Scattering Theory: Born Series

Stefan Blügel

This document has been published in

Manuel Angst, Thomas Brückel, Dieter Richter, Reiner Zorn (Eds.):
Scattering Methods for Condensed Matter Research: Towards Novel Applications at Future Sources
Lecture Notes of the 43rd IFF Spring School 2012
Schriften des Forschungszentrums Jülich / Reihe Schlüsseltechnologien / Key Technologies, Vol. 33
JCNS, PGI, ICS, IAS
Forschungszentrum Jülich GmbH, JCNS, PGI, ICS, IAS, 2012
ISBN: 978-3-89336-759-7

A 2 Scattering Theory: Born Series [1]

Stefan Blügel
Peter Grünberg Institut and
Institute for Advanced Simulation
Forschungszentrum Jülich GmbH

Contents

[1] Lecture Notes of the 43^{rd} IFF Spring School "Scattering Methods for Condensed Matter Research: Towards Novel Applications at Future Sources" (Forschungszentrum Jülich, 2012).

1 Introduction

Since Rutherford's surprise at finding that atoms have their mass and positive charge concentrated in almost point-like nuclei, scattering methods are of extreme importance for studying the properties of condensed matter at the atomic scale. Electromagnetic waves and particle radiation are used as microscopic probes to study a rich variety of structural and dynamical properties of solids and liquids. Atomistic processes in condensed matter take place at length scales on the order of an Ångström (1Å$= 10^{-10}$m) and an energy scale between a meV and a few eV. Obviously, detailed information concerning atomic systems require measurements related to their behavior at very small separations. Such measurements are in general not possible unless the de Broglie wavelength ($\lambda = \frac{h}{p} = \frac{h}{mv}$) of the relative motion of the probing particle is comparable to these distances. This makes x-ray scattering and neutron scattering, in addition to electron scattering and to a certain extent also Helium scattering, to the outstanding microscopic "measurement instruments" for studying condensed matter. To push electromagnetic waves in this area one uses either x-rays with wavelengths of a few Ångströms, but in the keV energy range, or light with energies in the eV range, but wavelengths of some 1000 Å. Neutrons (and Helium atoms) make it possible to match energy and wavelengths simultaneously to the typical atomic spacings and excitation energies of solids (solid surfaces). Thus, a simultaneous spatial and temporal resolution of atomistic or magnetic processes is possible. In addition, the photon, neutron, electron and under certain conditions also Helium possess internal degrees of freedom such as a polarization vector or a spin with which the probes couple to core and valence electrons. The photon, neutron and Helium result in only week interaction with matter, which simplifies considerably the analysis and interpretation of experiments as multiple scattering processes are frequently of minor importance and can often be ignored completely, which makes an interpretation of the scattering results valid within a kinematic scattering theory.
In this Chapter, we will provide a brief introduction to the elementary concepts and methodology of scattering theory. The focus lies on the introduction of the description of the scattering process in terms of the Hamiltonian of the scattering projectile at a finite range interaction potential of a single site target by the method of partial waves, i.e. using differential equation methods and the Lippmann-Schwinger equation, i.e. using an integral equation formulation of scattering that leads then to the first Born approximation of scattering and the distored wave Born approximation. The former is the approximation of choice if multiple scattering is unimportant and the latter is applied in the analysis of grazing-incidence small-angle scattering experiments discussed in more details chapter D2. The lecture closes with the discussion of the scattering on the lattice rather than a single site target resulting briefly the Bragg scattering, that will be discussed in more detail in the lecture Scattering Theory: Dynamical Theory (A3). The subject is typically part of an Advanced Quantum Mechanics curriculum and is therefore elaborated at textbooks on quantum mechanics. A selection is given as references [1, 2, 3, 4].

2 The Scattering Problem

In a scattering experiment a beam of particles is allowed to strike a target,[2] and the particles that emerge from the target area or *scattering volume*, respectively, are observed.

[2] In the language of elementary scattering theory one frequently refers to a target although we keep in mind that in the language of condensed matter, it is referred to as the sample.

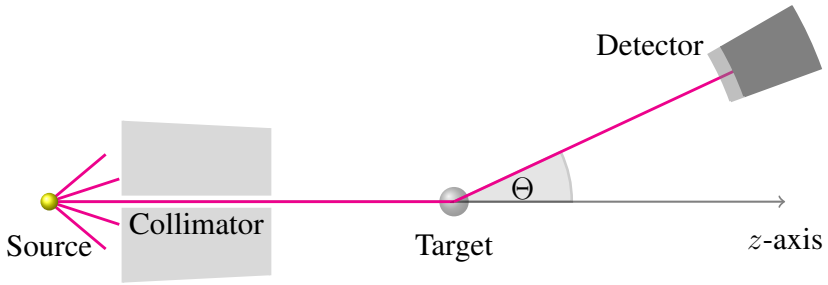


Fig. 1: *A set-up of a typical diffraction experiment consisting of a particle source, a scattering target and a particle detector. The beam passes through a collimator with an beam opening* Δr.

2.1 The Experimental Situation

A schematic representation of a standard scattering experiment appears in Fig. 1. Each scattering experiment consists of three indispensable elements: (i) The source of incident beam of particles or electromagnetic wave, to propagate with wave vector $\mathbf{k} = \frac{2\pi}{\lambda}\hat{\mathbf{k}}$ of wavelength λ along the direction $\hat{\mathbf{k}}$, which we assume without loss of generally to be the $\hat{\mathbf{z}}$-direction (the axis of the collimator). (ii) The target, that we consider stationary, a reasonable assumption in condensed matter physics and (iii) the detector, whose function is to simply count the number of particles of a particular type that arrive at its position $\mathbf{r}$ with the coordinate $\mathbf{r} = (x, y, z)$ in real space along the direction $\hat{\mathbf{r}}$ at the angle (θ, φ) with respect to the axis of the propagating incident beam. Ideally it may be set to count only particles of a given energy, spin or polarization vector, respectively. We assume throughout that the source and detector are classical objects that have a clearly defined, precisely controllable effect on the scattering process. The detector will be assumed to be 100% efficient and to have no effect on the scattered particle prior to the time it enters the detector.

The result of the scattering experiment will vary with the energy E of the incident beam. In order to simplify the analysis of the experimental data, the energy spectrum of the incident beam should be sharply peaked so that the experiment may be considered to take place at a unique energy eigenvalue E. To this end, in most experiments care is taken to achieve a monochromatic incident beam characterized by the wave vector $\mathbf{k}$. We shall assume here that the beam emerging from the collimator is both perfectly monochromatic and perfectly collimated, as well. Of course, according to the uncertainty principle, a beam of finite cross section (of the size of the collimator opening Δr) cannot be perfectly monochromatic ($\Delta k > 0$) and perfectly collimated as well. We may, however, assume the beam to be sufficiently well collimated that the angular divergence may be ignored in an actual experiment. In that case we must necessarily have not a monochromatic beam represented by a plane wave, but rather a beam describable as a superposition of such waves. In this respect the collimator can be considered the fourth indispensable element of a scattering experiment. It shields the detector from the incoming beam to the ideal extent that no count is measured in the detector without target, and produces a small beam of monochromatic energy. We further assume that the detector has a small opening angle $d\Omega$ and is positioned at large distance from the target. Under these conditions, the scattered beam can be characterized at the position of the detector by the wave vector $\mathbf{k}'$ and energy E'. Summarizing, in a scattering experiment a wave packet of incident particles characterized by the initial state $(\mathbf{k}, E, \mathbf{e})$, denoting the polarization vector $\mathbf{e}$ of an x-ray beam as a representative of an internal

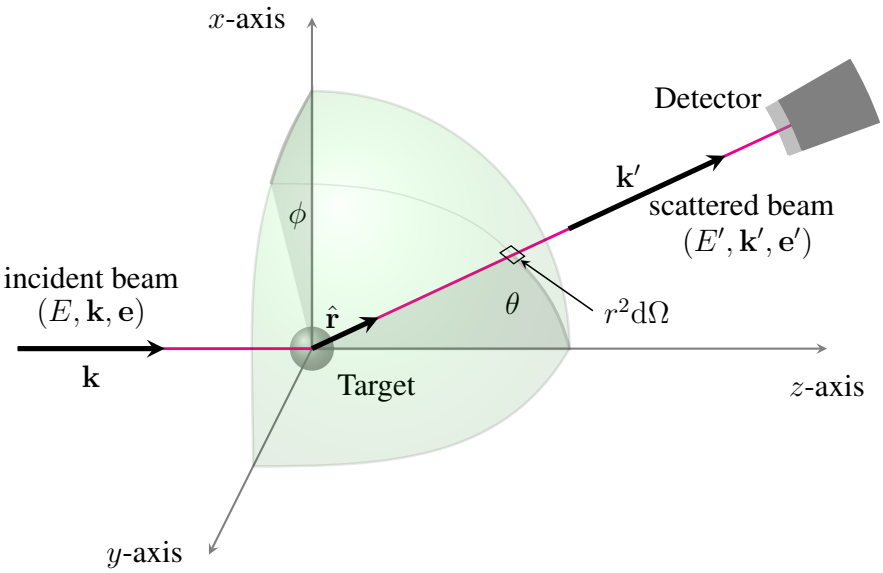


Fig. 2: *The geometry of the scattering experiment.*

degree of freedom of the particle, is scattered into the final state:

$$(\mathbf{k}, E, \mathbf{e}) \overset{\text{scattering}}{\longrightarrow} (\mathbf{k}', E', \mathbf{e}'). \tag{1}$$

The scattering process is characterized by the *scattering vector*

$$\mathbf{Q} = \mathbf{k}' - \mathbf{k} \tag{2}$$

and the *energy transition*

$$\hbar\omega = E' - E. \tag{3}$$

$\hbar\mathbf{Q}$ represents the momentum transfer during scattering, since according to de Broglie, the momentum of the particle corresponding to the wave with wave vector $\mathbf{k}$ is given by $\mathbf{p} = \hbar\mathbf{k}$. For *elastic scattering* (*diffraction*), it holds that $E' = E$ and $|\mathbf{k}'| = |\mathbf{k}|$ and all possible scattering vectors are located on a sphere, called *Ewald-sphere*. Structural investigations are always carried out by elastic scattering. The magnitude Q of the scattering vector can be calculated from wavelength λ and scattering angle θ as follows

$$Q = \sqrt{k^2 + k'^2 - 2kk'\cos\theta} = \sqrt{2k^2(1-\cos\theta)} = k\sqrt{2(1-\cos^2\frac{\theta}{2} + \sin^2\frac{\theta}{2})} = \frac{4\pi}{\lambda}\sin\frac{\theta}{2} \tag{4}$$

2.2 Description of Scattering Experiment

After the beam of particles is emitted from the collimated source, the experimenter has no control over the particles until they have reached his detector. During that time, the propagation is controlled solely by the laws of quantum mechanics and the Hamiltonian of the projectile-target system. We restrain our description to the nonrelativistic domain and may thus formulate the physical situation in terms of the solution of a Schrödinger equation using an appropriate

