with the typical time scale of the interaction. In quantum mechanics of molecules, atoms, and nuclei, the important methods of investigation are: scattering of particles, i.e. electrons, protons, neutrons, or α particles, on these systems; excitation and decay of their excited states by interaction with the electromagnetic radiation field.

Scattering processes which can be dealt with by means of the notions and methods developed in Chap. 1, are the subject of this chapter. The interaction with the radiation field requires further and more comprehensive preparation and is postponed to later chapters. Likewise, scattering theory in a physically more general, mathematically more formal framework will be taken up again later.

2.2 Scattering on a Central Potential

We assume that a potential $U(\mathbf{x})$ is given which describes the interaction of two particles and which is spherically symmetric and has finite range. Somewhat more formally this means

$$U(\mathbf{x}) \equiv U(r) \quad \text{with} \quad r = |\mathbf{x}|, \quad \lim_{r \rightarrow \infty} [rU(r)] = 0. \quad (2.1)$$

¹ Of course, the unstable state must have been created beforehand and one may ask why the preparation procedure is not taken to be part of the *in*-state, or under which condition this becomes a necessity. The answer is a qualitative one: The total decay probability of the unstable state, when multiplied by $\hbar$, yields the energy uncertainty, or width Γ of the unstable state. If $\Gamma \ll E_a$, i.e. if the width Γ is small as compared to the energy E_a of the state then this state is *quasi-stable*. The process used to prepare it can be separated from the decay process.

Spherically symmetric potentials such as

$$U(r) = U_0 \Theta(r_0 - r) \quad \text{or} \quad U(r) = g \frac{e^{-r/r_0}}{r},$$

the first of which vanishes outside of the fixed radius r_0 , while the second decreases exponentially, fulfill this condition. The Coulomb potential

$$U_C(r) = \frac{e_1 e_2}{r}$$

does not. The aim is to investigate the scattering of a particle of mass m on the potential and to calculate the corresponding differential cross section. (Note that in the case of the two-body system m is the reduced mass.) The differential cross section is an observable, i.e. a classical quantity. Its definition is the same as in classical mechanics (cf. [Scheck (2010)], Sect. 1.27): It is the ratio of the number dn of particles which are scattered, in the unit of time, into scattering angles between θ and $\theta + d\theta$, and of the number n_0 of incoming particles per unit of area and unit of time. In other terms, one determines the number of particles that were actually scattered, and normalizes to the incoming flux. In contrast to the classical situation these numbers are obtained from the current density (1.54) (with $\mathbf{A} \equiv 0$) describing the flow of probability, via Born's interpretation, not from classical trajectories (which no longer exist).

The correct way of proceeding would be to construct a state coming in along the 3-direction as a wave packet at $t = -\infty$ which clusters around the average momentum $\mathbf{p} = p\hat{\mathbf{e}}_3$, then to calculate the time evolution of this wave packet by means of the Schrödinger equation, and eventually analyze the outgoing flux at $t \rightarrow +\infty$. As this is tedious and cumbersome, one resorts to an intuitive method which is simpler and, yet, leads to the correct results. One considers the scattering process as a stationary situation. The incoming beam is taken to be a stationary plane wave, while the scattered state is represented by an outgoing spherical wave. At asymptotic distances from the scattering center the wave field then has the form

$$r \rightarrow \infty: \quad \psi_{\text{Somm}}(\mathbf{x}) \sim e^{ikx^3} + f(\theta) \frac{e^{ikr}}{r}, \quad k = \frac{1}{\hbar}|\mathbf{p}|, \quad (2.2)$$

whose first term is the incoming beam with momentum $\mathbf{p} = p\hat{\mathbf{e}}_3 = \hbar k\hat{\mathbf{e}}_3$ while the second is the outgoing spherical wave. This ansatz is called *Sommerfeld's radiation condition*

The role of the (in general) complex amplitude $f(\theta)$ is clarified by calculating the current densities of the incoming and outgoing parts. It is useful, here and below, to denote the skew-symmetric derivative of (1.54) by a symbol of its own,

$$f^*(\mathbf{x}) \overset{\leftrightarrow}{\nabla} g(\mathbf{x}) := f^*(\mathbf{x}) \nabla g(\mathbf{x}) - [\nabla f^*(\mathbf{x})] g(\mathbf{x}) \quad (2.3)$$

where f and g are complex functions which are at least C^1 (once continuously differentiable). For the incoming wave one finds

$$\mathbf{j}_{\text{in}} = \frac{\hbar}{2mi} e^{-ikx^3} \overset{\leftrightarrow}{\nabla} e^{ikx^3} = \frac{\hbar k}{m} \hat{\mathbf{e}}_3 = v\hat{\mathbf{e}}_3,$$

with $v\hat{\mathbf{e}}_3$ the velocity of the incoming particle.

Using spherical polar coordinates for which

$$\nabla = \left(\frac{\partial}{\partial r}, \frac{1}{r} \frac{\partial}{\partial \theta}, \frac{1}{r \sin \theta} \frac{\partial}{\partial \phi} \right),$$

and the following expressions for the gradient of $\psi = f(\theta)e^{ikr}/r$

$$(\nabla\psi)_r = \frac{\partial\psi}{\partial r} = \left(-\frac{1}{r^2} + \frac{ik}{r} \right) f(\theta)e^{ikr},$$

$$(\nabla\psi)_\theta = \frac{1}{r} \frac{\partial\psi}{\partial \theta} = \frac{1}{r^2} \frac{\partial f(\theta)}{\partial \theta} e^{ikr}, \quad (\nabla\psi)_\phi = 0,$$

the outgoing current density is easily calculated,

$$\mathbf{j}_{\text{out}} = \frac{\hbar k}{m} \frac{|f(\theta)|^2}{r^2} \hat{\mathbf{e}}_r + \frac{\hbar}{2mi} \frac{1}{r^3} f^*(\theta) \nabla f(\theta) \hat{\mathbf{e}}_\theta.$$

The first term, upon multiplication by the area element $r^2 d\Omega$ of a sphere with radius r and center at the origin, yields a probability current in the radial direction proportional to $|f(\theta)|^2$. The second term, in contrast, yields a current decreasing like $1/r$ which must be neglected asymptotically. The flux of particles across the cone with solid angle $d\Omega$ in an outgoing radial direction becomes (for large values of r)

$$\mathbf{j}_{\text{out}} \cdot \hat{\mathbf{e}}_r r^2 d\Omega = \frac{\hbar k}{m} \frac{|f(\theta)|^2}{r^2} r^2 d\Omega \quad (r \rightarrow \infty).$$

Normalizing to the incoming flux, the differential cross section is found to be

$$d\sigma_{\text{el}} = \frac{\mathbf{j}_{\text{out}} \cdot \hat{\mathbf{e}}_r r^2 d\Omega}{|\mathbf{j}_{\text{in}}|} = |f(\theta)|^2 d\Omega.$$

This result clarifies the physical interpretation of the amplitude $f(\theta)$: This amplitude determines the differential cross section

$$\boxed{\frac{d\sigma_{\text{el}}}{d\Omega} = |f(\theta)|^2}. \quad (2.4)$$

The function $f(\theta)$ is called *scattering amplitude*. It is a probability amplitude, in the spirit of Born's interpretation. The square of its modulus is the differential cross section and, hence, is a classical observable. As we will see soon it describes *elastic* scattering. The total elastic cross section is given by the integral taken over the complete solid angle

$$\boxed{\sigma_{\text{el}} = \int d\Omega |f(\theta)|^2 = 2\pi \int_0^\pi \sin \theta d\theta |f(\theta)|^2}. \quad (2.5)$$

Before continuing with a discussion of methods that allow to calculate the scattering amplitude and the cross sections we add a few complements to and comments on these results.

Remarks

1. The result obtained for the asymptotic form of j_{out} shows that it was justified to call the two terms in (1.135), Sect. 1.9.3, *outgoing* and *incoming* spherical waves, respectively.
2. In the two-body problem with central force, the variable r is the modulus of the relative coordinate, m is the reduced mass,

$$m \mapsto \frac{m_1 m_2}{m_1 + m_2}, \quad \text{and} \quad \theta \mapsto \theta^*$$

is the scattering angle in the center-of-mass system. Thus, the amplitude $f(\theta)$ is the *scattering amplitude in the center-of-mass system*.

3. The potential $U(r)$ must be real if the Hamiltonian is to be self-adjoint. If this is so, then there is only *elastic* scattering. No matter how it is scattered, the particle must be found somewhere in the final state, or, in the spirit of quantum mechanics, the probability to find the particle *somewhere* in space must be conserved. Therefore, the expression (2.4) describes the differential cross section for *elastic* scattering, the expression (2.5) gives the *integrated elastic* cross section.

However, there are processes where the final state is not the same as the initial state. An electron which is scattered on an atom, may loose energy and may leave behind the atom in an excited state. A photon used as a projectile may be scattered inelastically on the atom, or may even be absorbed completely. In those cases one says that the final state belongs to another *channel* than the initial state. Besides the real potential responsible for elastic scattering, the Hamiltonian must also contain interaction terms which allow to cross from the initial channel to other, inelastic channels. Loosely speaking, in such a situation the total probability is distributed, after the scattering, over the various final state channels. In Sect. 2.6 we will develop a bulk method for describing such a situation without knowing the details of the reaction dynamics.

4. Even though the ansatz (2.2) is intuitively compelling, in a strict sense the ensuing calculation is not correct. The condition (2.2) assumes a stationary wave function where both the incoming plane wave and the outgoing spherical wave are present at all times. In particular, when one calculates the current density (1.54) there should be terms arising from the interference between the incoming and outgoing parts. Instead, in our calculation of the current densities we proceeded as if at $t = -\infty$ there was only the plane wave, and at $t = +\infty$ there will be only the scattered spherical wave. Although this derivation rests on intuition and, strictly speaking, is not correct, it yields the right result. This is so because the plane wave is but an idealization and should be replaced by a suitably composed wave packet. We skip this painstaking calculation at this point and just report the essential result: One follows the evolution of a wave packet which at $t \rightarrow -\infty$ described a localized particle with average momentum $\mathbf{p} = p\hat{\mathbf{e}}_3$. For large positive times and at asymptotic distances there appears an outgoing spherical wave with the shape assumed above. There are indeed interference terms between the initial state and the final state, but, as

these terms oscillate very rapidly, integration over the spectrum of momenta renders them negligibly small. Except for the forward direction, that is for scattering where $\mathbf{p}' = \mathbf{p}$, the ansatz (2.2), together with the interpretation given above, is correct.

5. It is instructive to compare the quantum mechanical description with the theory of elastic scattering in classical mechanics. The definition of the differential cross section, of course, is the same (number of particles per unit of time scattered into the solid angle $d\Omega$, normalized to the incoming flux). The physical processes behind it are not the same. The classical particle that comes in with momentum $\mathbf{p} = p\hat{\mathbf{e}}_3$ and impact parameter b , moves on a well-defined trajectory. It suffices to follow this orbit from $t = -\infty$ to $t = +\infty$ to find out, with certainty, where the particle has gone. In quantum mechanics we associate a wave packet to the particle which, for example, contains only momenta in the 3-direction and which, at $t = -\infty$, is centered at a value $\mathbf{p} = p\hat{\mathbf{e}}_3$. Values for its 3-coordinate can be limited within what the uncertainty relation allows for. As the particle has no momentum components in the 1- and the 2-directions, or, in other terms, since p_1 and p_2 have the sharp values 0, the position of the particle in the plane perpendicular to the 3-axis is completely undetermined. At $t \rightarrow +\infty$ quantum mechanics yields a probability for detecting the particle in a detector which is positioned at a scattering angle θ with respect to the incoming beam. It is impossible to predict where any individual particle will be scattered. The probability $d\sigma_{\text{el}}/d\Omega$ which is defined by the complex scattering amplitude $f(\theta)$ will be confirmed only if one allows very many particles to scatter under identical experimental conditions.

2.3 Partial Wave Analysis

Clearly, the scattering amplitude must be a function of the energy $E = \hbar^2 k^2 / (2m)$ of the incoming beam, or, what amounts to the same, a function of the wave number k . Whenever this dependence matters we should write, more precisely, $f(k, \theta)$ instead of $f(\theta)$. The cross section has the physical dimension [area]. Hence, the scattering amplitude has dimension [length]. In the physically allowed region $\theta \in [0, \pi]$ or $z \equiv \cos \theta \in [-1, +1]$, and for fixed k , the amplitude $f(k, \theta)$ is a nonsingular, in general square integrable function of θ .² Therefore, it may be expanded in terms of spherical harmonics $Y_{\ell m}(\theta, \phi)$. However, as it depends on θ , by the spherical symmetry of the potential, and does not depend on ϕ , this expansion contains only spherical

² Assuming the restriction (2.1) the amplitude f is square integrable, indeed. In the case of the Coulomb potential the amplitude is singular in the forward direction $\theta = 0$, its behaviour being like $1/\sin \theta$, and, hence, is no longer square integrable. Nevertheless, the scattering amplitude can still be expanded in terms of Legendre polynomials. However, the series (2.6) is no longer convergent in the forward direction, and the expression (2.7) for the integrated cross section diverges.

harmonics with $m = 0$, $Y_{\ell 0}$, which are proportional to Legendre polynomials,

$$Y_{\ell 0} = \sqrt{\frac{2\ell + 1}{4\pi}} P_{\ell}(z = \cos \theta).$$

As a consequence one can always choose an expansion in terms of Legendre polynomials,

$$f(k, \theta) = \frac{1}{k} \sum_{\ell=0}^{\infty} (2\ell + 1) a_{\ell}(k) P_{\ell}(z). \quad (2.6)$$

The factor $1/k$ is introduced in order to keep track of the physical dimension of the scattering amplitude, the factor $(2\ell + 1)$ is a matter of convention and will prove to be useful. The complex quantities $a_{\ell}(k)$ which are defined by (2.6) are called *partial wave amplitudes*. They are functions of the energy only (or, equivalently, of the wave number). The spherical harmonics are orthogonal and are normalized to 1. Therefore, the integrated cross section (2.5) is

$$\sigma_{\text{el}}(k) = \frac{4\pi}{k^2} \sum_{\ell, \ell'} \sqrt{(2\ell + 1)(2\ell' + 1)} a_{\ell}(k) a_{\ell'}^*(k) \int d\Omega Y_{\ell' 0}^* Y_{\ell 0}$$

which, by the orthogonality of spherical harmonics, simplifies to

$$\sigma_{\text{el}}(k) = \frac{4\pi}{k^2} \sum_{\ell=0}^{\infty} (2\ell + 1) |a_{\ell}(k)|^2. \quad (2.7)$$

Like the formulae (2.4) and (2.5) these expressions are completely general, and make no use of the underlying dynamics, i.e. in the case being studied here, of the Schrödinger equation with a central potential $U(r)$.