Hamiltonian and suitable boundary conditions. The occurring phenomena can be very complex. We assume in the following that the incident particles do not interact with each other during the time of flight, rather that the particles fly one by one, and that incident particles and the target particles do not change their internal structures or states, but only scatter off each other. Internal excitations, rearrangements, charge or spin exchange are also excluded. In fact, internal degrees of freedom such as the spin or polarization vector are currently completely neglected. That means we shall consider only the purely *elastic scattering*. We further neglect the *multiple scattering* in the target and consider at first only the interaction of an incident particle with one target particle, the state of both is described by a two-particle wave function $\Psi(\mathbf{r}_\mathrm{P}, \mathbf{r}_\mathrm{T})$ and the interaction is described by a potential $V(\mathbf{r})$ which depends only on the relative distance $\mathbf{r} = \mathbf{r}_\mathrm{T} - \mathbf{r}_\mathrm{P}$, where the subscripts T and P denote the target and the incoming particle, respectively. We shall confine ourselves in this article to scattering processes in which only short-range central forces are present. In the presence of such potentials, the particle is not under influence of the target potential when they are emitted from the source or when they enter the detector. Since for the two-body problem the motion of the center of mass $\mathbf{R}$ can be separated out, the problem reduces to the scattering of a particle with the reduced mass $\frac{1}{m} = \frac{1}{m_\mathrm{T}} + \frac{1}{m_\mathrm{P}}$ at the potential $V(\mathbf{r})$. Since the potential does not depend explictly on the coordinate of the center of mass $\mathbf{R}$, the two-particle wave function can be expressed in terms of a product of single-particle wave functions $\Psi(\mathbf{r}_\mathrm{P}, \mathbf{r}_\mathrm{T}) = \phi(\mathbf{R})\psi(\mathbf{r})$,[3] both solutions of two separate Schrödinger equations. The elementary two-body scattering process could be intrinsically elastic, but recoil of the target particle might lead to a transfer of energy to the target. In the present context elastic scattering specifically excludes such effects. Considering a solid as target, depending on the energy of the projectile and the interaction of the constituent atoms in a solid, this can be a very good assumption, as for favorable circumstances all atoms contribute to the scattering mass of the solid (of course, in other chapters it becomes clear that atoms in a solid vibrate and a scattering event may cause inelastic excitations of phonons in the vicinity of the elastic energy). To think that the target particle or a target solid is infinitely heavy relative to the mass of the incident particle simplifies our thinking further. In this case the center of mass of the target remains stationary at the position of the target particle throughout the scattering process. Under these circumstances the relative coordinate $\mathbf{r}$ represents the actual laboratory coordinate of the light particle and the mass m is then the mass of the incident particle. These parameters enter the time-dependent Schrödinger equation

$$i\hbar\frac{\partial\psi}{\partial t} = \left[-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r})\right]\psi \qquad \text{with} \qquad V(\mathbf{r}) = 0 \qquad \text{except } \mathbf{r} \in \text{ target region } \mathbb{T} \quad (5)$$

to be solved.

The time-dependent Schrödinger equation seems a natural starting point for the description of a scattering event as it is not a stationary process but involves individual discrete particles as projectiles, but as we see a bit later the good news is, that under reasonable assumptions that are fulfilled in typical experimental situations, the same results are obtained using a time-independent description applying the stationary Schrödinger equation.

At the vicinity of the collimator and detector, the solution of the potential-free Schrödinger equation (5) is analytically known as the free-particle wave packet:

$$\psi(\mathbf{r}, t) = \frac{1}{(2\pi)^3}\int d^3k\, A(\mathbf{k})\,\psi_\mathbf{k}(\mathbf{r}, t) \qquad \text{with} \qquad \psi_\mathbf{k}(\mathbf{r}, t) = e^{i\mathbf{kr}}e^{-i\frac{\hbar k^2}{2m}t}. \quad (6)$$

[3] This does not hold if target and projectile are identical particles. Identical articles scattering about angle θ and $\pi - \theta$ cannot be distinguished.

The wave packet is expressed as a superposition of a complete set of stationary-state solutions $\psi_{\mathbf{k}}(\mathbf{r})$ of this Schrödinger equation, which are plane waves $\psi_{\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{kr}}$. The energy eigenvalue corresponding to the eigenfunction $\psi_{\mathbf{k}}$ is simply $E_{\mathbf{k}} = \frac{\hbar^2}{2m}k^2$. For convenience the target is placed at the origin of the coordinate system ($r = 0$). The coefficient $A(\mathbf{k})$ is the probability amplitude for finding the wave number $\mathbf{k}$, or momentum $\hbar\mathbf{k}$ in the initial state. We assume that the properties of the source are such that the wave packet is close to monochromatic and that the amplitude function $A(\mathbf{k})$ peaks about the average momentum $\hbar\mathbf{k} = \hbar\mathbf{k}_\circ$ with a spread in the wave number $\Delta\mathbf{k}$ that is small compared to $\mathbf{k}_\circ$ ($\Delta\mathbf{k} \ll \mathbf{k}_\circ$), related to the opening of the collimator $\Delta\mathbf{r}$ by Heisenberg's uncertainty principle ($\Delta\mathbf{k}\Delta\mathbf{r} \simeq 1$). If we finally impose the condition $\frac{(\Delta\mathbf{k})^2}{\mathbf{k}_\circ}L \ll 1$ (equivalent to the condition $\frac{\lambda_\circ}{\Delta r} \ll \frac{\Delta r}{L}$) the packet does not spread appreciably during the course of the experiment with the set-up of length L, and we can finally show that a stationary description of the scattering problem is sufficient. Under these conditions the energy-dependent phase factor of $\psi_{\mathbf{k}}(\mathbf{r},t)$ can be conveniently be approximated about the median energy $k^2 \simeq -k_\circ^2 + 2\mathbf{k}\cdot\mathbf{k}_\circ$ and Eq. (6) will become

$$\psi(\mathbf{r},t) = e^{i\frac{\hbar k_\circ^2}{2m}t}\,\frac{1}{(2\pi)^3}\int d^3k\, A(\mathbf{k})\, e^{i\mathbf{k}\cdot(\mathbf{r}-\mathbf{v}_\circ t)} = e^{i\frac{\hbar k_\circ^2}{2m}t}\psi(\mathbf{r}-\mathbf{v}_\circ t, 0), \tag{7}$$

i.e. a wave packet $\psi(\mathbf{r},t)$ centered about the origin $r = 0$ at $t = 0$ moves at the classical velocity $\mathbf{v}_\circ = \frac{\hbar\mathbf{k}_\circ}{m}$ and the packet at time $t > 0$ will have exactly the same shape, but centered about $\mathbf{r} = \mathbf{v}_\circ t$. Thus, the initial state $\lim_{t\to-\infty}\psi(\mathbf{r},t)$ and the final state $\lim_{t\to+\infty}\psi(\mathbf{r},t)$ can be expressed by Eq. (7), but with the coefficients $A(\mathbf{k})$ in the final state having been modified compared to the ones in the initial state due to the scattering, as we shall discuss immediately.
A solution of Eq. (5) requires, however, the specification of boundary conditions imposed on the solution that reflect the physical situation in the laboratory as discussed in section 2.1. The proper boundary condition is a condition on the wave function when the particle and target are far apart. It can be motivated from *Huygens' principle* [5] who proposed that every point which a luminous disturbance reaches becomes a source of a spherical wave, and the sum of these secondary waves determines the form of the wave at any subsequent time. For a single target scatterer we express the wave function

$$\psi_{\mathbf{k}}(\mathbf{r}) \overset{r\to\infty}{\longrightarrow} e^{i\mathbf{kr}} + \frac{1}{r}e^{ikr}f_{\mathbf{k}}(\theta,\phi) \qquad \forall\mathbf{k} \quad \text{and} \quad t > 0 \tag{8}$$

in terms of a superposition for the incoming wave plus an outgoing scattered wave emanating from the target, removing some of the incoming particles from the incident primary beam. $f(\theta,\phi)$, $f(\hat{\mathbf{r}})$ or $f(\hat{\mathbf{k}}')$, respectively, denotes the scattering amplitude. This form of the wave function is motivated by the fact that we expect, after scattering, an outgoing spherical wave, modified by the scattering amplitude, interfering with the incoming wave; we will later show a more rigorous justification of this expression. Consistent to the lab schematics in Fig. 1, $\mathbf{k}_\circ\|\hat{\mathbf{z}}$ and the azimuthal and polar scattering angle (θ,ϕ) are given by the projection of the direction of the wavevector $\hat{\mathbf{k}}$ of the scattered wave, e.g. into the detector at direction $\hat{\mathbf{r}}$ and the $\hat{\mathbf{z}}$ direction. If we replace $\psi_{\mathbf{k}}(\mathbf{r},t)$ in (6) by its asymptotic form given in (8), when the packet is far from the target, the wave function $\psi'(\mathbf{r},t)$ (where we use a prime to denote the wave function after scattering) breaks up into two terms

$$\psi'(\mathbf{r},t) = \psi_{\mathbf{k}}(\mathbf{r},t) + \psi_{\rm sc}(\mathbf{r},t), \qquad \text{with} \quad \psi_{\rm sc}(\mathbf{r},t) = 0 \quad \text{for} \quad t < 0 \tag{9}$$

with the incident beam $\psi_{\mathbf{k}}(\mathbf{r},t)$ identical to Eq. (7) and the scattered wave $\psi_{\rm sc}(\mathbf{r},t)$ according

to Eq. (6)

$$\psi_{\rm sc}(\mathbf{r},t) = \frac{1}{r}\,\frac{1}{(2\pi)^3}\int d^3k\, f_{\mathbf{k}}(\hat{\mathbf{r}})A(\mathbf{k})\,e^{ikr}\,e^{-i\frac{\hbar k^2}{2m}t}. \tag{10}$$

If we assume now that the scattering amplitude is slowly varying over the spread of the wave numbers $\Delta\mathbf{k}$, and thus approximate $f_{\mathbf{k}}(\hat{\mathbf{r}}) \simeq f_{\mathbf{k}_\circ}(\hat{\mathbf{r}})$ as well as making use of the approximations

$$k \simeq \hat{\mathbf{k}}_\circ \cdot \mathbf{k} \qquad \text{and} \qquad k^2 \simeq -k_\circ^2 + 2\mathbf{k}\cdot\mathbf{k}_\circ \qquad \text{for} \qquad (\Delta k)^2 \ll k_\circ^2 \tag{11}$$