We now show that the amplitudes $a_{\ell}(k)$ are obtained by solving the radial equation (1.127) for all partial waves. The arguments presented in Sect. 1.9.3 and the comparison to the analogous classical situation show that this is not only an exact method for studying elastic scattering but that it is also particularly useful from a physical point of view. By assumption the potential has finite range, i.e. it fulfills the condition (2.1). In the corresponding *classical* situation a particle with a large value of angular momentum ℓ_{cl} stays further away from the origin $r = 0$ than a particle with a smaller value of ℓ_{cl} , and the action of the potential on it is correspondingly weaker. Very much like in classical mechanics the quantum effective potential

$$U_{\text{eff}}(r) = \frac{\hbar^2 \ell(\ell + 1)}{2mr^2} + U(r),$$

for large values of ℓ , is dominated by the centrifugal term. Thus, one expects the amplitudes a_{ℓ} to decrease rapidly with increasing ℓ , so that the series (2.6) and (2.7) converge rapidly.

If the ℓ -th partial wave is taken to be

$$R_{\ell}(r) Y_{\ell m} = \frac{u_{\ell}(r)}{r} Y_{\ell m}$$

the radial function $u_\ell(r)$ obeys the differential equation

$$u_\ell''(r) - \left(\frac{2m}{\hbar^2} U_{\text{eff}}(r) - k^2 \right) u_\ell(r) = 0, \quad (2.8)$$

(see also Sect. 1.9.5). At the origin, $r = 0$, the radial function must be regular. This means that we must choose the solution which behaves like $R_\ell \sim r^\ell$, or $u_\ell \sim r^{\ell+1}$, respectively, in the neighbourhood of the origin. For $r \rightarrow \infty$ the effective potential becomes negligible as compared to k^2 so that (2.8) simplifies to the approximate form

$$r \rightarrow \infty : \quad u_\ell''(r) + k^2 u_\ell(r) \approx 0.$$

Therefore, the asymptotic behaviour of the partial wave must be given by

$$r \rightarrow \infty : \quad u_\ell(r) \sim \sin \left(kr - \ell \frac{\pi}{2} + \delta_\ell(k) \right). \quad (2.9)$$

The phase $\delta_\ell(k)$ which is defined by this equation is called the *scattering phase* in the partial wave with orbital angular momentum ℓ .

The following argument shows that the asymptotic form (2.9) is very natural: On the one hand, the function $u_\ell(r)$ is real (or can be chosen so) if the potential $U(r)$ is real. Under the same assumption the scattering phase must be real. On the other hand, the asymptotics of the force-free solution is known from the asymptotics (1.133) of spherical Bessel functions (which are regular at $r = 0$),

$$u_\ell^{(0)}(r) = (kr) j_\ell(kr) \sim \sin \left(kr - \ell \frac{\pi}{2} \right).$$

If the potential $U(r)$ is identically zero all scattering phases are equal to zero. Therefore, the scattering phases “measure” to which extent the asymptotic, oscillatory behaviour of the radial function $u_\ell(r)$ is shifted relative to the force-free solution $u_\ell^{(0)}(r)$.

There remains the problem of expressing the scattering amplitude, or, equivalently, the amplitudes $a_\ell(k)$ in terms of the scattering phases. In solving this problem, the idea is to write the unknown scattering solution $\psi(\mathbf{x})$ of the Schrödinger equation in terms of a series in partial waves,

$$\psi(\mathbf{x}) = \sum_{\ell=0}^{\infty} c_\ell R_\ell(r) Y_{\ell 0}(\theta) = \frac{1}{r} \sum_{\ell=0}^{\infty} c_\ell u_\ell(r) Y_{\ell 0}(\theta) \quad (2.10)$$

and to choose this expansion such that the incoming spherical wave $\alpha_{\text{in}} e^{-ikr}/r$ which is contained in it for $r \rightarrow \infty$, coincides with the incoming spherical wave contained in the condition (2.2). We begin with the latter: Expanding the plane wave in terms of spherical harmonics (cf. (1.136)),

$$e^{ikx^3} = \sum_{\ell=0}^{\infty} i^\ell \sqrt{4\pi(2\ell+1)} j_\ell(kr) Y_{\ell 0},$$

and making use of the asymptotics (1.133) of the spherical Bessel functions,

$$j_\ell(kr) \sim \frac{1}{kr} \sin\left(kr - \ell\frac{\pi}{2}\right) = \frac{1}{2ikr} (e^{ikr} e^{-i\ell\pi/2} - e^{-ikr} e^{i\ell\pi/2}),$$

the piece proportional to e^{-ikr}/r can be read off. The *outgoing* spherical wave, on the other hand, in (2.2), in addition to the term proportional to the scattering amplitude $f(\theta)$, also contains a piece of the plane wave that can be read off from the same expression. This is to say that the Sommerfeld condition (2.2) is rewritten in terms of spherical waves as follows:

$$\begin{aligned} \psi_{\text{Somm}}(\mathbf{x}) \sim & -\frac{e^{-ikr}}{2ikr} \left(\sum_{\ell=0}^{\infty} i^\ell \sqrt{4\pi(2\ell+1)} e^{i\ell\pi/2} Y_{\ell 0} \right) \\ & + \frac{e^{ikr}}{2ikr} \left(\sum_{\ell=0}^{\infty} i^\ell \sqrt{4\pi(2\ell+1)} e^{-i\ell\pi/2} Y_{\ell 0} + 2ikf(\theta) \right). \end{aligned}$$

This is to be compared to the representation (2.10) for the scattering solution for $r \rightarrow \infty$ which becomes, upon inserting (2.9) once more,

$$\psi(\mathbf{x}) \sim -\frac{e^{-ikr}}{2ir} \left(\sum_{\ell=0}^{\infty} c_\ell e^{-i\delta_\ell} e^{i\ell\pi/2} Y_{\ell 0} \right) + \frac{e^{ikr}}{2ir} \left(\sum_{\ell=0}^{\infty} c_\ell e^{i\delta_\ell} e^{-i\ell\pi/2} Y_{\ell 0} \right).$$

The *incoming* spherical waves in ψ_{Somm} and in ψ are equal provided the coefficients c_ℓ are chosen to be

$$c_\ell = \frac{i^\ell}{k} \sqrt{4\pi(2\ell+1)} e^{i\delta_\ell}.$$

For the rest of the calculation one just has to compare these formulae. Inserting the result for c_ℓ into the *outgoing* part of (2.10), one finds

$$\begin{aligned} f(\theta) &= \frac{1}{k} \sum_{\ell=0}^{\infty} \frac{e^{2i\delta_\ell} - 1}{2i} \sqrt{4\pi(2\ell+1)} Y_{\ell 0} \\ &= \frac{1}{k} \sum_{\ell=0}^{\infty} \frac{e^{2i\delta_\ell} - 1}{2i} (2\ell+1) P_\ell(\cos \theta), \end{aligned}$$

where use is made of the relation

$$Y_{\ell 0}(\theta) = \sqrt{\frac{2\ell+1}{4\pi}} P_\ell(\cos \theta).$$

Comparison with the general expansion (2.6) yields the following *exact* expression for the amplitudes $a_\ell(k)$ as functions of the scattering phases,

$$\boxed{a_\ell(k) = \frac{e^{2i\delta_\ell} - 1}{2i} = e^{i\delta_\ell(k)} \sin \delta_\ell(k)}. \quad (2.11)$$

Applications and Remarks

1. It was indeed useful to define the amplitudes a_ℓ by extracting an explicit factor $(2\ell+1)$ in (2.6). The so-defined amplitudes then have moduli which are smaller than or equal to 1. The second equation in (2.11) is correct because the phase δ_ℓ is real.³
2. The result (2.11) for the partial wave amplitudes which follows from the Schrödinger equation, has a remarkable property: The imaginary part of a_ℓ is positive-semidefinite

$$\text{Im } a_\ell(k) = \sin^2 \delta_\ell \geq 0.$$

Calculating the elastic scattering amplitude (2.6) in the forward direction $\theta = 0$, where $P_\ell(z = 1) = 1$, its imaginary part is seen to be

$$\text{Im } f(0) = \frac{1}{k} \sum_{\ell=0}^{\infty} (2\ell+1) \text{Im } a_\ell(k) = \frac{1}{k} \sum_{\ell=0}^{\infty} (2\ell+1) \sin^2 \delta_\ell(k).$$

In turn, the integrated elastic cross section (2.7) is found to be

$$\sigma_{\text{el}}(k) = \frac{4\pi}{k^2} \sum_{\ell=0}^{\infty} (2\ell+1) \sin^2 \delta_\ell(k).$$

In the case of a real potential there is elastic scattering only, the integrated cross section (2.7) is identical with the total cross section. Comparison of the results just obtained yields an important relation between the imaginary part of the elastic scattering amplitude in the forward direction and the total cross section, viz.

$$\boxed{\sigma_{\text{tot}} = \frac{4\pi}{k} \text{Im } f(0)} . \quad (2.12)$$

This relationship is called *the optical theorem*.⁴ Loosely speaking it is a consequence of the conservation of (Born) probability.

3. As we will see in Sect. 2.6 and in Chap. 8, the optical theorem also holds in more general situations. When two particles, A and B , are scattered on one another, besides elastic scattering $A + B \rightarrow A + B$, there will in general be inelastic processes as well, in which one of them, or both, are left in excited states, $A + B \rightarrow A + B^*$, $A + B \rightarrow A^* + B^*$, or where further particles are created, $A + B \rightarrow A + B + C + \dots$. As a short-hand allowed final states are denoted by “ n ”. The optical theorem then relates the imaginary part of the

³ This remark is important because the same analysis can be applied to the case of a complex, absorptive potential. In this case the scattering phases are complex functions. The first part of the formula (2.11) still applies, the second part does not.

⁴ Indeed, this term was coined in classical optics. It was known, in a different context, before quantum mechanics was developed.

elastic forward scattering amplitude at a given value of the energy, to the *total* cross section at this energy,

$$\sigma_{\text{tot}} = \sum_n \sigma(A + B \longrightarrow n) .$$

The more general form of the optical theorem (2.12) is

$$\sigma_{\text{tot}}(k) = \frac{4\pi}{k} \text{Im } f_{\text{el}}(k, \theta = 0) ,$$

the quantity k being the modulus of the momentum $\mathbf{k}^*$ in the center-of-mass system.

2.3.1 How to Calculate Scattering Phases

The asymptotic condition (2.9) can be interpreted in still a different way that, by the same token, gives a hint at possibilities of obtaining the scattering phases. As the potential has finite range the interval of definition of the radial variable r splits into an inner domain where the (true) potential $U(r)$ is different from zero, and an outer domain where either it vanishes or becomes negligibly small, and where only the centrifugal potential is active. Thus, in the outer domain every solution $u_\ell(r)$ is a linear combination of two fundamental solutions of the force-free case. For instance, these may be a spherical Bessel function $j_\ell(kr)$ and a spherical Neumann function $n_\ell(kr)$, so that

$$u_\ell(k, r) = (kr) [j_\ell(kr)\alpha_\ell(k) + n_\ell(kr)\beta_\ell(k)] ,$$

(for r such that $U(r) \approx 0$).

One now takes this formula to large values of r , and compares the asymptotic behaviour (2.9) with the asymptotics of the spherical Bessel and Neumann functions (1.133) and (1.140), respectively. Using the addition formula for Sines

$$\begin{aligned} & \sin \left(kr - \ell \frac{\pi}{2} + \delta_\ell(k) \right) \\ &= \sin \left(kr - \ell \frac{\pi}{2} \right) \cos \delta_\ell(k) + \cos \left(kr - \ell \frac{\pi}{2} \right) \sin \delta_\ell(k) \end{aligned}$$

then yields an equation for the scattering phase which is

$$\tan \delta_\ell(k) = \frac{\beta_\ell}{\alpha_\ell} . \quad (2.13)$$

This shows that the differential equation for the radial function must be solved only in the inner domain of the variable r : One determines the solution regular at $r = 0$, e.g. by numerical integration on a computer, and follows this solution to the boundary of the outer domain. At this point one writes it as a linear combination of j_ℓ and n_ℓ , and reads off the coefficients α_ℓ and β_ℓ whose ratio (2.13) yields the scattering phase in the interval $[0, \pi/2]$.