($k = |\mathbf{k}| = |\mathbf{k}_\circ + \Delta\mathbf{k}| = [k_\circ^2 + 2\mathbf{k}_\circ\cdot\Delta\mathbf{k} + (\Delta k)^2]^{1/2} \simeq k_\circ[1 + 2\mathbf{k}_\circ\cdot\Delta\mathbf{k}/k_\circ^2]^{1/2} \simeq k_\circ + \hat{\mathbf{k}}_\circ\cdot(\mathbf{k}-\mathbf{k}_\circ)$) in which k is equal to the projection along $\mathbf{k}_\circ$ we obtain

$$\psi_{\rm sc}(\mathbf{r},t) = e^{-i\frac{\hbar k_\circ^2}{2m}t}\,\frac{1}{r}\,f_{\mathbf{k}_\circ}(\hat{\mathbf{r}})\,\frac{1}{(2\pi)^3}\int d^3k\,A(\mathbf{k})\,e^{i\mathbf{k}\cdot(\hat{\mathbf{k}}_\circ r - \mathbf{v}_\circ t)} = e^{-i\frac{\hbar k_\circ^2}{2m}t}\,\frac{1}{r}\,f_{\mathbf{k}_\circ}(\hat{\mathbf{r}})\,\psi(\hat{\mathbf{k}}_\circ r - \mathbf{v}_\circ t, 0)\,. \tag{12}$$

Thus, after the incident packet has passed the target a spherical scattered wave shell of thickness Δr, equal to the size of the packet, centered on the origin and having a radius $r = v_\circ t$ emerges from the target. One finds further that the incoming wave packet given in (7) and the scattered wave, Eq. (12), share absolutely the same time dependence and are the same for all k. The solution is actually a superposition of all available wave numbers according to $\int d^3k A(\mathbf{k})\ldots$. Since there is no mode-mode coupling such as $\mathbf{k} \rightarrow \mathbf{k_1} + \mathbf{k_2}$, it is totally sufficient to solve the problem in terms of a scattering problem of $\psi_{\mathbf{k}}(\mathbf{r})$ on the basis of a stationary Schrödinger equation for all relevant wave vectors $\mathbf{k}$, which will be pursued during the rest of the manuscript, and keep thereby in mind that a wave packet is formed with a certain probability amplitude. This stationary problem with plane waves as incident beam simplifies the description of scattering significantly.

2.3 Coherence

The formation of a wave packet bears, however, a consequence on which we shall briefly touch upon: The scattering pattern or diffraction pattern, respectively, will be a superposition of patterns for different incident wave vectors $(\mathbf{k}, \mathbf{k}+\Delta\mathbf{k})$ and the question arises, which information is lost due to these non-ideal conditions. This "instrumental resolution" is intimately connected with the "coherence" of the beam and the size of the *scattering volume* in comparison to the *target volume*. Coherence is needed, so that the interference pattern is not significantly destroyed. Coherence requires a phase relation between the different components of the beam. A measure for the coherence length l is given by the distance, at which two components of the beam become fully out of phase, i.e. when one wave train at position $\mathbf{r}$ exhibits a maximum, meats a wave train exhibiting a minimum, thus experiencing a phase difference of $\lambda/2$. If the coherence length $l_\parallel$ is determined by the wavelength spread, λ and $\lambda + \Delta\lambda$ one refers to the temporal or longitudinal coherence. The condition $l_\parallel = n\lambda = (n - \frac{1}{2})(\lambda + \Delta\lambda)$ translates then into

$$l_\parallel = \frac{1}{2}\frac{\lambda^2}{\Delta\lambda} \qquad \text{for longitudinal coherence}$$

and

$$l_\perp = \frac{1}{2}\frac{\lambda}{\Delta\theta} \qquad \text{for transversal coherence.}$$

Analogously one obtains the transversal coherence length $l_\perp$ shown in above equation due to the divergence of the beam $\Delta\theta$ that results from the finite transverse beam size due to the finite extension of the source. In many instruments, the vertical and horizontal collimations are different and the vertical one can even be different along different spatial directions.
Together, the longitudinal and the two transversal coherence lengths define a coherence volume. This is a measure for a volume within the sample, in which the amplitudes of all scattered waves superimpose to produce an interference pattern. Normally, the coherence volume is significantly smaller than the sample size, typically a few 100 Å for neutron scattering, up to μm for synchrotron radiation. Scattering between different coherence volumes within the sample is no longer coherent, i.e. instead of the amplitudes, the intensities of the contributions to the scattering pattern have to be added. This limits the spatial resolution of a scattering experiment to the extension of the coherence volume.

2.4 The Cross Section

A general measure of the scattered intensity $I(\Omega)$ is the *differential cross section* ($\frac{d\sigma}{d\Omega}$). It is defined by the number of particles dN counted per unit time dt scattered into a cone of solid angle $d\Omega = \sin\theta\, d\theta\, d\phi$ in the detector located at the distance r along a ray specified by the direction $\hat{\mathbf{r}}$, at angle (θ, ϕ) or the solid angle Ω, respectively, normalized to the current of the incoming particles $j_{\rm in}$

$$\frac{1}{j_{\rm in}}\frac{dN}{dt} = \left(\frac{d\sigma}{d\Omega}\right) d\Omega = \left(\frac{d\sigma}{d\Omega}\right)\frac{1}{r^2} dA. \tag{13}$$

$d\sigma$ describes a cross-sectional area with a surface normal parallel to $\mathbf{k}_\circ$, through which the number of particles dN that get scattered into the angle Ω flow per unit time. The total cross section

$$\sigma_{\rm tot} = \int_0^{4\pi} \left(\frac{d\sigma}{d\Omega}\right) d\Omega \tag{14}$$

is the total effective geometrical cross-sectional area of the incident beam that is intercepted and the particles therein deflected by the target object.
From Eq. (13) the scattered current density is $j_{\rm sc} = \frac{1}{r^2} j_{\rm in}(\frac{d\sigma}{d\Omega})$. On the other hand $j_{\rm sc}$ can be calculated directly employing the expression of the probability current density given by

$$\mathbf{j}_{sc}(\mathbf{r}) = -i\frac{\hbar}{2m}\left[\psi^*_{\rm sc}(\mathbf{r})\nabla\psi_{\rm sc}(\mathbf{r}) - \psi_{\rm sc}(\mathbf{r})\nabla\psi^*_{\rm sc}(\mathbf{r})\right] \simeq j_{\rm in}\frac{1}{r^2}|f(\Omega)|^2\,\hat{\mathbf{r}} + \mathcal{O}\left(\frac{1}{r^3}\right)\ldots \tag{15}$$

where as $\psi_{\rm sc} = \frac{1}{r}e^{ikr}f(\Omega)$ is the asymptotic scattering wave, Eq. (8). We explicitly inserted here the current density $\mathbf{j}_{\rm in} = \frac{\hbar\mathbf{k}}{m}$ to the incoming plane wave $\psi_{\rm in}$. Equating the two expressions gives the relation

$$I(\Omega) \propto \left(\frac{d\sigma}{d\Omega}\right) = |f(\Omega)|^2 \tag{16}$$

for the differential cross section. This expression relates the experimental quantity, the differential cross section, to the scattering amplitude, which characterizes the wave function at large distances from the target. It is the fundamental relation between scattering theory and scattering experiments.

3 Lippmann Schwinger Equation

Having established the basic concepts for the scattering problem, we turn now to the illustration of the physical ideas that underlie the scattering analysis using integral equation methods. We recall that we are looking for the solution of the stationary Schrödinger equation

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r})\right]\psi_{\mathbf{k}}(\mathbf{r}) = E\psi_{\mathbf{k}}(\mathbf{r}) \qquad \text{with} \qquad V(\mathbf{r}) = 0 \qquad \text{except } \mathbf{r} \in \text{ target region } \mathbb{T}, \tag{17}$$

that is consistent with the boundary condition (8) of an incident plane wave $\psi_{\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{kr}}$ and an emanating scattered wave. The energy E is determined by the energy of the incident plane wave $E_{\mathbf{k}} = \frac{\hbar^2}{2m}k^2$. By introducing the Green function $G_\circ$,

$$\left[\frac{\hbar^2}{2m}\nabla^2 + E\right] G_\circ(\mathbf{r}, \mathbf{r}'|E) = \delta(\mathbf{r} - \mathbf{r}'), \tag{18}$$

for the potential-free Schrödinger equation, the Schrödinger equation for $\psi_{\mathbf{k}}(\mathbf{r})$,

$$\left[\frac{\hbar^2}{2m}\nabla^2 + E\right] \psi_{\mathbf{k}}(\mathbf{r}) = V(\mathbf{r})\,\psi_{\mathbf{k}}(\mathbf{r}), \tag{19}$$

can be transformed into an integral equation

$$\psi'_{\mathbf{k}}(\mathbf{r}) = \psi_{\mathbf{k}}(\mathbf{r}) + \int_{\mathbb{T}} d^3r' G_\circ(\mathbf{r}, \mathbf{r}'|E)\, V(\mathbf{r}')\, \psi'_{\mathbf{k}}(\mathbf{r}'), \tag{20}$$

in which the formal expression $V(\mathbf{r})\,\psi'_{\mathbf{k}}(\mathbf{r})$ is conceived as inhomogeneity of the differential equation (18). This integral equation is called the *Lippmann-Schwinger equation*. Hereby, $\psi_{\mathbf{k}}(\mathbf{r})$ is the above cited plane-wave solution of the potential-free Schrödinger equation. The index $\mathbf{k}$ in ψ' expresses the fact that this state has evolved from one that in the remote past was a plane wave of the particular wavevector $\mathbf{k}$. Obviously, in the limit of zero potential, $V(\mathbf{r}) \to 0$, the scattered and the incident wave are identical, $\psi'_{\mathbf{k}}(\mathbf{r}) = \psi_{\mathbf{k}}(\mathbf{r})$.
The Green function $G_\circ(\mathbf{r}, \mathbf{r}'|E)$ is not uniquely determined by the Schrödinger equation (18). Also here the unique solution requires a boundary condition, which is chosen such, that the solution $\psi'_{\mathbf{k}}(\mathbf{r})$ describes outgoing scattered waves. The Green function $G_\circ(\mathbf{r}, \mathbf{r}'|E)$,

$$G_\circ(\mathbf{r}, \mathbf{r}'|E) = -\frac{2m}{\hbar^2}\frac{1}{4\pi}\frac{e^{ik|\mathbf{r}-\mathbf{r}'|}}{|\mathbf{r} - \mathbf{r}'|} \qquad \text{with} \qquad k = \sqrt{\frac{2m}{\hbar^2}\,E}, \tag{21}$$

describes then the stationary radiation of a particle of energy E, that is generated at $\mathbf{r}'$, by a spherical wave outgoing from the target. In other words, the Green function $G_\circ(\mathbf{r}, \mathbf{r}'|E)$ gives the amplitude of this wave at location $\mathbf{r}$ due to its generation by the source at $\mathbf{r}'$, under the condition that the wave is not further scattered during its propagation from $\mathbf{r}'$ to $\mathbf{r}$. By the Lippmann-Schwinger equation, the incident wave $\psi_{\mathbf{k}}(\mathbf{r})$ is superimposed with spherical waves emitted from scattering at position $\mathbf{r}'$ in the target. The amplitude of these scattered waves is proportional to the interaction potential $V(\mathbf{r}')$ and the amplitude of the total wave field $\psi'(\mathbf{r}')$ at that point.
Recalling our experimental set-up that the distance between target and detector is significantly larger than the size of the sample, for large distances between $\mathbf{r}$ and the scattering center $\mathbf{r}'$