Here are some examples of potentials for which the reader may wish to determine the scattering phases:

1. The spherically symmetric potential well

$$U(r) = U_0 \Theta(r_0 - r); \quad (2.14)$$

2. The electrostatic potential

$$U(r) = -4\pi Q \left(\frac{1}{r} \int_0^r dr' \varrho(r') r'^2 + \int_r^\infty dr' \varrho(r') r' \right), \quad (2.15)$$

which is obtained from the charge distribution

$$\varrho(r) = N \frac{1}{1 + \exp[(r - c)/z]} \quad (2.16)$$

with normalization factor

$$N = \frac{3}{4\pi c^3} \left[1 + \left(\frac{\pi z}{c} \right)^2 - 6 \left(\frac{z}{c} \right)^3 \sum_{n=1}^{\infty} \frac{(-)^n}{n^3} e^{-nc/z} \right]^{-1}.$$

The distribution (2.16) is often used in the description of nuclear charge densities. The parameter c characterizes the radial extension while the parameter z characterizes the surface region. Its specific functional form is also known from statistical mechanics which is the reason why it is usually called *Fermi distribution*. Figure 2.1 shows an example applicable to realistic nuclei where z is very small as compared to c .

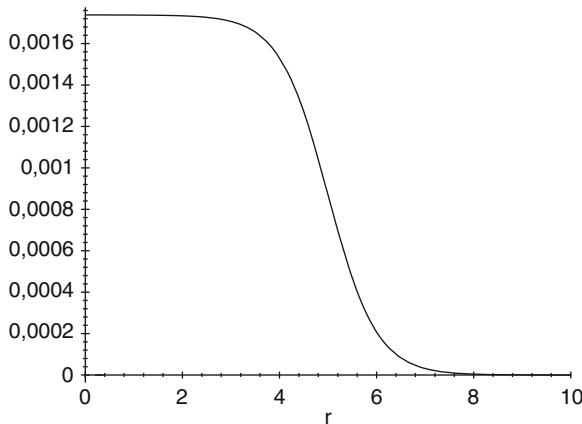


Fig. 2.1 Illustration of the model (2.16) for a normalized charge distribution. In the case shown here, $c \gg z$. The example shows the distribution with $c = 5$ fm, $z = 0.5$ fm. The parameter c is the distance from the origin to the radius where the function $\varrho(r)$ has dropped to half its value at $r = 0$. The two points where it assumes 90 and 10% of its value in $r = 0$, respectively, are situated at $r_{90} = c - 2z \ln 3$ and at $r_{10} = c + 2z \ln 3$, respectively. They are separated by the approximate distance $t \equiv 4z \ln 3 \approx 4.394z$.

3. The Yukawa potential, that we mentioned in the introduction to Sect. 2.2,

$$U_Y(r) = g \frac{e^{-r/r_0}}{r}. \quad (2.17)$$

We will show later that this potential describes the interaction of two particles which can exchange a scalar particle of mass $M = \hbar/(r_0 c)$ (c denotes the speed of light). The name is due to H. Yukawa who had postulated that the *strong* interactions of nucleons were due to the exchange of particles with spin 0, the π -mesons, long before these particles were actually discovered. The length $r_0 = \hbar c/(Mc^2)$ is interpreted as the range of the potential. It is the Compton wave length of particles of mass M . These remarks emphasize that the example (2.17) may have a deeper significance for physics than the pure model potentials (2.14), (2.15) and (2.16).

Consider now two potentials of finite range, $U^{(1)}$ and $U^{(2)}$, and compare their scattering phases. For equal values of the energy the corresponding radial functions obey the radial differential equations

$$u_\ell^{(j)''}(r) - \left[\frac{2m}{\hbar^2} U_{\text{eff}}^{(j)}(r) - k^2 \right] u_\ell^{(j)}(r) = 0, \quad j = 1, 2,$$

where the effective potentials differ only by the true, dynamical potentials

$$U_{\text{eff}}^{(2)}(r) - U_{\text{eff}}^{(1)}(r) = U^{(2)}(r) - U^{(1)}(r).$$

Both radial functions are assumed to be regular at $r = 0$. As we are factoring $1/r$, this means that $u_\ell^{(j)}(0) = 0$ ($j = 1, 2$). Compute then the following derivative, making use of the differential equations for $u_\ell^{(1)}$ and $u_\ell^{(2)}$,

$$\begin{aligned} \frac{d}{dr} (u_\ell^{(1)} u_\ell^{(2)'} - u_\ell^{(2)} u_\ell^{(1)'}) &= u_\ell^{(1)} u_\ell^{(2)''} - u_\ell^{(2)} u_\ell^{(1)''} \\ &= \frac{2m}{\hbar^2} (U^{(2)} - U^{(1)}) u_\ell^{(1)} u_\ell^{(2)}. \end{aligned}$$

Taking the integral over the interval $[0, r]$, one has

$$\begin{aligned} u_\ell^{(1)}(r) u_\ell^{(2)'}(r) - u_\ell^{(2)}(r) u_\ell^{(1)'}(r) \\ = \frac{2m}{\hbar^2} \int_0^r dr' (U^{(2)}(r') - U^{(1)}(r')) u_\ell^{(1)}(r') u_\ell^{(2)}(r'). \end{aligned}$$

In the limit of r going to infinity, and using the asymptotic form (2.9) as well as its derivative on the left-hand side of this equation, one obtains an integral representation for the difference of scattering phases:

$$k \sin(\delta_\ell^{(1)} - \delta_\ell^{(2)}) = \frac{2m}{\hbar^2} \int_0^\infty dr (U^{(2)}(r) - U^{(1)}(r)) u_\ell^{(1)}(r) u_\ell^{(2)}(r). \quad (2.18)$$

This formula is useful for testing the sensitivity of high, intermediate, and low partial waves to the potential, by letting $U^{(1)}$ and $U^{(2)}$ differ but little. Instead of the scattering phases themselves one calculates the change in any given partial wave as a function of the change in the potential.

Alternatively one may consider a situation where $U^{(2)}$ vanishes identically, i.e. where the corresponding radial functions are proportional to spherical Bessel functions,

$$u_\ell^{(2)}(r) = (kr)j_\ell(kr).$$

With $\delta_\ell^{(1)} \equiv \delta_\ell$ and $\delta_\ell^{(2)} = 0$ the integral representation reduces to

$$\sin(\delta_\ell) = -\frac{2m}{\hbar^2} \int_0^\infty r dr U(r) u_\ell(r) j_\ell(kr). \quad (2.19)$$

The Yukawa potential (2.17) may serve as an illustration of this formula. For the sake of simplicity we assume this potential to be weak enough so that the corresponding radial function can be approximated by the force-free solution,⁵

$$u_\ell^{(Y)}(r) \approx (kr)j_\ell(kr).$$

With this assumption one has

$$\begin{aligned} \sin \delta_\ell^{(Y)} &\approx -\frac{2mk}{\hbar^2} \int_0^\infty r^2 dr U_Y(r) j_\ell^2(kr) \\ &= -\frac{2mkg}{\hbar^2} \int_0^\infty r dr e^{-r/r_0} j_\ell^2(kr) \\ &= -\frac{mg\pi}{\hbar^2 k} \int_0^\infty d\varrho e^{-\varrho/(kr_0)} J_{\ell+1/2}^2(\varrho) \\ &= -\frac{mg}{\hbar^2 k} Q_\ell \left(1 + \frac{1}{2(kr_0)^2} \right). \end{aligned}$$

In this derivation the variable $\varrho = kr$ is introduced, and the spherical Bessel function is written in the standard form of Bessel functions found in monographs on special functions, viz.

$$j_\ell(\varrho) = \left(\frac{\pi}{2\varrho} \right)^{1/2} J_{\ell+1/2}(\varrho).$$

⁵ This approximation is nothing but the first Born approximation that is studied in more detail in Sect. 2.4.1.

The last step makes use of a known definite integral which is found, e.g. in [Gradshteyn and Ryzhik (1965)], Eq. 6.612.3. Here, Q_ℓ is a Legendre function of second kind whose properties are well known.⁶ These functions are known to decrease rapidly both for increasing ℓ and for increasing values of the argument ≥ 1 , cf., e.g., [Abramowitz and Stegun (1965)], Fig. 8.5.

2.3.2 Potentials with Infinite Range: Coulomb Potential

The Coulomb potential violates the condition (2.1). This means that its influence is still felt when the particle moves at very large distances from the scattering center. This is seen very clearly in the asymptotics of the partial waves, derived in Sect. 1.9.5, which in addition to the constant phase σ_ℓ , contain an r -dependent, logarithmic phase $-\gamma \ln(2kr)$ multiplied by the factor (1.156),

$$\gamma = \frac{ZZ'e^2m}{\hbar^2k}. \quad (2.20)$$

The scattering solutions of the Coulomb potential certainly do not obey the radiation condition (2.2). Both the outgoing spherical wave and the plane wave are modified due to the long range of the potential, and the formulae of partial wave analysis derived above, cannot be applied directly. A similar statement holds for any spherically symmetric potential which, though different from the $(1/r)$ -behaviour in the inner domain, approaches the Coulomb potential for large values of r . An example is provided by the electrostatic potential corresponding to the charge distribution (2.16) in Example 2 of Sect. 2.3.1. In order to solve this new problem we proceed in two steps:

In the first step we show that the condition (2.2) is modified to

$$r \rightarrow \infty : \quad \psi \sim e^{i\{kx^3 + \gamma \ln[2kr \sin^2(\theta/2)]\}} + f_C(\theta) \frac{e^{i[kr - \gamma \ln(2kr)]}}{r}, \quad (2.21)$$

with r -dependent, logarithmic phases both in the incoming wave and in the outgoing spherical wave, and calculate the scattering amplitude $f_C(\theta)$ for the pure Coulomb potential.

In the second step we study spherically symmetric potentials which deviate from the $(1/r)$ -form in the inner region but decrease like $1/r$ in the outer region, in other words, which approach the Coulomb potential for $r \rightarrow \infty$. In this case it is sufficient to calculate the *shift* of the scattering phases relative to their values in the pure Coulomb potential, and not relative to the force-free case.

Step 1: Although we already know the scattering phases for the Coulomb potential from Sect. 1.9.5 it is instructive to calculate the scattering amplitude directly, using

⁶ The function $Q_\ell(z)$ and the Legendre polynomial $P_\ell(z)$ form a fundamental system of solutions of the differential equation (1.112) with $\lambda = \ell(\ell+1)$ and $m = 0$. In contrast to $P_\ell(z)$ the function $Q_\ell(z)$ is singular in $z = 1$, the singularity being a branch point. For all values $|z| > 1$ of the argument $Q_\ell(z)$ is a one-valued function.

a somewhat different method. Indeed, the (nonrelativistic) Schrödinger equation can be solved exactly in a way adapted to the specific scattering situation at hand.⁷ With $k^2 = 2mE/\hbar^2$, $U(r) = ZZ'e^2/r$, and with the definition (2.20) for γ , the stationary Schrödinger equation (1.160) reads

$$\left(\Delta + k^2 - \frac{2\gamma k}{r}\right)\psi(\mathbf{x}) = 0. \quad (2.22)$$

This is solved using parabolic coordinates

$$\xi = \sqrt{r - x^3}, \quad \eta = \sqrt{r + x^3}, \quad \phi$$

and by means of the ansatz

$$\psi(\mathbf{x}) = c_\psi e^{ikx^3} f(r - x^3) = c_\psi e^{ik(\eta^2 - \xi^2)/2} f(\xi^2),$$

in which c_ψ is a complex number still to be determined. As before, the direction of the incoming, asymptotic momentum is taken to be the 3-direction. Since no other, perpendicular direction is singled out in the *in*-state and since the potential is spherically symmetric, the scattering amplitude does not depend on ϕ . Surprisingly, the differential equation (2.22) separates in these coordinates, too. The variable $\xi^2 = r - x^3$ is denoted by u , first and second derivatives with respect to that variable are written f' and f'' , respectively. Then, for $i = 1, 2$:

$$\begin{aligned} \frac{\partial \psi}{\partial x^i} &= e^{ikx^3} f'(u) \frac{\partial r}{\partial x^i} = e^{ikx^3} f'(u) \frac{x^i}{r}, \quad \frac{\partial^2 \psi}{\partial (x^i)^2} \\ &= e^{ikx^3} \left[f'' \frac{(x^i)^2}{r^2} + f' \left(\frac{1}{r} - \frac{(x^i)^2}{r^3} \right) \right]. \end{aligned}$$

The derivatives with respect to x^3 give

$$\begin{aligned} \frac{\partial \psi}{\partial x^3} &= e^{ikx^3} \left[ikf + f'(u) \left(\frac{x^3}{r} - 1 \right) \right], \quad \frac{\partial^2 \psi}{\partial (x^3)^2} \\ &= e^{ikx^3} \left[-k^2 f + 2ikf' \left(\frac{x^3}{r} - 1 \right) + f'' \left(\frac{x^3}{r} - 1 \right)^2 + f' \left(\frac{1}{r} - \frac{(x^3)^2}{r^3} \right) \right]. \end{aligned}$$

Inserting these formulae in (2.22) one obtains

$$\left(u \frac{d^2}{du^2} + (1 - iku) \frac{d}{du} - \gamma k \right) f(u) = 0.$$

This differential equation is again of Fuchsian type and appears to be very close to Kummer's equation (1.145). The identification becomes perfect if one replaces the variable u by the variable $v := iku$. Indeed, the differential equation then becomes

$$v \frac{d^2 f(v)}{dv^2} + (1 - v) \frac{df(v)}{dv} + i\gamma f(v) = 0.$$

⁷ This no longer holds true when the relativistic form of the wave equation is used.

The solution which is regular at $r = 0$ is

$$f(v) = c_\psi {}_1F_1(-i\gamma; 1; v) = c_\psi {}_1F_1[-i\gamma; 1; ik(r - x^3)].$$

The asymptotics of the confluent hypergeometric function is obtained from the formula (1.147),

$${}_1F_1 \sim \frac{1}{\Gamma(1 + i\gamma)} e^{\pi\gamma} [ik(r - x^3)]^{i\gamma} + \frac{1}{\Gamma(-i\gamma)} e^{ik(r - x^3)} [ik(r - x^3)]^{-i\gamma+1}.$$

Setting

$$i\gamma = e^{-\pi\gamma/2}$$

and choosing the coefficient c_ψ as follows

$$c_\psi = \Gamma(1 + i\gamma) e^{-\pi\gamma/2},$$

the solution ψ takes the asymptotic form postulated above

$$\psi \sim e^{i\{kx^3 + \gamma \ln[k(r - x^3)]\}} - \frac{\Gamma(1 + i\gamma)}{\Gamma(1 - i\gamma)} \frac{\gamma}{k(r - x^3)} e^{i\{kr - \gamma \ln[k(r - x^3)]\}}.$$

Inserting $r - x^3 = r(1 - \cos \theta) = 2r \sin^2(\theta/2)$ shows that this is the asymptotic decomposition, (2.21), into an incoming, but deformed plane wave, and an outgoing, deformed spherical wave. The complex Γ -function is written in terms of modulus and phase,

$$\Gamma(1 \pm i\gamma) = |\Gamma(1 + i\gamma)| e^{\pm i\sigma_C},$$

so that the scattering amplitude for the pure Coulomb potential is seen to be

$$f_C(\theta) = -\frac{\gamma}{2k \sin^2(\theta/2)} e^{i\{2\sigma_C - \gamma \ln[\sin^2(\theta/2)]\}}. \quad (2.23)$$

This amplitude contains a phase factor that depends on the scattering angle, and which is characteristic for the long range of the Coulomb potential. This phase factor drops out of the differential cross section (2.4) for which one obtains

$$\frac{d\sigma_{el}}{d\Omega} = \frac{\gamma^2}{4k^2} \frac{1}{\sin^4(\theta/2)} = \left(\frac{ZZ'e^2}{4E} \right)^2 \frac{1}{\sin^4(\theta/2)}, \quad (2.24)$$

where the definition (2.20) and $E = \hbar^2 k^2 / (2m)$ were used. The result (2.24) is called the *Rutherford cross section*. Note that it agrees with the corresponding expression of classical mechanics (cf. [Scheck (2010)], Sect. 1.27). This important formula was essential in analyzing the scattering experiments of α particles on nuclei, performed by Rutherford, Geiger, and Marsden from 1906 on. These experiments proved that nuclei are practically point-like as compared to typical radii of atoms.

Step 2: Consider now a spherically symmetric charge distribution which is no longer concentrated in a point but is localized in the sense that it lies inside a sphere with a given, finite radius R . One calculates the electrostatic potential by means of the formula (2.15) and notes that for values $r > R$ it coincides, either completely or to a very good approximation, with the pure Coulomb potential but deviates from it for values $r < R$. It should be clear immediately, in the light of the general discussion of

Sect. 2.3, that high partial waves are insensitive to these deviations. The information on the precise shape of the charge distribution is contained in the low and intermediate partial waves. This suggests to design the partial wave analysis for these cases such that it is not the force-free case but the Coulomb potential which is taken as the reference potential. This means that the phase shift analysis should be designed such as to yield the difference

$$\delta_\ell = \delta_{U(r)} - \delta_C$$

between the true phase and the Coulomb phase.

2.4 Born Series and Born Approximation

We emphasize again that the expansion in terms of partial waves is an *exact* method to calculate the cross section for spherically symmetric potentials which, in addition, has the advantage of making optimal use of the information about the range of the potential. In the case of potentials which are not spherically symmetric but may be expanded in terms of spherical harmonics the cross section can also be computed by expanding the scattering amplitude in partial waves. However, this method becomes technically complex and cumbersome, and loses much of the simplicity and transparency it has for spherically symmetric potentials.

The Born series that we describe in this section, does not have this disadvantage. It yields an exact, though formal, solution of the scattering problem by means of the technique of Green functions, and can equally well be applied to potentials with or without spherical symmetry. Its most stringent disadvantage is the fact that beyond first order it is not very practicable and becomes cumbersome. The first iteration, or *first Born approximation*, in turn, is easy to calculate and allows for simple and convincing physical interpretation, but it violates the optical theorem.

The starting point is again the stationary Schrödinger equation (1.160) in the form

$$(\Delta + k^2)\psi(\mathbf{x}) = \frac{2m}{\hbar^2}U(\mathbf{x})\psi(\mathbf{x}), \quad (2.25)$$

where $k^2 = 2mE/\hbar^2$. If one deals with a two-body problem the parameter m is the reduced mass; if one studies scattering of a single particle on a fixed external potential then m is just the mass of that particle.⁸ The differential equation (2.25) is solved by means of Green functions, i.e. of functions (more precisely: distributions) $G(\mathbf{x}, \mathbf{x}')$, which obey the differential equation

$$(\Delta + k^2)G(\mathbf{x}, \mathbf{x}') = \delta(\mathbf{x} - \mathbf{x}').$$

⁸ The latter case can also be viewed as the limit of the former in which the mass of the heavier partner is very large as compared to the one of the lighter partner.

The well-known relation

$$(\Delta + k^2) \frac{e^{\pm ik|z|}}{|z|} = -4\pi\delta(z)$$

shows that the general solution can be given in the form

$$G(\mathbf{x}, \mathbf{x}') = -\frac{1}{4\pi} \frac{1}{|\mathbf{x} - \mathbf{x}'|} \left[a e^{ik|\mathbf{x} - \mathbf{x}'|} + (1 - a) e^{-ik|\mathbf{x} - \mathbf{x}'|} \right].$$

Formally, the differential equation (2.25) then has the solution

$$\psi_{\mathbf{k}}(\mathbf{x}) = e^{i\mathbf{k} \cdot \mathbf{x}} + \frac{2m}{\hbar^2} \int d^3x' G(\mathbf{x}, \mathbf{x}') U(\mathbf{x}') \psi_{\mathbf{k}}(\mathbf{x}'). \quad (2.26)$$

It is formal because the differential equation (2.25) is replaced by an *integral equation* which contains the unknown wave functions both on the left-hand side and in the integrand of the right-hand side. Nevertheless, it has two essential advantages: The constant a in the Green function can be chosen such that the scattering solution fulfills the right boundary condition, which in our case is the Sommerfeld radiation condition (2.2). Furthermore, if the strength of the potential is small in some sense, this integral equation can be used as the starting basis for an iterative solution, i.e. an expansion of the scattering function around the force-free solution (the plane wave).

The correct asymptotics (2.2) is reached with the choice $a = 1$. This is seen as follows: Define $r := |\mathbf{x}|$, $r' := |\mathbf{x}'|$, and assume the potential $U(\mathbf{x}')$ to be localized. As r goes to infinity one has

$$r \gg r' : \quad |\mathbf{x} - \mathbf{x}'| = \sqrt{r^2 + r'^2 - 2\mathbf{x} \cdot \mathbf{x}'} \approx r - \frac{1}{r} \mathbf{x} \cdot \mathbf{x}'.$$

The scattering function takes the asymptotic form

$$r \rightarrow \infty : \quad \psi_{\mathbf{k}}(\mathbf{x}) \sim e^{i\mathbf{k} \cdot \mathbf{x}} - \frac{2m}{4\pi\hbar^2} \frac{e^{ikr}}{r} \int d^3x' e^{-ik'\mathbf{x}'} U(\mathbf{x}') \psi_{\mathbf{k}}(\mathbf{x}').$$

The reader will have noticed that we defined $k\mathbf{x}/r =: \mathbf{k}'$ in this expression. Indeed, the momentum of the scattered particle is $\hbar\mathbf{k}'$. It moves in the direction of $\mathbf{x}/r$ and, because the scattering is elastic, one has $|\mathbf{k}'| = |\mathbf{k}|$.

By the same token, this result yields a general formula for the scattering amplitude, viz.

$$\boxed{f(\theta, \phi) = -\frac{2m}{4\pi\hbar^2} \int d^3x e^{-i\mathbf{k}' \cdot \mathbf{x}} U(\mathbf{x}) \psi_{\mathbf{k}}(\mathbf{x})}. \quad (2.27)$$

(As this equation no longer contains the point of reference $\mathbf{x}$, the integration variable $\mathbf{x}'$ was renamed $\mathbf{x}$.)

This equation is an interesting result. If the potential has a strictly finite range we need to know the exact scattering function only in the domain where $U(\mathbf{x})$ is sizeably different from zero.⁹

⁹ An approximation which makes use of this fact and which is particularly useful for scattering at high energies, is provided by the *eikonal expansion*. The reader will find an extended description of this method in, e.g., [Scheck (2012)], Chap. 5, and illustrated by explicit examples.

If one knew the exact scattering solution this formula would yield the *exact* scattering amplitude. Although this ambitious goal cannot be reached, the formula serves as a basis for approximation methods which are relevant for various kinematic conditions. One of these is the *Born series* which is obtained from an iterating solution of the integral equation (2.26). The idea is simple: one imagines the potential as a perturbation of the force-free solution

$$\psi_{\mathbf{k}}^{(0)} = e^{i\mathbf{k} \cdot \mathbf{x}}$$

such that in a decomposition of the full wave function

$$\psi_{\mathbf{k}}(\mathbf{x}) = \sum_{n=0}^{\infty} \psi_{\mathbf{k}}^{(n)}(\mathbf{x})$$

the n -th term is obtained from the $(n-1)$ -st by means of the integral equation (2.26), i.e.

$$\psi_{\mathbf{k}}^{(n)}(\mathbf{x}) = -\frac{1}{4\pi} \frac{2m}{\hbar^2} \int d^3x' \frac{e^{ik|\mathbf{x}-\mathbf{x}'|}}{|\mathbf{x}-\mathbf{x}'|} U(\mathbf{x}') \psi_{\mathbf{k}}^{(n-1)}(\mathbf{x}'), \quad n \geq 1 \quad (2.28)$$

Even without touching the (difficult) question of its convergence, one realizes at once that this provides a method of representing the scattering amplitude as a series whose structure is very different from the expansion in terms of partial waves. While in the latter one expands in increasing values of ℓ , the former is an expansion in the strength of the potential.

2.4.1 First Born Approximation

It is primarily the first and simplest approximation which matters for practical applications. It consists in truncating the series (2.28) at $n = 1$. In this case the full scattering function in the integrand of the right-hand side of (2.27) is replaced by $\psi_{\mathbf{k}}^{(0)} = \exp(i\mathbf{k} \cdot \mathbf{x})$ so that one obtains

$$f^{(1)}(\theta, \phi) = -\frac{2m}{4\pi \hbar^2} \int d^3x e^{-i\mathbf{k}' \cdot \mathbf{x}} U(\mathbf{x}) e^{i\mathbf{k} \cdot \mathbf{x}}.$$

Introducing the momentum transfer

$$\mathbf{q} := \mathbf{k} - \mathbf{k}' \quad \text{with} \quad |\mathbf{k}| = |\mathbf{k}'| = k, \quad \hat{\mathbf{q}} = (\theta, \phi),$$

the *first Born approximation* for the scattering amplitude reads

$$f^{(1)}(\mathbf{q}) = -\frac{2m}{4\pi \hbar^2} \int d^3x e^{i\mathbf{q} \cdot \mathbf{x}} U(\mathbf{x}). \quad (2.29)$$

This formula tells us that in first Born approximation the scattering amplitude is the Fourier transform of the potential with respect to the variable $\mathbf{q}$.

The formula (2.29) simplifies further if the potential has spherical symmetry, $U(\mathbf{x}) \equiv U(r)$. One inserts the expansion (1.136) of $\exp(i\mathbf{q} \cdot \mathbf{x})$ in terms of spherical

harmonics and notes that by integrating over $d\Omega_x$ only the term with $\ell = 0$ survives. This follows from the fact that $Y_{00} = 1/\sqrt{4\pi}$ is a constant and that

$$\int d\Omega_x Y_{\ell m}(\hat{x}) = \sqrt{4\pi} \delta_{\ell 0} \delta_{m 0}.$$

Thus, one obtains the expression

$$f^{(1)}(\theta) = -\frac{2m}{\hbar^2} \int_0^\infty r^2 dr U(r) j_0(qr) \quad (2.30)$$

where

$$q \equiv |\mathbf{q}| = 2k \sin(\theta/2), \quad \text{and where} \quad j_0(u) = \frac{\sin u}{u}$$

is the spherical Bessel function with $\ell = 0$ (see Sect. 1.9.3). The functional dependence of the scattering amplitude could be written as $f(q)$, or, even more precisely, $f(q^2)$ because the result (2.30) shows that it depends only on the modulus of $\mathbf{q}$ and is invariant under the exchange $q \rightarrow -q$. As an alternative, one may express q by the scattering angle θ and write the scattering amplitude in the form

$$f^{(1)}(\theta) = -\frac{m}{\hbar^2 k \sin(\theta/2)} \int_0^\infty r dr U(r) \sin[2kr \sin(\theta/2)].$$

We illustrate this result by the following example.