it is useful to expand the Green function $G_\circ$ in powers of $\frac{r'}{r} \ll 1$ assuming that the extent of $\mathbf{r}'$ is restricted to the space of a small target or scattering volume, respectively, $\mathbf{r}' \in \mathbb{T}$. Approximating for $r' \ll r$

$$\frac{1}{|\mathbf{r}-\mathbf{r}'|} = \frac{1}{r} + \mathcal{O}\left(\frac{1}{r^2}\right) \qquad \text{and} \qquad |\mathbf{r}-\mathbf{r}'| \approx r - \hat{\mathbf{r}}\cdot\mathbf{r}' \qquad \text{with} \qquad \hat{\mathbf{r}} = \frac{\mathbf{r}}{r} \tag{22}$$

and inserting this into the relation (21) one obtains the asymptotic form, or far-field limit, respectively, of the Green function $G_\circ$,

$$G_\circ(\mathbf{r},\mathbf{r}'|E) = -\frac{2m}{\hbar^2}\frac{1}{4\pi}\frac{e^{ikr}}{r}e^{-ik\hat{\mathbf{r}}\cdot\mathbf{r}'} + \mathcal{O}\left(\frac{1}{r^2}\right). \tag{23}$$

Inserting this expression into the Lippmann-Schwinger equation (20) one obtains the asymptotic solution of the wave function $\psi'_{\mathbf{k}}(\mathbf{r})$ for large distances $\mathbf{r}$

$$\psi'_{\mathbf{k}}(\mathbf{r}) \simeq e^{i\mathbf{k}\mathbf{r}} + \frac{1}{r}e^{ikr} f_{\mathbf{k}}(\hat{\mathbf{r}}), \tag{24}$$

which is exactly the boundary condition (8) we conjectured from Huygens' principle, whereas the scattering amplitude $f(\hat{\mathbf{r}}) = f(\theta,\phi)$ is given by the integral,

$$f_{\mathbf{k}}(\hat{\mathbf{r}}) = -\frac{2m}{\hbar^2}\frac{1}{4\pi}\int d^3r'\, e^{-i\mathbf{k}'\mathbf{r}'} V(\mathbf{r}')\,\psi'_{\mathbf{k}}(\mathbf{r}') = -4\pi\frac{\hbar^2}{2m}\,T(\mathbf{k}',\mathbf{k}) \tag{25}$$

that can be interpreted as a transition-matrix element from the scattering state described by $\psi'_{\mathbf{k}}(\mathbf{r}')$ to the scattered state at far distances, which is a plane-wave state described by $\mathbf{k}' = k\cdot\hat{\mathbf{r}}$, the wave vector of the scattered wave in the direction of the detector, which is known in the experiment. $T(\mathbf{k}',\mathbf{k})$ is referred to as the T matrix or transition amplitude, a quantity proportional to the scattering amplitude. Due to the far-field approximation (22) the scattering pattern $f_{\mathbf{k}}(\hat{\mathbf{r}})$ is independent of the distance between target and detector, depending only on the angles to the detector from the target. In optics this is known as the Fraunhofer diffraction and in this context approximation (23) is also referred to as the Fraunhofer approximation of the Green function.

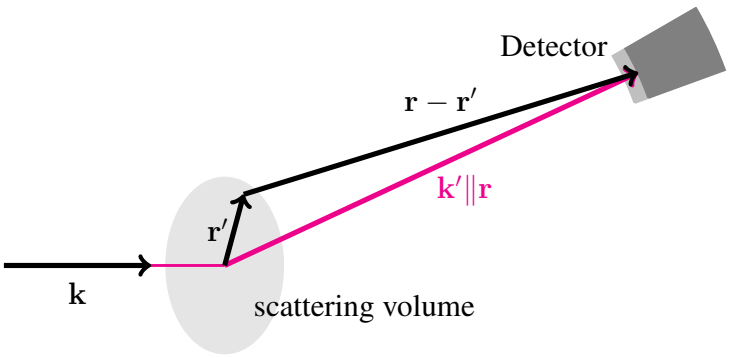


Fig. 3: *Scattering geometry for the calculation of the far-field limit at the detector. In the Fraunhofer approximation, we assume that* $|\mathbf{r}| \gg |\mathbf{r}'|$.

4 Born Approximation

Note that in the Lippmann-Schwinger equation (20) the wave function $\psi'(\mathbf{k})$ appears both on the left and right hand side. In a general case, there is no simple way to find exact solutions of the Lippmann-Schwinger equation. The form of the Lippmann-Schwinger equation provides a natural but approximate means that can be used for any potential, under the proper conditions, to proceed by an iterative procedure. At zeroth order in V, the scattering wave function is specified by the unperturbed incident plane wave,

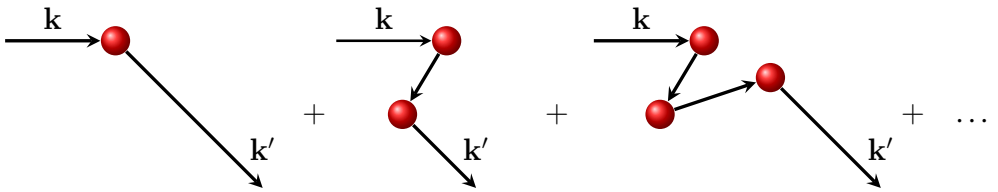
$$\psi'^{(0)}_{\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{kr}}. \tag{26}$$

Then one can iterate the Lippmann-Schwinger equation (20) according to the rule

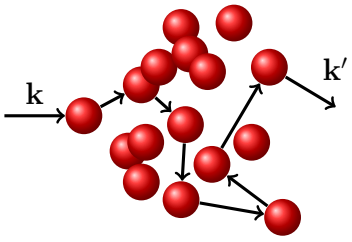
$$\psi'^{(n+1)}_{\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{kr}} + \int d^3r' G_\circ(\mathbf{r},\mathbf{r}'|E)\, V(\mathbf{r}')\, \psi'^{(n)}_{\mathbf{k}}(\mathbf{r}') \tag{27}$$

that results in the *Born expansion* of the wave function in powers of the interaction potential V written here in a symbolic form[4]

$$\begin{aligned}
\psi'_{\mathbf{k}} &= \psi'^{(0)}_{\mathbf{k}} + \psi^{(1)}_{\mathbf{k}} + \psi^{(2)}_{\mathbf{k}} + \psi^{(3)}_{\mathbf{k}} + \cdots + && (28)\\
&= \psi'^{(0)}_{\mathbf{k}} + G_\circ V \psi'^{(0)}_{\mathbf{k}} + G_\circ V G_\circ V \psi'^{(0)}_{\mathbf{k}} + G_\circ V G_\circ V G_\circ V \psi'^{(0)}_{\mathbf{k}} + \cdots + && (29)\\
&= (1 + G_\circ T)\, \psi'^{(0)}_{\mathbf{k}} \quad \text{with} \quad T = V + G_\circ V + \cdots + = \frac{1}{1 - VG_\circ} && (30)
\end{aligned}$$



A term-by-term convergence of this series is in general not guaranteed and depends on the potential and the energy of the incident particle, even though the final expression is always valid. Physically, an incoming particle undergoes a sequence of *multiple scattering* events from the potential. The first term in the series expansion (29) describes single scattering processes of the incident wave, while the following terms describe then scattering processes of successively higher order. Rarely are higher-order terms calculated analytically, since the complications then become so great that one might as well use a numerical method to obtain the exact solution if this is possible at all. Thus, only the first iteration of the series is taken into account, i.e. only single scattering, and the T matrix is approximated by the potential matrix $V(\mathbf{k}',\mathbf{k})$,



$$T(\mathbf{k}',\mathbf{k}) \simeq V(\mathbf{k}',\mathbf{k}). \tag{31}$$

This first order term, in which the exact wave function $\psi'_{\mathbf{k}}(\mathbf{r}')$ in the integral kernel is replaced by the plane wave $e^{i\mathbf{kr}'}$ is the *first Born approximation* and typically abbreviated as the *Born approximation*.[5] This approximation is most useful when calculating the scattering amplitude.

[4] Please note that $\psi^{(n)}_{\mathbf{k}} = (G_\circ V)^n \psi'^{(0)}_{\mathbf{k}}$. This is different from definition $\psi'^{(n)}_{\mathbf{k}}(\mathbf{r})$ in (27).

[5] It should not be confused with the Born-Oppenheimer approximation.

In first Born approximation the general equation for the scattering amplitude (25) reads then

$$f_{\mathbf{k}}^{(1)}(\hat{\mathbf{r}}) = -\frac{2m}{\hbar^2}\frac{1}{4\pi}\int d^3r'\, e^{-i\mathbf{k}'\mathbf{r}'}V(\mathbf{r}')\, e^{i\mathbf{k}\mathbf{r}'} = -\frac{2m}{\hbar^2}\frac{1}{4\pi}V(\mathbf{Q}) \quad \text{with} \quad \mathbf{Q}=\mathbf{k}-\mathbf{k}', \tag{32}$$

with $V(\mathbf{Q})$ denoting the Fourier transform of the potential with the momentum transfer $\mathbf{Q}$.[6] $V(\mathbf{Q})$ can be interpreted as a transition-matrix describing the transition from the incoming plane-wave of state $\mathbf{k}$ into the outgoing plane-wave state $\mathbf{k}'$ due to the action of the potential expressed in the reciprocal space at scattering angle $\mathbf{Q}$. From (16) follows then the differential cross section

$$\left(\frac{d\sigma}{d\Omega}\right)^{(1)} = \left(\frac{2m}{\hbar^2}\right)^2\frac{\pi}{2}|V(\mathbf{Q})|^2. \tag{33}$$

The physics behind the 1st Born approximation is provided by the assumption that the incoming wave scatters only *once* inside the target potential before forming the scattered wave $\psi^{(1)}$. This is the concept behind the *kinematic theory of scattering*, that simplifies the interpretation of the scattering experiment substantially. For example, for the case of elastic scattering that we assumed all the time during the derivations, energy is conserved $|\mathbf{k}|^2 = |\mathbf{k}'|^2$, all possible scattering vectors are placed on the so-called *Ewald sphere* with radius $|\mathbf{k}|$. The length of the *scattering vector* $\mathbf{Q}$ is then given by

$$Q(\Omega) = |\mathbf{Q}| = 2\,|\mathbf{k}|\,\sin\frac{1}{2}\Omega = \frac{4\pi}{\lambda}\,\sin\frac{1}{2}\Omega \qquad \text{with} \qquad \Omega=(\theta,\phi)\sphericalangle(\mathbf{k}',\mathbf{k}). \tag{34}$$

Note, and this is the essence of the Ewald-sphere, that this shows that the differential cross section (33) does not depend on scattering angle and beam energy independently, but on a single parameter through the combination $Q = 2k\,\sin\frac{1}{2}\Omega$. By using a range of energies, $\mathbf{k}$, for the incoming particles, this dependence can be used to test whether experimental data can be well described by the Born approximation. A very common use of the Born approximation is, of course, in reverse. Having found $\frac{d\sigma}{d\Omega}$, experimentally, a reverse Fourier transform can be used to obtain the form of the potential.

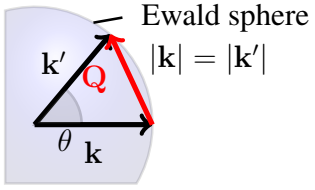


Fig. 4: *The Ewald sphere.*

4.1 Example of Born Approximation: Central Potential

For a centrally symmetry potential, $V(\mathbf{r}) = V(r)$, we can make some progress with the matrix element integral (32) if we choose a polar coordinate system with $\mathbf{Q}$ along the z-axis, so that $\mathbf{Q}\cdot\mathbf{r} = Qr\cos\theta$. Then, the scattering amplitude in Born approximation $f^{(1)}(\theta)$ is written after some manipulations in the form

$$f_k^{(1)}(\theta) = -\frac{2m}{\hbar^2}\frac{1}{Q}\int_0^\infty V(r)\, r\, \sin Qr\, dr \tag{35}$$

and is seen to be independent of ϕ due to the cylindrical symmetry of the problem at hand and all scattering vectors are placed on an Ewald-circle. An example, is the *Rutherford* scattering or Coulomb scattering, respectively, where a charged particle with charge $Z_1\mathrm{e}$ impinges on an

[6] It would be mathematically more correct to denote the Fourier transformation $\mathcal{F}$ of $V(\mathbf{r})$ by a different function name e.g. $\widetilde{V}(\mathbf{Q}) = \mathcal{F}[V(r)]$. To avoid incomprehension of reading due to unduly complicated notation we replace $\widetilde{V}(\mathbf{Q})$ by $V(\mathbf{Q})$.

other charged particle with charge $Z_2\mathrm{e}$ under the action of a Coulomb potential, which results into the scattering amplitude

$$f_k^{(1)}(\theta) = -\frac{2m}{\hbar^2}\frac{Z_1 Z_2}{Q^2}\mathrm{e}^2 = -\frac{1}{4}\frac{Z_1 Z_2}{\sin^2\frac{1}{2}\theta}\mathrm{e}^2\frac{1}{E} \tag{36}$$

and the differential cross section,

$$\left(\frac{d\sigma}{d\theta}\right)^{(1)} = \left|\frac{1}{4}\frac{Z_1 Z_2}{\sin^2\frac{1}{2}\theta}\mathrm{e}^2\right|^2 \frac{1}{E^2} \tag{37}$$

known as the *Rutherford formula*. Due to the long-range nature of the Coulomb scattering potential, the boundary condition on the scattering wave function does not apply. We can, however, address the problem by working with the screened (Yukawa) potential, $V(r) = \frac{Z_1 Z_2}{r}e^{-\kappa r}$, leading to $f^{(1)} \propto \frac{1}{Q^2+\kappa^2}$ and taking $\kappa \to 0$, which leads then to the Rutherford formula (37). Accidentally, the first Born approximation gives the correct result of the differential cross section for the Coulomb potential.

4.2 Example of Born Approximation: Square Well Potential

Consider scattering of particles interacting via a spherical three dimensional (3D) square well potential $V(r) = V_\circ$ for $r \le R_\circ$ and zero outside ($V(r) = 0$ for $r > R_\circ$). The integral (35) for the scattering amplitude required here is then

$$f_k^{(1)}(\theta) = \frac{2m}{\hbar^2}\frac{1}{Q}\int_0^{R_\circ} V_\circ\, r\, \sin Qr\, dr = \frac{2m}{\hbar^2}\frac{1}{Q}V_\circ\left[\frac{\sin Qr - Qr\cos Qr}{Q^2}\right]_0^{R_\circ} \tag{38}$$

[7] and whence to the differential cross section

$$\left(\frac{d\sigma}{d\theta}\right)^{(1)} = \left(\frac{2m}{\hbar^2}\frac{V_\circ}{Q}\right)^2 R_\circ^2\, j_1^2(QR_\circ) \simeq \left(\frac{2m}{\hbar^2}\frac{V_\circ}{Q}\right)^2 \begin{cases} \frac{1}{9}\left(1-\frac{1}{5}Q^2R_\circ^2\right) & \text{for low } E, \quad kR_\circ < 1 \\ \frac{R_\circ^2}{Q^2} & \text{for high } E, \quad kR_\circ > 1 \end{cases}. \tag{39}$$

From integrating over θ and ϕ the low and high energy limits for the total cross section are

$$\sigma(E\to\infty) = \pi\left(\frac{2m}{\hbar^2}\right)^2\left(\frac{V_\circ R_\circ^3}{kR_\circ}\right)^2 \qquad \sigma(E\to 0) = \sigma(E\to\infty)\frac{8}{9}\left(k^2R_\circ^2 - \frac{2}{5}k^4R_\circ^4 + \cdots\right). \tag{40}$$

The two examples illustrate some general features of scattering in the Born approximation:
(i) Born approximation is based on perturbation theory, so it works best for high energy particles.
(ii) At high energy, the scattering amplitude and the cross section are inversely proportional to the energy ($E = \hbar^2k^2/2m$). E.g. both become smaller and the scattering weaker with increasing energy. This is a general phenomenon, if no bound states appear in the vicinity of the energy. This can be seen best by inspecting the Fourier transformed Green function $G_\circ(k|E) \propto 1/(E - \frac{h^2k^2}{2m})$ that is inverse proportional to the energy.
(iii) Scattering depends on square of the interaction potential, e.g. $V_\circ^2$, so both attractive and

[7] $j_0(Qr) = \sin Qr/Qr$ is the spherical Bessel function for angular momentum $\ell = 0$. Radial integration leads to Bessel function $j_1(Qr)$.

repulsive potentials behave the same.
(iv) The dependence on the energy of the incident beam k and scattering angle θ arises only through the combination $Q = 2k \sin \frac{\theta}{2}$. Thus as energy increases, the scattering angle θ is reduced and the scattered beam becomes more peaked in the forward direction.
(v) Angular dependence depends on the range of the potential $R_\circ$ but not on the strength $V_\circ$.
(vi) The total cross section depends on both range $R_\circ$ and depth $V_\circ$ of the potential.

4.3 Validity of first Born Approximation

This raises the practical questions (i) under which conditions the Born expansion converges and (ii) whether the first term is a good approximation. In the Born approximation the T matrix is approximated by the potential matrix V. This will not work if the denominator $|1 - VG_\circ|$ in (30) is small or zero. This is the situation at low energy, when the energy of the incoming beam coincides with bound states of the potential. Then, the Born approximation is invalid and the Born expansion will not converge. The solution to this problem is provided by the *dynamical scattering theory* discussed in Chapter A3. According to (30) the Born approximation $T \simeq V$ is equivalent to the condition

$$\left| \int\int_{\mathbb{T}} d^3r \, d^3r' \, V(\mathbf{r}) G_\circ(\mathbf{r}, \mathbf{r}'|E) V(\mathbf{r}') \right| \ll 1 \,. \tag{41}$$

At the same time this condition determines the radius of convergence of the Born series with respect to the strength of the potential. This condition means that the first Born approximation is valid and the Born series converges if the potential is sufficiently weak and the approximation improves as the energy is increased. Concerning the question whether the first term is itself a good approximation to the wave function, a convenient, although nonrigorous, criterion can be obtained by requiring that the first-order correction to the wave function be small compared to the incident wave in the region of the potential, i.e. $|\psi_{\mathbf{k}}^{\prime(1)}(\mathbf{r})| \ll |\psi_{\mathbf{k}}^{\prime(0)}(\mathbf{r})|$ which results to

$$\frac{2m}{\hbar^2} \frac{1}{4\pi} \left| \int_{\mathbb{T}} d^3r' \, e^{-ikr'} V(\mathbf{r}') \, e^{-i\mathbf{k}\mathbf{r}'} \right| \ll 1. \tag{42}$$

For the above introduced spherical 3D square well potential $V(r \leq R_\circ) = V_\circ$ and $V(r > R_\circ) = 0$, this implies

$$\left| \frac{mV_\circ}{\hbar^2 k^2} \left(e^{ikR_\circ} \sin kR_\circ - kR_\circ \right) \right| \ll 1. \tag{43}$$

or

$$\frac{m}{\hbar^2} |V_\circ| R_\circ^2 \ll 1 \qquad \text{for low energies } kR_\circ < 1 \tag{44}$$

$$\frac{m}{\hbar^2} |V_\circ| R_\circ \frac{1}{k} \ll 1 \qquad \text{for high energies } kR_\circ > 1. \tag{45}$$

Since a bound state for this potential exists when $\frac{m}{\hbar^2}|V_\circ|R_\circ^2 \gtrsim 1$, as said above, the Born approximation will not be valid at low energies if the potential is so strong that it has a bound state. On the other hand criterion (45) can be satisfied for any potential by going to sufficiently high energy. When we square criterion (45) and multiply it by the geometrical cross section $\sigma_{\text{geo}} = \pi R_\circ^2$, criterion (45) reads

$$\pi \left(\frac{2m}{\hbar^2} \right)^2 \left(\frac{V_\circ R_\circ^3}{kR_\circ} \right)^2 \ll \pi R_\circ^2 \qquad \Longleftrightarrow \qquad \sigma_{\text{tot}} \ll \sigma_{\text{geo}}. \tag{46}$$

and provides a hand-waving criterion when the potential is sufficiently weak so that the Born approximation gives reliable results: If the ratio of the scattering cross section and the geometrical extension of the potential is small, $u := \frac{\sigma_{\rm tot}}{\sigma_{\rm geo}} \ll 1$, the Born approximation can be used. For x-ray and neutron scattering, the scattering cross sections amount to a few 10^{-24} cm^2, the cross-sectional area per atom is of the order of several 10^{-16} cm^2. This results indeed in a very small potential strength of $u \sim 10^{-8} \div 10^{-7}$ for scattering on different atoms: that means, the Born approximation is justified and the easy-to-interpret kinematic interpretation of scattering results is sufficient. The arguments become invalid for the nuclear scattering of neutrons by individual nuclei as the cross-sectional area of a nucleus is eight orders of magnitude smaller and the scattering cross section and the geometrical gross section can be of similar size and the potential strength u can be even larger than 1, $u > 1$. Due to the strong Coulomb interaction potential, the probability for multiple scattering processes of electrons in solids is extremely high, making the interpretation of electron diffraction experiments very difficult. Although in neutron and x-ray scattering, the first Born approximation is almost always adequate, even for neutrons and x-rays, the kinematic scattering theory can break down, for example in the case of Bragg scattering from large nearly perfect single crystals. In this case as in the case of electron scattering the wave equation has to be solved exactly under the boundary conditions given by the crystal geometry. This is then called the dynamic scattering theory discussed in Chapter A3. For simple geometries, analytical solutions can be obtained. Other examples where the Born series do not converge are neutron optical phenomena like internal total reflection in a neutron guide, or grazing-incidence small-angle neutron scattering (GISANS). The same holds for x-ray scattering for example in combination with grazing-incidence small-angle x-ray scattering (GISAXS) experiments. The *grazing-incidence small-angle scattering (GISAS)* techniques and their application will be discussed in Chapter D2. The theoretical analysis makes use of the *distorted-wave Born approximation (DWBA)*.