Example 2.1

Let us return to the Yukawa potential (2.17),

$$U_Y(r) = g \frac{e^{-\mu r}}{r}, \quad \text{where} \quad \mu = \frac{1}{r_0}.$$

The following integral is obtained in an elementary way

$$\int_0^\infty dr e^{-\mu r} \sin(\alpha r) = \frac{\alpha}{\mu^2 + \alpha^2}.$$

With $\alpha = 2k \sin(\theta/2)$ the formula (2.30) yields

$$f_Y^{(1)}(\theta) = -\frac{2mg}{\hbar^2} \frac{1}{4k^2 \sin^2(\theta/2) + \mu^2}. \quad (2.31)$$

Two properties of the result (2.31) should be noticed

1. In the limit $\mu \rightarrow 0$ (though not allowed), and with $g = ZZ'e^2$ and $\hbar^2 k^2 = 2mE$, the amplitude becomes

$$f_C^{(1)}(\theta) = -\frac{ZZ'e^2}{4E} \frac{1}{\sin^2(\theta/2)}.$$

This is the scattering amplitude for the pure Coulomb potential, except for the phase factor in (2.23). Its absolute square gives the correct expression (2.24) of the differential cross section.

2. There is a well-known expansion of $1/(z-t)$ in terms of Legendre polynomials and Legendre functions of the second kind, (see [Gradshteyn and Ryzhik (1965)], Eq. 8.791.1)

$$\frac{1}{z-t} = \sum_{\ell=0}^{\infty} (2\ell+1) Q_{\ell}(z) P_{\ell}(t).$$

Write the amplitude (2.31) as

$$\begin{aligned} f_Y^{(1)}(\theta) &= -\frac{mg}{\hbar^2 k^2} \frac{1}{2\sin^2(\theta/2) + \mu^2/(2k^2)} \\ &= -\frac{mg}{\hbar^2 k^2} \frac{1}{1 + \mu^2/(2k^2) - \cos\theta}, \end{aligned}$$

set $1 + \mu^2/(2k^2) = z$ and $\cos\theta = t$. This yields

$$f_Y^{(1)}(\theta) = -\frac{mg}{\hbar^2 k^2} \sum_{\ell=0}^{\infty} Q_{\ell} \left(1 + \frac{\mu^2}{2k^2} \right) P_{\ell}(\cos\theta).$$

One now compares this with the general expansion in terms of partial waves (2.6) and notices that the coefficients of this series are

$$a_{\ell} = e^{i\delta_{\ell}} \sin \delta_{\ell} \approx \sin \delta_{\ell} = -\frac{mg}{\hbar^2 k} Q_{\ell} \left(1 + \frac{\mu^2}{2k^2} \right)$$

and that they agree with the example (2.19) in Sect. 2.3.1. Note that here and in that example, the scattering phases δ_{ℓ} are small.

Remark

The results (2.27) and (2.30) show that the scattering amplitude in first Born approximation is real, i.e. $\text{Im } f^{(1)} = 0$. This is in contradiction with the optical theorem. The first Born approximation does not respect the conservation of probability.

2.4.2 Form Factors in Elastic Scattering

The first Born approximation leads in a natural way to a new notion, called *form factor*, which is important for the analysis of scattering experiments. This section gives its definition and illustrates it by a few examples. The question and the idea are the following: Suppose a localized distribution $\varrho(\mathbf{x})$ of elementary scattering centers is given whose interaction with the projectile is known. If we know the scattering amplitude for the elementary process, i.e. for the scattering of the projectile off a single, isolated elementary scattering center, can we calculate the scattering amplitude off the *distribution* $\varrho(\mathbf{x})$?

The answer to this question is simple if the Born approximation is sufficiently accurate for the calculation of the scattering amplitudes. In this case, the amplitude

for the distribution is equal to the product of the elementary scattering amplitude and a function which depends only on the density $\varrho(\mathbf{x})$ and on the momentum transfer $\mathbf{q}$. We show this by means of an example:

Suppose the projectile is scattered by a number A of particles whose distribution in space is described by the density $\tilde{\varrho}(\mathbf{x}) = A\varrho(\mathbf{x})$. This is to say that

$$\int d^3x \tilde{\varrho}(\mathbf{x}) = A \quad \text{and} \quad \int d^3x \varrho(\mathbf{x}) = 1.$$

It is customary to normalize the density $\varrho(\mathbf{x})$ to 1, i.e. to take out an explicit factor A . Let the elementary interaction be described by the Yukawa potential (2.17). The potential created by all particles, with their density $\varrho(\mathbf{x})$, then is, using $\mu = 1/r_0$

$$U(\mathbf{x}) = gA \int d^3x' \frac{e^{-\mu|\mathbf{x}-\mathbf{x}'|}}{|\mathbf{x}-\mathbf{x}'|} \varrho(\mathbf{x}'). \quad (2.32)$$

It obeys the differential equation

$$(\Delta_x - \mu^2)U(\mathbf{x}) = -4\pi A\varrho(\mathbf{x}). \quad (2.33)$$

In first Born approximation the scattering amplitude $F^{(1)}$ describing scattering on the distribution $\varrho(\mathbf{x})$ is given by the formula (2.29), upon insertion of the potential (2.32). The exponential function is replaced by the identity

$$e^{i\mathbf{q}\cdot\mathbf{x}} = -\frac{1}{\mathbf{q}^2 + \mu^2}(\Delta_x - \mu^2)e^{i\mathbf{q}\cdot\mathbf{x}}.$$

The differential operator $(\Delta_x - \mu^2)$ is shifted to $U(\mathbf{x})$, by partially integrating twice, and the differential equation (2.33) replaces the potential by the density. One obtains the expression

$$F^{(1)}(\mathbf{q}) = A f_Y^{(1)}(\theta) \cdot F(\mathbf{q}) \quad (2.34)$$

for the scattering amplitude. The first factor is the elementary amplitude (2.31), the second factor is defined by

$$F(\mathbf{q}) = \int d^3x e^{i\mathbf{q}\cdot\mathbf{x}} \varrho(\mathbf{x}). \quad (2.35)$$

This factor which depends on the density $\varrho(\mathbf{x})$ and on the momentum transfer only, is called *form factor*. Its physical interpretation is clarified by its properties the most important of which are summarized here:

Properties of the Form Factor:

1. If it were possible to measure the form factor for *all* values of the momentum transfer then the density would be obtained by inverse Fourier transform,

$$\varrho(\mathbf{x}) = \frac{1}{(2\pi)^3} \int d^3q e^{-i\mathbf{q}\cdot\mathbf{x}} F(\mathbf{q})$$

The density $\varrho(\mathbf{x})$ describes a *composite* target such as, e.g., an atomic nucleus composed of A nucleons. If the interaction of the projectile with the individual particle in the target is known (in our example this is a nucleon), the form factor measures the spatial distribution of the target particles.

2. Scattering in the forward direction, $\mathbf{q} = \mathbf{0}$, tests the normalization

$$F(\mathbf{q} = \mathbf{0}) = 1.$$

If the target is point-like, i.e. has no spatial extension at all, the form factor equals 1 for *all* momentum transfers,

$$\varrho(\mathbf{x}) = \delta(\mathbf{x}) \longrightarrow F(\mathbf{q}) = 1 \quad \forall \mathbf{q}.$$

3. For a spherical density, $\varrho(\mathbf{x}) = \varrho(r)$ where $r := |\mathbf{x}|$, the formulae for the form factor simplify further. Like in the derivation of (2.30) one shows that the form factor only depends on q^2 ($q := |\mathbf{q}|$),

$$F(\mathbf{q}) \equiv F(q^2) = \frac{4\pi}{q} \int_0^\infty r dr \varrho(r) \sin(qr), \quad (2.36)$$

the density being given by the inversion of this formula:

$$\varrho(r) = \frac{4\pi}{(2\pi)^3 r} \int_0^\infty q dq F(q) \sin(qr).$$

Expanding (2.36) for small values of q , one has

$$F(q) \approx 4\pi \int_0^\infty r^2 dr \varrho(r) - \frac{4\pi}{6} q^2 \int_0^\infty r^2 dr r^2 \varrho(r) = 1 - \frac{1}{6} q^2 \langle r^2 \rangle.$$

The first term is independent of q and is equal to 1 (using the normalization as defined above). The second term contains the *mean square radius*

$$\langle r^2 \rangle := 4\pi \int_0^\infty r^2 dr r^2 \varrho(r), \quad (2.37)$$

which is characteristic for the given distribution $\varrho(\mathbf{x})$. If the density is not known, but the scattering amplitude and, hence, the form factor, are measured for small values of q , the mean square radius is obtained from the first derivative of the form factor by q^2 ,

$$\langle r^2 \rangle = -6 \frac{dF(q^2)}{dq^2}. \quad (2.38)$$

That is to say, in order to obtain the root-mean-square radius one plots the form factor as a function of q^2 , reads off the slope at the origin, and multiplies by (-6) .

Example 2.2

The following density is normalized to 1,

$$\varrho(r) = \frac{1}{\pi^{3/2} r_0^3} e^{-r^2/r_0^2}, \quad 4\pi \int_0^\infty r^2 dr \varrho(r) = 1.$$

It is easy to verify that it leads to the form factor

$$F(q^2) = e^{-q^2 r_0^2/4}.$$

The mean square radius is found to be

$$\langle r^2 \rangle = \frac{3}{2} r_0^2,$$

so that the form factor and the density can be written equivalently as

$$F(q^2) = e^{-(1/6)\langle r^2 \rangle q^2}, \quad \text{and} \quad \varrho(r) = \frac{3\sqrt{6}}{4} \frac{1}{(\pi \langle r^2 \rangle)^{3/2}} e^{-(3/2)r^2/\langle r^2 \rangle}$$

respectively.

This example is more than an academic one. Indeed, to a good approximation, the function $\varrho(r)$ describes the distribution of electric charge in the interior of a proton, with

$$\langle r^2 \rangle_{\text{Proton}} = (0.86 \times 10^{-15} \text{ m})^2$$

as a typical value for the mean square radius as obtained from electron scattering on protons.

Remarks

1. Although the definition of the form factor is based on Born approximation it has a more general significance. When the potential becomes too strong for Born approximation to be applicable, this will be felt in a deformation of the partial waves (in comparison to the force-free case) which is the stronger the smaller ℓ is. Nevertheless, the information on the distribution of the scattering centers that is contained in the scattering amplitude, is not modified in any essential way. Thus, there are methods which allow to isolate this effect and to define an effective Born approximation which enables one to draw conclusions on the density $\varrho(\mathbf{x})$ from the form factor (2.35).
2. The case of the Coulomb potential which is of infinite range must be treated with special care. Although this is mathematically not correct, we let the parameter μ in the formulae for the Yukawa potential tend to zero. This limit gives the correct scattering amplitude, except for the characteristic logarithmic phases, and, hence, the correct differential cross section. This cross section then takes the form

$$\frac{d\sigma}{d\theta} = \left(\frac{d\sigma}{d\theta} \right)_{\text{point}} F^2(\mathbf{q}), \quad (2.39)$$

the first factor being the cross section for a point-like target, i.e.

$$\left(\frac{d\sigma}{d\theta} \right)_{\text{point}} = \left(\frac{ZZ'e^2}{4E} \right)^2 \frac{1}{\sin^4(\theta/2)},$$

while $F(\mathbf{q})$ is the electric form factor (2.35) of the target. The density $\varrho(\mathbf{x})$ now is the charge density and is normalized to 1 provided the total charge $Q = Ze$ is factored.

Example 2.3

Assume the charge distribution of an atomic nucleus to be given by the homogeneous density

$$\varrho(r) = \frac{3}{4\pi r_0^3} \Theta(r_0 - r).$$

Equation (2.36), by elementary integration, yields the form factor

$$F(q^2) = \frac{3}{(qr_0)^3} [\sin(qr_0) - (qr_0) \cos(qr_0)] = \frac{3}{(qr_0)} j_1(qr_0),$$

where $j_1(z)$ is the spherical Bessel function with $\ell = 1$, cf. Sect. 1.9.3. This function has zeroes at the points

$$z_1 = 4.493, \quad z_2 = 7.725, \quad z_3 = 10.904, \dots$$

While the cross section for the point charge has no zeroes, the cross section for scattering on a homogeneous charge density has zeroes at the values of the product $qr_0 = 2kr_0 \sin(\theta/2)$ given above. These are artifacts of Born approximation. Yet, they are not unphysical: An exact calculation of the cross section will differ from Born approximation only by the varying deformation of individual partial waves. As a result, the zeroes are “smeared out”, that is, they are replaced by minima of the cross section which are less pronounced than the zeroes of Born approximation and are shifted slightly as compared to those. These minima are called *diffraction minima*, they contain essentially the same physical information as the zeroes obtained in first Born approximation.

2.5 *Analytical Properties of Partial Wave Amplitudes

Up to this point all important concepts of scattering theory were introduced. As far as *observables* are concerned these were carried over from classical to quantum mechanics, all other concepts were new. In particular, we developed some practical methods for calculating scattering amplitudes and cross sections.