4.4 Distorted-Wave Born Approximation (DWBA)

In the previous Section we discussed that the Born approximation is accurate if the scattered field is small, compared to the incident field, in the scatterer. The scatterer is treated as a perturbation to free space or to a homogeneous medium, and the incident wave is a plane wave. When this smallness criteria is not met, it is often possible to generalize the idea of the Born approximation, which is frequently referred to as the distorted-wave Born approximation (DWBA). In generalization to the Born approximation, the free space zero-potential, $V_\circ(\mathbf{r}) = 0$, is replaced by a non-trivial reference potential $V_1(\mathbf{r})$ to which the scattered field $\psi'^1_{\mathbf{k}}$ is known analytically, numerically, e.g. due to the solution of the Lippmann-Schwinger equation (20),

$$\psi'^1_{\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{kr}} + \int_{\mathbb{T}} d^3r' G_\circ(\mathbf{r},\mathbf{r}'|E)\, V_1(\mathbf{r}')\, \psi'^1_{\mathbf{k}}(\mathbf{r}'), \tag{47}$$

or experimentally. The interaction of interest V

$$V(\mathbf{r}) = V_1(\mathbf{r}) + \delta V(\mathbf{r}) \qquad \text{with} \qquad |\delta V| \ll |V_1| \tag{48}$$

is treated as a perturbation δV to the reference system V_1. In the distorted-wave Born approximation, the scattering field $\psi'_{\mathbf{k}}(\mathbf{r})$ due to the potential V is then determined applying the Born approximation

$$\psi'_{\mathbf{k}}(\mathbf{r}) = \psi'^1_{\mathbf{k}}(\mathbf{r}) + \int d^3r' G_1(\mathbf{r},\mathbf{r}'|E)\, \delta V(\mathbf{r}')\, \psi'^1_{\mathbf{k}}(\mathbf{r}') \tag{49}$$

to the description of the scattering of the incident wave $\psi'^1_{\mathbf{k}}(\mathbf{r})$, the so-called "distorted" wave, due the perturbative potential $\delta V(\mathbf{r})$. The "distorted" incident wave, is the outgoing-wave solution of

$$\left[\frac{\hbar^2}{2m}\nabla^2 - V_1(\mathbf{r}) + E\right]\psi'^1_{\mathbf{k}}(\mathbf{r}) = 0, \tag{50}$$

that is supposed to be known, and $G_1(\mathbf{r},\mathbf{r}'|E)$ is the corresponding Green function with the outgoing boundary condition for the same potential,

$$\left[\frac{\hbar^2}{2m}\nabla^2 - V_1(\mathbf{r}) + E\right]G_1(\mathbf{r},\mathbf{r}'|E) = \delta(\mathbf{r}-\mathbf{r}'). \tag{51}$$

In analogy to the potential-free case (19), the difference to the reference system that appears in the Schrödinger equation, $\delta V(\mathbf{r})\psi'^1_{\mathbf{k}}(\mathbf{r})$, can be considered as inhomogeneity that constitutes a Lippmann-Schwinger equation with $\psi'^1_{\mathbf{k}}(\mathbf{r})$ as homogeneous solution. The Born approximation to this equation is given by Eq. (49).
To satisfy the boundary conditions we must also require that the "distorted" wave function behaves in the asymptotic limit as plane wave plus an outgoing wave

$$\psi'^1_{\mathbf{k}}(\mathbf{r}) \stackrel{r\to\infty}{\longrightarrow} e^{i\mathbf{k}\mathbf{r}} + \frac{1}{r}e^{ikr}f^1_{\mathbf{k}}(\theta,\phi), \tag{52}$$

where, as in (25)

$$f^1_{\mathbf{k}}(\theta,\phi) = -\frac{2m}{\hbar^2}\frac{1}{4\pi}\int d^3r'\, e^{-i\mathbf{k}'\mathbf{r}'}V_1(\mathbf{r}')\,\psi'^1_{\mathbf{k}}(\mathbf{r}'). \tag{53}$$

This is simply the scattering amplitude for the potential $V_1(\mathbf{r})$, as if it were the only potential present, assumed to be known. The total scattering amplitude $f_{\mathbf{k}}(\theta,\phi)$ is

$$f_{\mathbf{k}}(\theta,\phi) = f^1_{\mathbf{k}}(\theta,\phi) + \delta f_{\mathbf{k}}(\theta,\phi) \tag{54}$$

where $\delta f_{\mathbf{k}}(\theta,\phi)$ is calculated in the Born approximation ($\psi'_{\mathbf{k}}(\mathbf{r}) \simeq \psi'^1_{\mathbf{k}}(\mathbf{r})$)

$$\delta f_{\mathbf{k}}(\theta,\phi) \simeq -\frac{2m}{\hbar^2}\frac{1}{4\pi}\int d^3r'\,\psi'^{1(-)*}_{\mathbf{k}'}(\mathbf{r}')\delta V(\mathbf{r}')\,\psi'^1_{\mathbf{k}}(\mathbf{r}'). \tag{55}$$

The scattering amplitude describes the scattering strength of an outgoing spherical wave. By inspection of Eq. (53) one finds that the first wave function of the integrand is a plane wave $e^{-i\mathbf{k}'\mathbf{r}'}$, whose negative sign in the exponent represents an incoming plane wave. According of the standard definition of plane waves we can write $e^{-i\mathbf{k}'\mathbf{r}'} = \psi^{(-)*}_{\mathbf{k}}$, where $(-)$ denotes the incoming boundary condition. Quite in the same way $\psi'^{1(-)*}_{\mathbf{k}'}(\mathbf{r}')$ is the known incoming wave function corresponding to the reference potential V_1.
Clearly Eq. (55) will be a good approximation if $\delta V(\mathbf{r})$ is sufficiently small, so that the additional scattering that is generated does not significantly modify the wave function. Some example in which this method is useful include scattering in which $\delta V(\mathbf{r})$ may be the spin-orbit interaction or a perturbation due to many-particle excitations, atomic scattering where $\delta V(\mathbf{r})$ may be a deviation from the Coulomb potential or from a Hartree average potential, or in case of scattering at a magnetic superlattice where $V_1(\mathbf{r})$ contains the scattering at the nuclei or electron charge distribution plus the interaction to an average magnetization, and $\delta V(\mathbf{r})$ describes the interaction to the modulated magnetic structure of the superlattice. The DWBA is at place analyzing grazing-incidence small-angle scattering (GISAS) experiments to resolve the magnetic structure of superlattices [6].

5 Method of Partial Wave Expansion

The differential equation formulation of scattering provides additional insights that are not readily apparent from the integral equation discussed in the previous section. Many potentials in nature are spherically symmetric, or nearly so, and thus for simplicity, here we will focus on the properties of a centrally symmetric potential, $V(r)$, where the scattering wave function, $\psi'(\mathbf{r})$ (and indeed that scattering amplitudes, $f(\theta)$) must be symmetrical about the axis of incidence, and hence independent of the azimuthal angle, ϕ. The method of partial wave expansion is inspired by the observation that a plane wave $\psi_{\mathbf{k}} = e^{i\mathbf{kr}}$ can actually be written as a sum over spherical waves

$$\psi_{\mathbf{k}} = e^{i\mathbf{kr}} \;=\; e^{ikr\cos\theta} \;=\; \sum_{\ell=0}^{\infty}(2\ell+1)\, i^{\ell} j_{\ell}(kr) P_{\ell}(\cos\theta)\,, \tag{56}$$

known as the Rayleigh expansion. As we shall discuss in more detail below, the real function is a standing wave, made up of incoming and outgoing waves of equal amplitude. The radial functions $j_\ell(kr)$ appearing in the above expansion of a plane wave in its spherical components are the *spherical Bessel functions*, discussed below.
Generalizing this concept, if we define the direction of the incident wave $\mathbf{k}$ to lie along the z-axis, and θ denotes the scattering angle to the detector, $\theta = \sphericalangle(\mathbf{k}, \mathbf{r})$, then the azimuthal rotational symmetry of plane waves and the spherical potential around the direction of the ingoing wave ensures that the wave function can be expanded in a series

$$\psi(\mathbf{r}) = \psi(r,\theta) = \sum_{\ell=0}^{\infty} (2\ell+1) i^{\ell}\, R_{\ell}(r)\, P_{\ell}(\cos\theta) \tag{57}$$

of Legendre polynomials $P_\ell(\cos\theta) = \sqrt{\frac{4\pi}{2\ell+1}} Y_{\ell 0}(\theta)$, where $Y_{\ell m}$ denotes the spherical harmonics. Each term in the series is known as a *partial wave*, and is a simultaneous eigenfunction of the angular momentum operators $\mathbf{L}^2$ and L_z having eigenvalue $\hbar^2\ell(\ell+1)$, and 0, respectively. Following standard spectroscopic notation, $\ell = 0, 1, 2, \cdots$ are referred to as $s, p, d, \cdots$ waves. The *partial wave amplitudes*, f_ℓ are determined by the radial functions, $R_\ell(r)$, defined by

$$\left[\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr} - \frac{\ell(\ell+1)}{r^2} - v(r) + k^2\right] R_{\ell}(r,E) = 0 \qquad \text{with} \qquad V(r) = 0 \quad \text{except } r \in \mathbb{RT}, \tag{58}$$

where $v(r) = \frac{2m}{\hbar^2} V(r)$ represents the effective potential and k^2 refers to the energy of the incoming beam $k^2 = \frac{2m}{\hbar^2} E_{\mathbf{k}}$. The energy $E_{\mathbf{k}}$ can be chosen positive and equal to the kinetic energy of the projectile when it is far from the scattering center. The potential $V(r)$ or $v(r)$, respectively, will be assumed to vanish sufficiently rapidly with increasing r that it may be neglected beyond some finite radius, that defines the radial target region $\mathbb{RT}$ or scattering volume, respectively. We are looking for the solution of the stationary Schrödinger equation that is consistent with the boundary condition (8) of an incident plane wave $\psi_{\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{kr}}$ and an emanating spherical scattered wave. Beyond the range of the potential, i.e. r outside the radial target region $\mathbb{RT}$, the $R_\ell(r,E)$ may be expressed in terms of the solutions of the potential free radial differential equation

$$\left[\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr} - \frac{\ell(\ell+1)}{r^2} + k^2\right] R_{\ell}(r,E) = 0. \tag{59}$$