Quantum theoretic scattering theory has a number of further aspects which need more comprehensive analysis and which become important in various applications. Among them we list the following

1. Generalization to the case where, besides elastic scattering, also scattering into inelastic channels is possible.
2. The more general expression of the optical theorem announced above, and its relation to the conservation of probability.
3. A formal, operator theoretic description of potential scattering which makes extensive use of the theory of integral equations.
4. A more detailed description of scattering on composite targets, i.e. the calculation of the scattering amplitude for a target composed of elementary constituents, from the amplitude for the individual scattering centers.

5. The analysis of scattering processes, by means of Heisenberg's scattering matrix, in which the projectiles may have relativistic velocities and where the dynamics and the kinematics allow for creation or annihilation of particles.
6. The analytical properties of scattering amplitudes and their consequences for the physics of scattering.

Some of these subjects will be taken up later when the concepts and methods will be ready that are needed to treat them. At this stage I sketch one of these topics which gives a good impression for the richness of quantum scattering theory: the analytic properties of scattering amplitudes for definite values of the angular momentum ℓ (i.e. item 6 on our list). This section which makes use of some function theory, is slightly more difficult than the previous ones and this is why it is marked by an asterisk. This also means that there is no harm if one decides to skip it in a first reading.

The starting point is the differential equation (2.8) for the radial function $u_\ell(r)$. We repeat it here, for the sake of convenience:

$$u_\ell''(r) - \left(\frac{\ell(\ell+1)}{r^2} + \frac{2m}{\hbar^2} U(r) - k^2 \right) u_\ell(r) = 0, \quad k^2 = \frac{2mE}{\hbar^2}. \quad (2.40)$$

As this equation is homogeneous we can normalize the solution which is regular at $r = 0$ such that

$$u_\ell(r) = r^{\ell+1} f_\ell(r) \quad \text{with} \quad f_\ell(r=0) = 1,$$

that is, we take out the centrifugal tail and put the remainder to 1 at the origin.

2.5.1 Jost Functions

In this section we study the analytic properties of the wave function, of the scattering phase δ_ℓ , and of the scattering amplitude, as functions of k^2 , taken as a variable in the complex plane. What do we know about the differential equation (2.40)? It is of Fuchsian type, (1.113). The regular solution is free of the singularities that the coefficients of (1.113) have at $r = 0$. As is obvious, the coefficients are analytic functions of the complex variable k^2 . The boundary conditions imposed on u_ℓ (the condition at $r = 0$ and the asymptotics for $r \rightarrow \infty$) are analytic as well. One can then show that the solutions are analytic functions of k^2 . Hence, we write $u_\ell(r) \equiv u_\ell(r, k^2)$, in order to emphasize this property, and formulate their asymptotic behaviour as follows,

$$r \rightarrow \infty : \quad u_\ell(r, k^2) \sim \varphi_\ell^{(-)}(k^2) e^{ikr} + \varphi_\ell^{(+)}(k^2) e^{-ikr}. \quad (2.41)$$

The functions $\varphi_\ell^{(\pm)}(k^2)$ are called *Jost functions*.¹⁰ Comparison to the asymptotic formula (2.9),

$$u_\ell \sim \frac{1}{2i} [e^{i(-\ell\pi/2 + \delta_\ell)} e^{ikr} - e^{i(\ell\pi/2 - \delta_\ell)} e^{-ikr}]$$

¹⁰ After Res Jost (1918–1990), who developed the mathematical foundations of scattering theory in a series of important publications.

yields the relation of the scattering phase to the Jost functions

$$S_\ell(k^2) := e^{2i\delta_\ell} = (-)^{\ell+1} - \frac{\varphi_\ell^{(-)}(k^2)}{\varphi_\ell^{(+)}(k^2)}. \quad (2.42)$$

In a physical scattering process, i.e. for real k , the definition (2.41) implies that the Jost functions are complex conjugates of each other. Indeed, with a real potential the radial function $u_\ell(r, k^2)$ is real and, hence,

$$\varphi_\ell^{(+)}(k^2) = [\varphi_\ell^{(-)}(k^2)]^* \quad (k \text{ real}).$$

One of the reasons why these functions are important is the fact that one can derive and understand the analytic properties of the function $S_\ell(k^2)$ (just defined) and of the partial wave amplitude $a_\ell(k^2)$ from the Jost functions. The following remarks and examples may serve to illustrate this statement.

When the energy is negative, E , then also $k^2 < 0$ and $k = i\kappa$, with real κ , is pure imaginary. The asymptotic form (2.41) then has a term that decreases exponentially, and a term that grows exponentially. There will be a bound state with energy $E = E_n < 0$ if the wave function is square integrable, i.e. if the second term is absent. This means that

$$\varphi^{(+)}\left(k^2 = -\frac{2m|E_n|}{\hbar^2}\right) = 0 \quad (k = i\kappa \text{ pure imaginary}).$$

As a consequence the function $S_\ell(k^2)$ defined in (2.42) has a *pole* at this point. A more detailed analysis of the singularities of the partial wave amplitude a_ℓ will show where this pole is situated.

2.5.2 Dynamic and Kinematic Cuts

Here and below we analyze partial wave amplitudes which already contain the factor $1/k$ of the expansion (2.6), i.e we write

$$f(k, \theta) = \sum_{\ell=0}^{\infty} (2\ell+1) f_\ell(k) P_\ell(\cos \theta) \quad \text{with} \quad f_\ell := \frac{1}{k} a_\ell,$$

a_ℓ being defined by (2.11). The amplitude f_ℓ is studied both as a function of k^2 and of k . The convention is that k as a square root of k^2 is always chosen such that it has *positive* imaginary part. Furthermore, the potential in (2.40) is assumed to be the bare Yukawa potential (2.17). As $u_\ell(r, k^2)$ is analytic, $f_\ell(k^2)$ is analytic as long as one stays clear of the negative real half-axis of k^2 .

Note that the asymptotic form (2.41) holds under the assumption that the two first terms in the parentheses of (2.40) (centrifugal and true potentials) are negligible against k^2 . If $k^2 = -\kappa^2$, i.e. is negative real, the first term in (2.41) decreases like $e^{-\kappa r}$. If it does so more rapidly than this, one can no longer neglect the potential which decreases like e^{-r/r_0} . Therefore, it seems plausible that the Jost function $\varphi_\ell^{(-)}(k^2)$ is no longer defined. Indeed, one can show that this function has a singularity at

$k_c^2 = -\kappa_c^2 = -1/(4r_0^2)$ and is not defined below this point, $k^2 < k_c^2$. Qualitatively speaking, the value κ_c is the point where the exponentially growing part, when multiplied by the term e^{-r/r_0} of the potential, equals the exponentially decreasing term,

$$e^{(\kappa_c - 1/r_0)r} = e^{-\kappa_c r}.$$

The interval $[-\infty, -1/(4r_0^2)]$ of the negative real half-axis in the complex k^2 -plane is called *left cut*, or *dynamical cut*.

Let us analyze the dynamical cut by means of first Born approximation. We showed in Sect. 2.4.1 that the amplitude which belongs to the angular momentum ℓ , in first Born approximation, is given by

$$f_\ell(k^2) \equiv \frac{a_\ell}{k} = -\frac{mg}{\hbar^2 k^2} Q_\ell \left(1 + \frac{1}{2(kr_0)^2} \right).$$

The Legendre function of the second kind $Q_\ell(z)$ is known to be an analytic function of z if the complex plane is cut from -1 to $+1$ along the real axis. It is singular on the cut $[-1, +1]$. As a matter of illustration, we quote the first three Legendre functions of the second kind,

$$\begin{aligned} Q_0(z) &= \frac{1}{2} \ln \left(\frac{z+1}{z-1} \right), & Q_1(z) &= \frac{z}{2} \ln \left(\frac{z+1}{z-1} \right) - 1, \\ Q_2(z) &= \frac{3z^2 - 1}{4} \ln \left(\frac{z+1}{z-1} \right) - \frac{3z}{2}, \end{aligned}$$

whose singularity structure is evident.

The point -1 corresponds to $k^2 = k_c^2 = -1/(2r_0)^2$, while the point $+1$ corresponds to the infinity in the k^2 -plane that we choose to lie at $-\infty$. This shows that the amplitude $f_\ell(k^2)$, in first Born approximation, already exhibits the left cut. The position of this cut depends on r_0 and, hence, on the range of the potential.

It is not difficult to compute the discontinuity of $f_\ell(k^2)$ across the cut $[-1, +1]$. In Sect. 2.4.1, Example 2.1, we quoted the expansion

$$\frac{1}{z-t} = \sum_{\ell'=0}^{\infty} (2\ell'+1) Q_{\ell'}(z) P_{\ell'}(t) = \sum_{\ell'=0}^{\infty} \sqrt{4\pi(2\ell'+1)} Q_{\ell'}(z) Y_{\ell'0}(\theta, \phi)$$

with $t = \cos \theta$. This equation can be solved for Q_ℓ by multiplying with $Y_{\ell m}^*(\theta, \phi)$, and integrating over the entire solid angle. Making use of the orthogonality of the spherical harmonics, we have

$$Q_\ell(z) = \frac{1}{\sqrt{4\pi(2\ell+1)}} \int d\Omega \frac{1}{z - \cos \theta} Y_{\ell 0}(\theta, \phi) = \frac{1}{2} \int_{-1}^{+1} dt \frac{P_\ell(t)}{z-t}.$$

The discontinuity then follows from

$$f_\ell(k^2 + i\varepsilon) - f_\ell(k^2 - i\varepsilon) = -\frac{mg}{\hbar^2 k^2} [Q_\ell(z + i\varepsilon) - Q_\ell(z - i\varepsilon)]$$

and the formula

$$\frac{1}{w \pm i\varepsilon} = \mathcal{P} \frac{1}{w} \mp i\pi \delta(w) \quad (2.43)$$

with $w = z - t$ and, as before, $z = 1 - 1/(2(kr_0)^2)$. The formula refers to the evaluation of integrals along the real axis. The pole at $w = 0$ of the left-hand side is shifted to the upper or to the lower half-plane, respectively. The right-hand side contains the principal value¹¹ and Dirac's δ -distribution. Inserting this formula into the expression for the discontinuity, the contribution of the principal value cancels out and one obtains

$$f_\ell(k^2 + i\varepsilon) - f_\ell(k^2 - i\varepsilon) = i\pi \frac{mg}{\hbar^2 k^2} P_\ell \left(1 + \frac{1}{2(kr_0)^2} \right).$$

As a result we note that the *position* of the left cut is determined by the *range*, its *discontinuity* by the *strength* g of the potential. This is the reason why this cut is called dynamical cut.

The partial wave amplitude f_ℓ exhibits yet another cut whose nature is purely kinematical. This is the reason it is called *kinematic cut*. In order to show this we return to the Jost functions and study them both in the complex k^2 -plane and in the complex k -plane.

The asymptotic expansion (2.41) is not defined in the point $k^2 = 0$. Physically speaking, the reason is that at this point the centrifugal term and the potential cannot be neglected as compared to k^2 . Let $z := k^2 = re^{i\alpha}$ with r very small, α positive and small, too. After a complete rotation about the origin this becomes $z \mapsto z' = re^{i(\alpha+2\pi)}$, while its square root becomes $k = \sqrt{z} \mapsto k' = -k$. At the same time the two Jost functions, taken as functions of k , exchange their roles,

$$\varphi_\ell^{(+)}(k) = \varphi_\ell^{(-)}(-k).$$

It follows from this observation that the point $k^2 = 0$ is a two-sheeted branch point (one also says a branch point of order 1). Let us investigate in somewhat more detail this singularity and the Riemann surface that is related to it. To do so we define

$$\phi_\ell(k) := \varphi_\ell^{(-)}(k^2).$$

This function is analytic in the upper half-plane $\text{Im } k > 0$, cut along the interval $[i/(2r_0), +i\infty]$ of the imaginary axis. If k is replaced by $-k$, the solution $u_\ell(r, k^2)$ remains unchanged. However, the two exponential functions in its asymptotic expansion (2.41) are interchanged. From this follows an important relation for the Jost functions,

$$\phi_\ell(k) = \phi_\ell(-k)$$

which shows that the analytic continuation of $\phi_\ell(k)$ to the lower half-plane $\text{Im } k < 0$ is precisely the function $\varphi_\ell^{(+)}(k^2)$. This function has no other singularities in that half-plane.

¹¹ As a reminder: The principal value is half the sum of the integrals for which the integration path is deformed once above, once below the point 0.

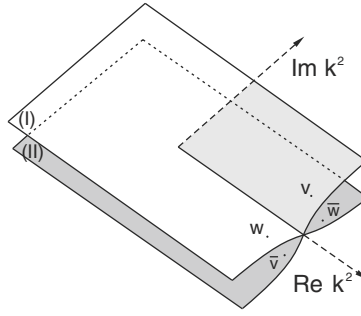


Fig.2.2 Because of the kinematic cut the origin of the complex k^2 -plane is a branch point of order 1. The scattering amplitude with fixed ℓ is defined on a two-sheet Riemann surface. The physical and the unphysical sheets are denoted by (I) and (II), respectively

We conclude that the manifold of the k^2 is a two-sheeted Riemann surface whose sheets, for fixed k^2 , are distinguished by the two values of k . This surface is sketched in Fig.2.2. The two sheets are tangent to each other along the positive real axis. In scattering theory the customary nomenclature is the following:

Sheet (I) with $\text{Im } k > 0$ is called the *physical sheet*, sheet (II) with $\text{Im } k < 0$ is the *unphysical sheet*.

2.5.3 Partial Wave Amplitudes as Analytic Functions

The formula (2.11) for the partial wave amplitude, upon insertion of the definition (2.42), gives the scattering amplitude in terms of the S -matrix,

$$f_\ell(k^2) = \frac{a_\ell}{k} = \frac{1}{2ik} [S_\ell(k^2) - 1].$$

Thus, $f_\ell(k^2)$ is seen to be a function of the two Jost functions. Therefore, the analytic properties of $f_\ell(k^2)$ can be deduced from the analytic properties of the Jost functions. By convention and for the sake of clarity let us denote the function (2.42) by $S_\ell(k^2)$ on the first, physical sheet, and by $\bar{S}_\ell(k^2)$ its continuation to the second, unphysical sheet. Consider a point v on the physical sheet (i.e. the square root of $k^2 + i\eta$),

$$z = k^2 + i\eta \equiv r e^{i\alpha}, \quad v = \sqrt{z} = \sqrt{r} e^{i\alpha/2},$$

and its neighbour $\bar{v} = \sqrt{z^*} = \sqrt{r} e^{-i\alpha/2}$ (square root of $k^2 - i\eta$) on the unphysical sheet. The other square root of z , $\bar{w} = -v$, lies on the unphysical sheet, while the other root of z^* , $w = -\bar{v}$, lies on the physical sheet. The four points $\{v, \bar{v}, w, \bar{w}\}$ are shown in Fig.2.2 on the Riemann surface of complex k^2 , and in Fig.2.3 in the complex k -plane.

The function (2.42), taken on the unphysical sheet, is given by

$$\bar{S}_\ell(k^2) = (-)^{\ell+1} \frac{\varphi_\ell^{(-)}(-k)}{\varphi_\ell^{(+)}(-k)} = (-)^{\ell+1} \frac{\varphi_\ell^{(+)}(k)}{\varphi_\ell^{(-)}(k)} = \frac{1}{S_\ell(k^2)}. \quad (2.44)$$

This relation provides the key for analytic continuation of the amplitude f_ℓ from the physical to the unphysical sheet. Indeed, the amplitude on the second sheet is

$$\bar{f}_\ell(k^2) = \frac{1}{2ik} [\bar{S}_\ell(k^2) - 1] = \frac{1}{2ik} \left(\frac{1}{S_\ell} - 1 \right) = \frac{f_\ell(k^2)}{1 + 2ikf_\ell(k^2)}.$$

Thus, $\bar{f}_\ell(k^2)$ is expressed in terms of the same amplitude on the first sheet. (Note that a first minus sign in the transformation is compensated by another minus sign: in performing the analytic continuation the factor $1/k$ goes over into $\bar{k} = -k$.) This analysis shows, in particular, that f_ℓ has the left cut $[-\infty, -1/(2r_0)^2]$ both on the first and on the second sheets.

2.5.4 Resonances

We know from Sect. 2.5.1 that poles on the negative real half-axis in the complex k^2 -plane correspond to genuine bound states. We now want to show that poles that appear on the second, unphysical sheet play a physical role, too.

In a first step we show that the function $S_\ell(k^2)$ (studied both in the first *and* the second sheets) takes complex conjugate values for complex conjugate arguments k^2 , i.e. that

$$S_\ell[(k^2)^*] = [S_\ell(k^2)]^*. \quad (2.45)$$

The differential equation (2.40) has real coefficients. Hence, its solutions obey the relation

$$u_\ell(r, k^2) = \{u_\ell[r, (k^2)^*]\}^*.$$

The left-hand side has the asymptotic behaviour (2.41). If $v = \sqrt{k^2 + i\eta}$ is the root of k^2 then the root of $(k^2)^*$ (which also lies in the first sheet) equals $w = -\bar{v} = -v^*$. Therefore, the asymptotics of the right-hand side is

$$r \rightarrow \infty : u_\ell[r, (k^2)^*] \sim \varphi_\ell^{(-)}[(k^2)^*] e^{-ik^*r} + \varphi_\ell^{(+)}[(k^2)^*] e^{ik^*r}.$$

Comparing this to the complex conjugate of (2.41) yields

$$\varphi_\ell^{(\pm)}[(k^2)^*] = [\varphi_\ell^{(\pm)}(k^2)]^*,$$

so that the assertion (2.45) holds true. For any pair of two points in the first or the second sheet whose positions are symmetric with respect to the real axis, the function S_ℓ takes complex conjugate values.

Suppose the function $\bar{S}_\ell(k^2)$ has a first-order pole in

$$\bar{v}, \quad \text{positive square root of } k^2 = k_0^2 - i\Gamma/2,$$

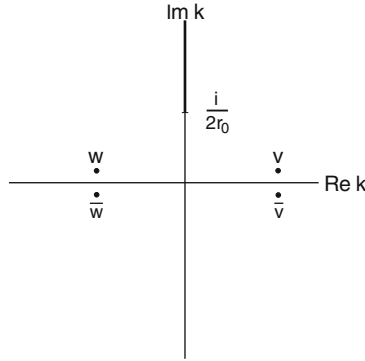


Fig. 2.3 The function $\phi_\ell(k) = \varphi_\ell^{(-)}(k^2)$ is analytic in the cut k -plane. The points marked here are the same as in Fig. 2.2

where k_0 and Γ are real. By the symmetry (2.45) it then has also a pole in

$$\bar{w}, \quad \text{negative square root of } k^2 = k_0^2 + i\Gamma/2;$$

both of which lie in the second sheet. The relation (2.44) implies that $S_\ell(k^2)$ has zeroes in the points v and w of the *first* sheet, see Fig. 2.3. If one approaches the point k_0 of the real, positive axis from above, it is clear that the variation of S_ℓ , as a function of k^2 , is dominated by the pole in $\bar{v}$ and by the zero in v . Thus, in the neighbourhood of k_0 one can write

$$S_\ell(k^2) = \frac{k^2 - k_0^2 - i\Gamma/2}{k^2 - k_0^2 + i\Gamma/2} S_\ell^{(\text{n.r.})}(k^2)$$

where the “nonresonant” function $S_\ell^{(\text{n.r.})}$ is slowly varying. The factor $(k^2 - k_0^2 - i\Gamma/2)/(k^2 - k_0^2 + i\Gamma/2)$ is a pure phase factor. As the product has the form indicated in (2.42), the second factor must also be a pure phase. Thus, both factors can be written as follows

$$\frac{k^2 - k_0^2 - i\Gamma/2}{k^2 - k_0^2 + i\Gamma/2} = e^{2i\delta_\ell^{(\text{res})}}, \quad S_\ell^{(\text{n.r.})} = e^{2i\delta_\ell^{(\text{n.r.})}},$$

where the “resonant” phase is given by

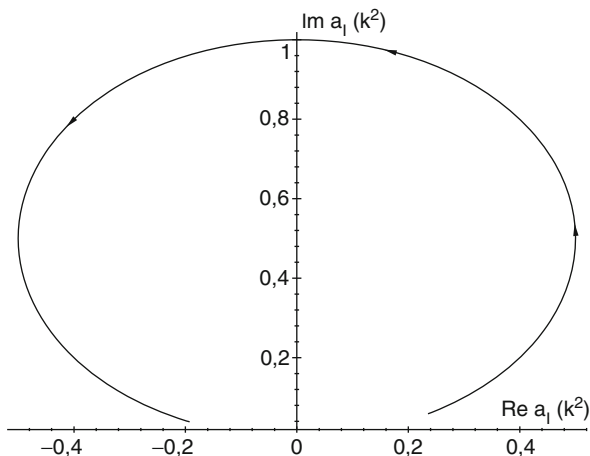
$$\delta_\ell^{(\text{res})} = \arctan\left(\frac{\Gamma/2}{k_0^2 - k^2}\right). \quad (2.46)$$

The other phase, $\delta_\ell^{(\text{n.r.})}$, is a parametrization of the nonresonant amplitude, and is a slowly varying function of k^2 . Inserting this in (2.11) the partial wave amplitude is

$$f_\ell(k) = \frac{1}{k} e^{i(\delta_\ell^{(\text{res})} + \delta_\ell^{(\text{n.r.})})} \sin(\delta_\ell^{(\text{res})} + \delta_\ell^{(\text{n.r.})}). \quad (2.47)$$

It is not difficult to interpret these results. Suppose first that the nonresonant phase is negligibly small as compared to the resonant phase. If we let k^2 run through an

Fig. 2.4 With increasing k^2 the amplitude $a_\ell = kf_\ell$ runs along a curve in the complex plane that crosses the point $(0, i)$ for $k^2 = k_0^2$. In the example shown here, we chose $k_0^2 = 10$, $\Gamma = 4$ (in arbitrary units)



interval I on the real axis that includes the point k_0^2 , the phase $\delta_\ell^{(\text{res})}$ runs from nearly zero to values close to π , while at $k^2 = k_0^2$ it takes the value $\pi/2$. The amplitude

$$f_\ell(k^2) \approx f_\ell^{(\text{res})} = \frac{1}{k} e^{i\delta_\ell^{(\text{res})}} \sin \delta_\ell^{(\text{res})} = -\frac{1}{k} \frac{\Gamma/2}{k^2 - k_0^2 + i\Gamma/2}$$

runs through the curve sketched in Fig. 2.4, in the complex plane for f_ℓ . For $k^2 = k_0^2$ it is pure imaginary and has the value i/k . The special role of this point becomes clear if we note that the cross section (2.7) for a partial wave ℓ ,

$$\sigma_\ell(k^2) = 4\pi(2\ell + 1) |f_\ell(k^2)|^2 = \frac{4\pi(2\ell + 1)}{k^2} \frac{\Gamma^2/4}{(k^2 - k_0^2)^2 + \Gamma^2/4}$$

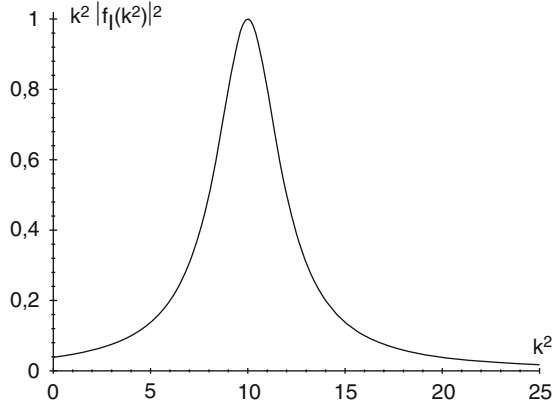
is proportional to $|a_\ell^{(\text{res})}(k^2)|^2$, and if we plot this quantity over k^2 in the interval I . Indeed, Fig. 2.5 shows that this function has a sharp maximum at the point $k^2 = k_0^2$. For $k^2 = k_0^2 \pm \Gamma/2$ it takes half the value of the maximum. A graph of this type is called Breit–Wigner curve, or Lorentz curve.

The pole at $(k_0^2, i\Gamma/2)$ leads to a resonance in the partial wave cross section σ_ℓ , the quantity Γ is the width of the resonance. It is not difficult to find out qualitatively how these results change when the nonresonant phase is not small, or when the contributions of other partial waves $\ell' \neq \ell$ to the cross section (2.7) are not negligible. I just mention in passing that there are methods which allow to reconstruct the individual partial wave amplitudes from experimental data and thereby to check whether one of these exhibits a resonance of this type at some value k_0^2 in the physical range. Like bound states, resonances contain physical information on the potential.

2.5.5 Scattering Length and Effective Range

This section is devoted to a discussion of two notions of special importance for scattering at very low energies: the *scattering length* and the *effective range*.

Fig. 2.5 Resonance curve of $|a_\ell|^2 = k^2 |f_\ell|^2$ as a function of k^2 . The parameters are chosen as in Fig. 2.4, i.e. $k_0^2 = 10$, $\Gamma = 4$



With decreasing energy the modulus k of the momentum tends to zero. With some more mathematics one can show rigorously that when $k \rightarrow 0$, the amplitude a_ℓ , (2.11), tends to zero like $k^{2\ell+1}$. I skip the proof of this result but give a plausibility argument based on the formula (2.19) for $\sin \delta_\ell$ and on simple dimensional analysis. The potential $U(r)$, as well as the kinetic energy $\hbar^2 k^2 / (2m)$ have dimension [energy]. The left-hand side of (2.19) being dimensionless, this must also be true for its right-hand side which can be written in terms of the ratio of potential to kinetic energy, viz.

$$\int_0^\infty (kr) d(kr) u_\ell(r) j_\ell(kr) \frac{U(r)}{\hbar^2 k^2 / (2m)}.$$

We already know that for

$$r \rightarrow 0 : \quad u_\ell(r) \sim r^{\ell+1}, \quad j_\ell(kr) \sim (kr)^\ell,$$

and, of course, that the product (kr) carries no dimension. Thus, in order to balance physical dimensions, u_ℓ must behave like $(kr)^{\ell+1}$. This shows that the integral goes to zero for $k \rightarrow 0$. More specifically, for small k , it is proportional to $k^{2\ell+1}$. If this is so then, as k tends to zero,

$$k \rightarrow 0 : \quad f_\ell = \frac{1}{k} e^{i\delta_\ell} \sin \delta_\ell \approx \frac{1}{k} \sin \delta_\ell \approx \frac{1}{k} \delta_\ell \sim k^{2\ell}.$$

This consideration shows that it is meaningful to define the limit

$$\lim_{k \rightarrow 0} \left(\frac{f_\ell(k)}{k^{2\ell}} \right) = \lim_{k \rightarrow 0} \left(\frac{\delta_\ell(k)}{k^{2\ell+1}} \right) =: a^{(\ell)}. \quad (2.48)$$

The quantities $a^{(\ell)}$ determine the cross section at the threshold, i.e. at very small positive energy. They are called *scattering lengths*. This nomenclature is somewhat inaccurate because only $a^{(\ell=0)}$ really has the dimension of a length L . For $\ell = 1$ the amplitude $a^{(1)}$ is a volume, the more general $a^{(\ell)}$ has dimension $L^{2\ell+1}$.