This is a differential equation of 2nd order which has two linearly independent solutions at each energy E, known as the spherical Bessel function

$$R_\ell(r,E) = j_\ell(kr) \quad \text{with} \quad j_\ell(kr) \stackrel{rk\ll 1}{\longrightarrow} \frac{z^\ell}{(2l+1)!!} \quad \text{and} \quad j_\ell(kr) \stackrel{rk\gg 1}{\longrightarrow} \frac{1}{kr}\sin\left(kr-\ell\frac{\pi}{2}\right) \tag{60}$$

and the spherical Neumann function

$$R_\ell(r,E) = n_\ell(kr) \quad \text{with} \quad n_\ell(kr) \stackrel{rk\ll 1}{\longrightarrow} \frac{(2\ell-1)!!}{z^{\ell+1}} \quad \text{and} \quad n_\ell(kr) \stackrel{rk\gg 1}{\longrightarrow} \frac{1}{kr}\cos\left(kr-\ell\frac{\pi}{2}\right), \tag{61}$$

whereas j_ℓ and n_ℓ show a regular and irregular solutions, respectively, in the origin $r=0$ and $n!! = n(n-2)(n-4)\cdots 1$. That means any solution $R_\ell(r)$ of the radial Schrödinger equation (59) can be expressed at a given energy E for r outside $\mathbb{RT}$ as linear combination of j_ℓ and n_ℓ or in the form spherical Hankel functions

$$h_\ell^{(\pm)}(kr) = n_\ell(kr) \pm i\, j_\ell(kr) \stackrel{rk\gg 1}{\longrightarrow} \frac{1}{kr} e^{\pm i\left(kr-\ell\frac{\pi}{2}\right)}, \tag{62}$$

a different set of independent solutions that correspond to incident $(-)$ and emanating $(+)$ radial waves at large distances r. This holds also for the wave function of the incident beam before scattering expressed in terms of a plane wave

$$\psi_{\mathbf{k}} = e^{i\mathbf{kr}} = \sum_{\ell=0}^{\infty}(2\ell+1)\, i^\ell j_\ell(kr) P_\ell(\cos\theta) = \frac{i}{2}\sum_{\ell=0}^{\infty}(2\ell+1)\, i^\ell \left(h_\ell^{(-)}(kr) - h_\ell^{(+)}(kr)\right) P_\ell(\cos\theta), \tag{63}$$

that can be recast according to Rayleigh into incoming and outgoing spherical Hankel functions. After scattering, the incoming spherical wave $h_\ell^{(-)}$ is unaffected by the scattering process, while the outgoing wave $h_\ell^{(+)}$ is modified by a herewith introduced quantity,

$$S_\ell(k) \quad \text{or} \quad S_\ell(E) = e^{i2\delta_\ell(E)}, \tag{64}$$

the *partial wave scattering matrix*, subject to the constraint $|S_\ell(k)| = 1$ following from the conservation of particle flux (current density times area). $\delta_\ell(E)$ is the *phase shift* (the name becomes clear below as the phase difference between incoming and outgoing wave). For scattering processes where the net flux of particles is zero, the phase shift is real, and thus only the phase and not the amplitude of the outgoing spherical wave is affected but the presence of the potential. The wave after scattering $\psi'(\mathbf{r})$ reads then

$$\psi'_{\mathbf{k}}(\mathbf{r}) = \psi'_{\mathbf{k}}(r,\cos\theta) = \frac{i}{2}\sum_{\ell=0}^{\infty}(2\ell+1) i^\ell \left(h_\ell^{(-)}(kr) - S_\ell(k)\, h_\ell^{(+)}(kr)\right) P_\ell(\cos\theta) \tag{65}$$

$$= \sum_{\ell=0}^{\infty}(2\ell+1) i^\ell \left(j_\ell(kr) + T_\ell(k)\, h_\ell^{(+)}(kr)\right) P_\ell(\cos\theta) \quad r \notin \mathbb{RT}. \tag{66}$$

The first term in the parenthesis proportional to j_ℓ sums up according to the Rayleigh expansion (56) to the incoming plane wave, the second describes the outgoing spherical wave multiplied by a *partial wave scattering amplitude* $f_\ell(k)$ or the *partial wave transition matrix element* $T_\ell(k)$

$$T_\ell(k) = \frac{1}{2i}(S_\ell(k)-1) = e^{i\delta_\ell(k)}\sin\delta_\ell(k) = \frac{1}{\cot\delta_\ell - i} = k f_\ell(k) \tag{67}$$

due to the presence of the interaction potential. The wave function after scattering takes the asymptotic form

$$\psi'_{\mathbf{k}}(\mathbf{r}) \simeq e^{i\mathbf{k}r} + \sum_{\ell=0}^{\infty}(2\ell+1)i^{\ell}\,T_{\ell}(k)\,\frac{1}{kr}e^{i\left(kr-\ell\frac{\pi}{2}\right)}P_{\ell}(\cos\theta) \;= e^{i\mathbf{k}r} + \frac{1}{r}e^{ikr}f_{\mathbf{k}}(\theta). \tag{68}$$

consistent with the scattering boundary condition (8) where the scattering amplitude $f_{\mathbf{k}}(\theta)$ can be related to the partial wave scattering amplitude and the phase shift as

$$f_{\mathbf{k}}(\theta) = \sum_{\ell=0}^{\infty}(2\ell+1)f_{\ell}(k)P_{\ell}(\cos\theta)\,. \tag{69}$$

Making use of the identity $\int d\Omega P_{\ell}(\cos\theta)P_{\ell'}(\cos\theta) = \frac{4\pi}{2\ell+1}\delta_{\ell\ell'}$ and the definition of the total cross section (14) one obtains

$$\sigma_{\rm tot}(k) = \int |f_{\mathbf{k}}(\theta)|^2 d\Omega = \sum_{\ell=0}^{\infty}\sigma_{\ell}(k) = \frac{4\pi}{k^2}\sum_{\ell=0}^{\infty}(2\ell+1)|T_{\ell}(k)|^2 = \frac{4\pi}{k^2}\sum_{\ell=0}^{\infty}(2\ell+1)\sin^2\delta_{\ell}(k)\,. \tag{70}$$

The total cross section is additive in the contribution of the $\sigma_{\ell}(k)$ of each partial wave. This does not mean, though, that the differential cross-section for scattering into a given solid angle is a sum over separate ℓ values, no the different components interfere. It is only when all angles are integrated over, that the orthogonality of the Legendre polynomials guarantees that the cross-terms vanish.

Notice that the scattering cross-section for particles in angular momentum state ℓ is upper bounded by

$$\sigma_{\ell}(k) \le \frac{4\pi}{k^2}(2\ell+1)\,, \tag{71}$$

which is four times the classical cross section for that partial wave impinging on, e.g. a hard sphere: Imagine semi-classically particles in an annular area, with the angular momentum $L = rp$, but $L = \hbar\ell$ and $p = \hbar k$ so $\ell = rk$. Therefore, the annular area corresponding to angular momentum between ℓ and $\ell+1$ has inner and outer radii, ℓ/k and $(\ell+1)/k$, respectively, and therefore the area $\frac{\pi}{k^2}(2\ell+1)$. The quantum result is essentially a diffractive effect.

The maximal contribution is obtained for the phase shifts $\delta_{\ell}(k) = (n+\frac{1}{2})\pi$, with $n = 0, \pm1, \pm2, \cdots$. For these energies $E_{\mathbf{k}}$, resonant scattering occurs if in addition $\delta_{\ell}(k)$ changes rapidly. On the other hand, for energies leading to phase shifts $\delta_{\ell}(k) = n\pi$ with $n = 0, \pm1, \pm2, \cdots$, the scattering amplitude and the cross section vanish.

Since for the imaginary part of the partial wave scattering amplitude (67) holds

$$\Im f_{\ell}(k) = \frac{1}{k}\sin^2\delta_{\ell}(k) = k|f_{\ell}(k)|^2 \quad \text{or more simply} \quad \Im\frac{1}{f_{\ell}(k)} = -k \tag{72}$$

and the Legendre polynomial at unity are always unity, $P_{\ell}(1) = 1$ for $\forall\ell$, and apply this to equation (69) we find that

$$\Im f_{\mathbf{k}}(0) = \frac{k}{4\pi}\,\sigma_{\rm tot}(k)\,, \tag{73}$$

a relation known as the *optical theorem*. It is a direct consequence of the flux conversation in elastic scattering and says for example that the scattering amplitudes are complex valued quantities.

Comparing equation (57) with equation (66) and replacing the definition of the partial wave transition matrix T_ℓ by the phase shift given in (67) we can write the radial wave function $R_\ell(r,E)$ after scattering outside the target region, $r \notin \mathbb{RT}$, as

$$\begin{aligned} R_\ell(r,E) &= j_\ell(kr) + h_\ell^{(+)}(kr)\, e^{i\delta_\ell(k)} \sin\delta_\ell(k) \qquad \text{for} \quad r \notin \mathbb{RT} \quad (74)\\ &= e^{i\delta_\ell(k)} \left(\cos\delta_\ell(k) j_\ell(kr) + \sin\delta_\ell(k) n_\ell(kr)\right) \quad (75)\\ &\simeq e^{i\delta_\ell(k)} \frac{1}{kr} \left(\cos\delta_\ell(k) \sin\left(kr - \ell\frac{\pi}{2}\right) + \sin\delta_\ell(k) \cos\left(kr - \ell\frac{\pi}{2}\right)\right) \quad (76)\\ &\simeq e^{i\delta_\ell(k)} \frac{1}{kr} \sin\left(kr - \ell\frac{\pi}{2} + \delta_\ell(k)\right) \qquad \text{for} \quad kr \gg 1\,. \quad (77) \end{aligned}$$

In the asymptotic limit, the radial incoming wave $j_\ell(kr) \simeq \frac{1}{kr}\sin\left(kr - \ell\frac{\pi}{2}\right)$ and the scattered wave differ by just a phase $\delta_\ell(k)$ known as the scattering phase, which gives $\delta_\ell(k)$ the name phase shift, as well as a phase phase factor $e^{i\delta_\ell(k)}$.
I would like to end this section with remarking that the scattering and transition matrices S, T, respectively, describe the scattering at different boundary condition. The scattering matrix describes the scattering from the incoming spherical wave into an outgoing spherical wave, while the transition matrix describes scattering from an incoming plane wave into an emanating spherical wave. The scattering matrix contains all the scattered and the unscattered states and the matrix elements are unity without scattering. The T matrix contains only the scattered states and it has only zero valued matrix elements in the absence of scattering.