The expansion in small values of k can be pushed one step further. For this purpose define the function

$$R_\ell(k) := \frac{1 + ikf_\ell(k)}{f_\ell(k)} = k \frac{1 + ie^{i\delta_\ell} \sin \delta^{(\ell)}}{e^{i\delta_\ell} \sin \delta_\ell} = k \cot \delta_\ell.$$

The analytical properties of this function, when understood as a function of the complex variable k , are derived from those of the amplitude f_ℓ . For our discussion the most relevant feature is that the function $R_\ell(k)$, in contrast to $f_\ell(k)$, does *not* have the right, or kinematic, cut. This is shown as follows. Starting from the specific form (2.11) of the amplitude one sees that

$$\frac{1}{f_\ell^*(k)} - \frac{1}{f_\ell(k)} = k \frac{e^{i\delta} - e^{-i\delta}}{\sin \delta} = 2ik.$$

Thus, if one calculates the discontinuity of R_ℓ one finds that it vanishes,

$$R_\ell^*(k) - R_\ell(k) = \left(\frac{1 - ikf_\ell^*(k)}{f_\ell^*(k)} - \frac{1 + ikf_\ell(k)}{f_\ell(k)} \right) = k(2i - 2i) = 0,$$

the discontinuity of $1/f_\ell$ (which is not zero) is cancelled.

With $k \rightarrow 0$, $R_\ell(k)$ behaves like $k^{-2\ell}$. From this fact and the fact that R_ℓ has no cut on the real positive axis one concludes that the product $r^{2\ell} R_\ell(k)$ can be expanded around the origin,

$$k^{2\ell} R_\ell(k) = k^{2\ell+1} \cot \delta_\ell(k) = \frac{1}{a^{(\ell)}} + \frac{1}{2} r_0^{(\ell)} k^2 + \mathcal{O}(k^3). \quad (2.49)$$

The first term contains the scattering length defined in (2.48). The second term contains the new parameter $r_0^{(\ell)}$, called *effective range*. (Note that $r_0^{(\ell)}$ has physical dimension [length] only for s -waves.)

The formula (2.49) is a good approximation for sufficiently low values of k . The following example serves to illustrate these concepts and their usefulness at low energies.

Example 2.4

We consider s -wave scattering in an attractive square-well potential, $U(r) = -U_0 \Theta(R - r)$, in which case (2.40) reduces to

$$u''(r) + \left(k^2 + \frac{2m}{\hbar^2} U_0 \Theta(R - r) \right) u(r) = 0.$$

The index $\ell = 0$ is dropped, for convenience. In the outside domain, $r > R$, the relation between wave number and energy is, as before, $k^2 = 2mE/\hbar^2$. Inside the radius R we define

$$\kappa^2 := k^2 + K^2 \quad \text{where} \quad K^2 := \frac{2mU_0}{\hbar^2}.$$

The inner solution which is regular at $r = 0$, is seen to be $u^{(i)}(r) = \sin(\kappa r)$. For the outer solution we write $u^{(o)}(r) = \sin(kr + \delta)$, with δ still to be determined.

The requirement that the wave function and its first derivative be continuous at $r = R$,

$$\left. \frac{u^{(i)'}}{u^{(i)}} \right|_{r=R} = \left. \frac{u^{(o)'}}{u^{(o)}} \right|_{r=R} \quad (2.50)$$

yields the condition

$$k \cot \delta = \frac{\kappa + k \tan(kR) \tan(\kappa R)}{\tan(\kappa R) - \sqrt{1 + K^2/k^2} \tan(kR)}.$$

This result is expanded in k^2 and is compared to (2.49). The scattering length and the effective range then are found to be

$$a^{(0)} = -R + \frac{1}{K} \tan(KR), \quad r_0^{(0)} = R - \frac{1}{3} \frac{R^3}{(a^{(0)})^2} + \frac{1}{K^2 a^{(0)}}.$$

The scattering amplitude $f_{\ell=0}$ proper is easily expressed in terms of scattering length and effective range. Writing $\sin \delta = 1/\sqrt{1+u^2}$, $\cos \delta = u/\sqrt{1+u^2}$, and $u \equiv \cot \delta$ one has

$$f_0 = \frac{1}{k} e^{i\delta} \sin \delta = \frac{1}{u - i} \approx \frac{a^{(0)}}{1 - ia^{(0)}k + a^{(0)}r_0^{(0)}k^2/2}.$$

This amplitude has poles on the negative real axis in the complex k^2 -plane which correspond to the bound states in this potential. If one wants to know the exact values of their energy one would have to solve the condition (2.50), with $k = i\sqrt{2m(-E)}$, either analytically or numerically. However, if the term of the denominator containing the effective range is small, the pole, or bound state, is obtained from $1 - ia^{(0)}k = 1 + a^{(0)}\sqrt{2m(-E)} = 0$. Thus,

$$E \approx -\frac{\hbar^2}{2m(a^{(0)})^2}$$

gives an approximate value for the binding energy.

2.6 Inelastic Scattering and Partial Wave Analysis

Examination of the differential equation for the radial function $u_\ell(r)$ in the form of (2.8) or of (2.40) shows that a real, attractive or repulsive potential leads to real scattering phases. In these cases there is only elastic scattering. If, on the other hand, the initial state can make transitions to other states that differ from it, there will be both elastic and inelastic scattering amplitudes whose absolute square yield the cross sections for the various inelastic channels. Loosely speaking, the elastic final state will be “depopulated” in favour of new, inelastic channels. Whether such channels are “open”, and, if so, how many there are, depends on the dynamics of the scattering

process and of the energy of the incoming state. For example, an electron which scatters on an atom, can lift this atom to an excited discrete state,

$$e + (Z, A) \longrightarrow (Z, A)^* + e',$$

if its energy is high enough as to furnish the finite, discrete difference $E(Z, A)^* - E(Z, A)$.

An exact quantum theoretic description would have to be a *multi-channel* calculation of the transition probabilities into all channels, the elastic one as well as all open inelastic channels, by solving a finite number of coupled wave equations. Depending on the kind and on the complexity of the system on which the scattering takes place, this may be an extensive, technically challenging calculation. If, on the other hand, one is primarily interested in the back-reaction onto the elastic channel, there is a simpler bulk procedure to parametrize the partial wave contributions to (2.6). The key to this method is provided by the optical theorem (2.12) which says that the *total* cross section

$$\sigma_{\text{tot}} = \sigma_{\text{el}} + \sigma_{\text{abs}}$$

is proportional to the imaginary part of the *elastic* scattering amplitude in the forward direction,

$$\sigma_{\text{tot}} = \sigma_{\text{el}} + \sigma_{\text{abs}} = \frac{4\pi}{k} \text{Im } f_{\text{el}}(k, \theta = 0). \quad (2.51)$$

The elastic cross section, integrated over the whole solid angle, is given by

$$\sigma_{\text{el}} = \int d\Omega |f_{\text{el}}|^2 = \frac{4\pi}{k^2} \sum_{\ell=0}^{\infty} (2\ell+1) |a_{\ell}(k)|^2 = 4\pi \sum_{\ell=0}^{\infty} (2\ell+1) |f_{\ell}(k)|^2.$$

The remainder σ_{abs} is the sum of all cross sections into inelastic channels open at the given energy. It represents the absorption out of the elastic channel.

So far, we did not prove the optical theorem in this general form because we did not yet develop all tools needed for its proof. In the theory of potential scattering the theorem follows essentially from the conservation of probability: if the particle can be scattered away from the elastic channel, the probability to find it *somewhere* in one of the kinematically (and dynamically) allowed final states must be equal to 1.

The expansion in partial waves being so useful and well adapted to the physics of scattering, it is suggestive to define total, elastic, and absorption cross sections for each partial wave ℓ ,

$$\begin{aligned} \sigma_{\text{el}}^{(\ell)} &:= 4\pi(2\ell+1) |f_{\ell}(k)|^2, \\ \sigma_{\text{tot}}^{(\ell)} &:= \frac{4\pi}{k} (2\ell+1) \text{Im } f_{\ell}(k), \\ \sigma_{\text{abs}}^{(\ell)} &:= \sigma_{\text{tot}}^{(\ell)} - \sigma_{\text{el}}^{(\ell)}. \end{aligned}$$

Note that we have made use of the optical theorem in the second definition. As $\sigma_{\text{(tot)}}^{(\ell)} \geq \sigma_{\text{el}}^{(\ell)}$ there follows an important condition on the partial wave amplitudes:

$$\boxed{\text{Im } f_{\ell}(k) \geq k |f_{\ell}(k)|^2}. \quad (2.52)$$

The condition (2.52) is called *positivity condition*. This condition implies that $f_\ell(k)$ must have the general form

$$f_\ell(k) = \frac{1}{2ik} (e^{2i\delta_\ell(k)} - 1) \quad (2.53)$$

where δ_ℓ is a phase which may be complex, and whose imaginary part must be positive or zero. This is shown as follows:

The polar decomposition of the complex function $1 + 2ikf_\ell$ is written as follows

$$1 + 2ikf_\ell = \eta_\ell e^{2i\varepsilon_\ell} \quad \text{with} \quad \eta_\ell = e^{-2 \operatorname{Im} \delta_\ell}, \quad \varepsilon_\ell = \operatorname{Re} \delta_\ell.$$

(The factor 2 in the exponent is introduced for convenience in order to facilitate comparison with the results of Sect. 2.3.) One calculates

$$\operatorname{Im} f_\ell = \frac{1}{2k} [1 - \eta_\ell \cos(2\varepsilon_\ell)], \quad |f_\ell|^2 = \frac{1}{4k^2} [1 + \eta_\ell^2 - 2\eta_\ell \cos(2\varepsilon_\ell)].$$

The positivity condition (2.52) implies the inequalities

$$1 \geq \frac{1 + \eta_\ell^2}{2} \quad \text{or} \quad 0 \leq \eta_\ell^2 \leq 1.$$

This was precisely the assertion: If $\eta_\ell = 1$, then $\operatorname{Im} \delta_\ell = 0$; if $\eta_\ell < 1$, then $\operatorname{Im} \delta_\ell > 0$. The quantity η_ℓ , which, by definition, is positive semi-definite and which obeys the inequality

$$\boxed{0 \leq \eta_\ell \leq 1} \quad (2.54)$$

is called *inelasticity*. Indeed, qualitatively speaking, the inelasticity is a measure for the amount taken out of the ℓ -th partial wave of elastic scattering, due to absorption.

The result (2.53) with the property (2.54) is quite remarkable: The same form (2.11) for the amplitude $f_\ell = a_\ell/k$ was obtained from the Schrödinger equation, though with *real* potentials and, hence, real scattering phases. In deriving the more general formulae of this section we need no more than the optical theorem (2.51)!

The cross sections of fixed partial wave, defined above, when written as functions of the inelasticity and the real scattering phase, are given by

$$\sigma_{\text{tot}}^{(\ell)} = \frac{2\pi}{k^2} (2\ell + 1) [1 - \eta_\ell \cos(2\varepsilon_\ell)], \quad (2.55)$$

$$\sigma_{\text{el}}^{(\ell)} = \frac{\pi}{k^2} (2\ell + 1) [1 + \eta_\ell^2 - 2\eta_\ell \cos(2\varepsilon_\ell)], \quad (2.56)$$

$$\sigma_{\text{abs}}^{(\ell)} = \sigma_{\text{tot}}^{(\ell)} - \sigma_{\text{el}}^{(\ell)} = \frac{\pi}{k^2} (2\ell + 1) [1 - \eta_\ell^2]. \quad (2.57)$$

The interpretation of the results (2.55)–(2.57) is simple:

1. If $\eta_\ell = 1$ there is no absorption at all in this partial wave. The inelastic contribution vanishes, the elastic cross section (2.57) equals the total cross section (2.55),

$$\sigma_{\text{abs}}^{(\ell)} = 0, \quad \sigma_{\text{el}}^{(\ell)} = \sigma_{\text{tot}}^{(\ell)}.$$

In this case the scattering phase δ_ℓ is real, and (2.53) can be written in the form known from (2.11),

$$f_\ell(k) = \frac{1}{k} e^{i\delta_\ell} \sin \delta_\ell.$$

2. The other extreme case is $\eta_\ell = 0$. The absorption is maximal in the partial wave with angular momentum ℓ . This does not mean that there is no elastic scattering at all! Rather, the elastic and the inelastic cross sections are equal. The results (2.55)–(2.57) which were derived from the optical theorem, give the result

$$\sigma_{\text{abs}}^{(\ell)} = \sigma_{\text{el}}^{(\ell)} = \frac{1}{2} \sigma_{\text{tot}}^{(\ell)} .$$

The scattering amplitude proper is pure imaginary and is equal to

$$f_\ell = \frac{i}{2k} .$$

3. A case of interest is one where there is a resonance in the ℓ -th partial wave, accompanied by absorption. The resonance curve Fig. 2.4 remains qualitatively similar to the case without absorption. However, it no longer intersects the ordinate in the point i (or i/k), but at a smaller value from which the inelasticity can be read off.

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