5.1 The Born Approximation for Partial Waves

From the boundary condition (8) and the solution of the Lippmann-Schwinger equation (see Section 3) in far-field limit

$$\psi'_{\mathbf{k}}(\mathbf{r}) \simeq e^{i\mathbf{kr}} - \frac{2m}{\hbar^2}\frac{1}{4\pi}\int d^3r'\, e^{-i\mathbf{k}'\mathbf{r}'} V(\mathbf{r}')\, \psi'_{\mathbf{k}}(\mathbf{r}') \quad (78)$$

we obtained the respective definition of scattering amplitude $f(\theta)$ (25). On inserting expression (56) and (57) for the plane wave and the wave function after scattering, respectively, and integrating over the angle $d\Omega'$ one yields the radial Lippmann-Schwinger equation for the far field limit,

$$R_\ell(r,k) \simeq j_\ell(kr) - \int_{\mathbb{RT}} r'^2 dr'\, j_\ell(kr')\, v(r')\, R_\ell(r',k) \quad (79)$$

and an explicit formulation of the partial scattering amplitudes

$$f_\ell(\theta) = \frac{1}{k} e^{i\delta_\ell(k)} \sin\delta_\ell(k) = -\int_{\mathbb{RT}} r'^2 dr'\, j_\ell(kr')\, v(r')\, R_\ell(r',k) \quad (80)$$

which provides an elegant procedure to calculate the phase shift. We recall that in the first Born Approximation the exact wave function $R_\ell(r',k)$ in the integral kernel is replaced by the plane wave represented by the Bessel function $j_\ell(kr')$ and the partial-wave Born approximation of the scattering matrix and the transition matrix, respectively, reads

$$f_\ell^{(1)}(\theta) = \frac{1}{k} T_\ell^{(1)}(k) = \frac{1}{k} e^{i\delta_\ell^{(1)}(k)} \sin\delta_\ell^{(1)}(k) = -\int_{\mathbb{RT}} r'^2 dr'\, j_\ell(kr')\, v(r')\, j_\ell(kr') \approx \frac{1}{k}\delta_\ell^{(1)}(k) \quad (81)$$

with an approximate expression for the phase shift in Born approximation $\delta_\ell^{(1)}(k)$ valid for small phase shifts (the only place where the Born approximation is valid).
Concerning the Distorted-Wave Born Approxmiation (DWBA) one can also perform a partial-wave analysis of Eq. (54) to obtain an approximate expression for the phase shift. This result is

$$e^{i\delta_\ell^{(1)}(k)} \sin\delta_\ell^{(1)}(k) = e^{i\delta_\ell^1(k)} \sin\delta_\ell^1(k) - \int_{\mathbb{RT}} r'^2 dr' \, \left(R_\ell^1(kr')\right)^2 \, v(r') \,, \tag{82}$$

where $\delta_\ell^1(k)$ are the phase shifts to the nontrivial reference potential V_1, and the Bessel function representing the plane waves are replaced by the exact radial scattering solution $R_\ell^1(kr)$.

5.2 Low Energy Scattering: Scattering Phases and Scattering Length

From (81) follows that the sign of $\delta_\ell(k)$ is determined by the sign of the potential. For an attractive potential, the phase shift $\delta_\ell > 0$ is positive and the phase shift is negative, $\delta_\ell < 0$, for a repulsive potential. At large distances r, the zeros of $R_\ell(r,k) \simeq \frac{1}{kr}\sin\left(kr - \ell\frac{\pi}{2} + \delta_\ell(k)\right)$ are at $r_0 = \frac{1}{k}\left(n\pi + \ell\frac{\pi}{2} - \delta_\ell(k)\right)$. Positive (negative) $\delta_\ell(k)$ relate to an inward (outward) shift of the nodes. That means, for an attractive potential, the probability of a particle to stay in the potential range becomes greater, so that the wave function is drawn into the potential range: the nodes shift inwards, i.e. $\delta_\ell > 0$. For a repulsive potential the wave function is squeezed out of the potential range. In consequence the nodes move to the outside, i.e. $\delta_\ell > 0$.
If $kr' \ll 1$ or $\lambda \gg r'$, respectively, we shall be able to approximate the Bessel function $j_\ell(kr') \simeq \frac{1}{(2\ell+1)!!}(kr')^\ell$ and one obtains the simple estimate

$$\delta_\ell(k) \approx \left(\frac{1}{(2\ell+1)!!}\right)^2 k^{2\ell+1} \int_{\mathbb{RT}} dr' r'^{\,2\ell+2} \, v(r) \tag{83}$$

for the scattering phase. For low energies and high angular momenta the scattering phases $\delta_\ell(k)$ behave proportional to $\delta_\ell(k) \propto k^{2\ell+1}$. In particular one expects that only *s-wave scattering* ($\ell = 0$) survives for $k \to 0$ since the cross section scales as

$$\sigma_\ell(k) = \frac{4\pi}{k^2}(2\ell+1)\sin^2\delta_\ell(k) \propto k^{4\ell} \,. \tag{84}$$

When a slow particle scatters off a short ranged scatterer it cannot resolve the structure of the object since its de Broglie wavelength λ is very long, larger than the scatterer. The idea is that then it should not be important what precise potential $V(\mathbf{r})$ one scatters off, but only how the potential looks at long length scales. At very low energy the incoming particle does not see any structure, therefore to lowest order one has only a spherical symmetric outgoing wave, the so called s-wave scattering (angular momentum $\ell = 0$). At higher energies one also needs to consider p and d-wave (l = 1,2) scattering and so on.
Although exact at all energies, the partial wave method is most useful for dealing with scattering of low energy particles. This is because for slow moving particles to have large angular momentum ($\hbar kb$) they must have large impact radii b. Classically, particles with impact radius larger than the range of the potential miss the potential. Thus, for scattering of slow-moving particles we need only to consider a few partial waves, all the others are unaffected by the potential ($\delta_\ell \approx 0$). Thus at a given incoming momentum, $\hbar k$, we can determine how many terms in the partial wave expansion to consider from $\hbar k b_{\max} \approx \ell_{\max}\hbar$, where $b_{\max}$ is the maximum impact parameter for classical collision, i.e. the range of the potential $\mathbb{RT}$. Since the angular

variation of the Legendre polynomial for the angular momentum $\ell = 0$ is $P_{\ell=0}(\cos\theta) = 1$, the s-wave scattering is isotropic, consistent with the thought of averaging over the potential. Since in practical applications the expansion into Legendre polynomials has to be truncated for higher ℓ values, since otherwise the effort becomes too large, the partial wave analysis is primarily a method of approximation for low energies. It generally requires an exact (numerical) solution of the radial equations, since the Born approximation fails at low energies in general. Thus partial waves and the Born approximation are complementary methods, good for slow and fast particles, respectively.
At energy $E \to 0$, the radial Schrödinger equation for $rR_{\ell=0}$ away from the potential becomes $\frac{d^2}{dr^2} rR_{\ell=0} = 0$ with a straight line solution $rR_{\ell=0} = (r - a_s)$.[8] For the s-wave solution the approximation (77) becomes exact and the radial wave function $rR_0(r,k) = \sin(kr + \delta_0(k)) \stackrel{k\to 0}{\longrightarrow} k\left(r + \frac{1}{k}\delta_\ell(k)\right)$ can only become a straight line in r, if $\delta_0(k)$ is itself linear in k for sufficiently small k. Then $\delta_0(k) = -ka_s$, a_s being the point at which the extrapolated external wave function intersects the axis (maybe at negative r). So, as k goes to zero, the term

$$\lim_{k\to 0} k \cot\delta_0(k) = -\frac{1}{a_s} \tag{85}$$

dominates in the denominator of expression (67) where the scattering amplitude and the cross section take the expression

$$f_{\ell=0}(k \to 0) = -a_s \qquad \text{and} \qquad \sigma_{\ell=0}(k \to 0) = 4\pi a_s^2 \,. \tag{86}$$

The parameter a_s of dimension length is called the *scattering length*. At low energies it determines solely the elastic cross section. This is a nontrivial construction from the potential itself and the wave function of the state. We see that for momenta much less than the inverse radius of the potential the scattering length is sufficient to describe all of the interactions. It is clear that by measuring the scattering length of a system alone we cannot reconstruct the potential uniquely. There are infinitely many different shapes, depths and ranges of potentials that will reproduce a single scattering length.

5.3 S-Wave Scattering at Square Well Potential

The properties of scattering phases are studied for the problem of quantum scattering from an attractive spherically symmetric three-dimensional (3D) square well potential $V(r) = -\frac{\hbar^2}{2m} v_0 \Theta(R_\circ - r)$. For convenience we write $v_0 = k_v^2$. The continuity condition of the wave function R_ℓ

$$\begin{aligned} R_\ell(r,k) &= A_\ell(\kappa)\, j_\ell(\kappa r) \qquad \text{with} \qquad \kappa^2 = k^2 + k_v^2 \qquad \text{for} \quad r \le R_\circ & (87)\\ R_\ell(r,k) &= e^{i\delta_\ell(k)} \left(\cos\delta_\ell(k)\, j_\ell(kr) \,+\, \sin\delta_\ell(k)\, n_\ell(kr)\right) \qquad \text{for} \quad r \ge R_\circ & (88) \end{aligned}$$

and its derivative $R'_\ell = \frac{d}{dr} R_\ell$ at the boundary, $r = R_\circ$, where $A_\ell(\kappa)$ is a normalization constant. The wave function outside of $R_\circ$ is normalized to to incoming plane wave normalized to unity.

$$\begin{aligned} A_\ell(\kappa)\, j_\ell(\kappa R_\circ) &= e^{i\delta_\ell(k)} \left(\cos\delta_\ell(k)\, j_\ell(kR_\circ) \,+\, \sin\delta_\ell(k)\, n_\ell(kR_\circ)\right) & (89)\\ \kappa\, A_\ell(\kappa)\, j'_\ell(\kappa R_\circ) &= k\, e^{i\delta_\ell(k)} \left(\cos\delta_\ell(k)\, j'_\ell(kR_\circ) \,+\, \sin\delta_\ell(k)\, n'_\ell(kR_\circ)\right) & (90) \end{aligned}$$

[8] Normalization constant A_0 is neglected for simplicity.

translates to the following relation for the phase shifts

$$\tan\delta_\ell(k) = -\frac{k\,j'_\ell(kR_\circ) - L_\ell(E)\,j_\ell(kR_\circ)}{k\,n'_\ell(kR_\circ) - L_\ell(E)\,n_\ell(kR_\circ)} = \frac{1}{\cot\delta_\ell(k)} \qquad \text{with} \qquad L_\ell(E) = \kappa\,\frac{j'_\ell(\kappa R_\circ)}{j_\ell(\kappa R_\circ)}, \tag{91}$$

where L_ℓ is the logarithmic derivative of the wave function at the potential boundary. Here $j'_\ell(x) = \frac{d}{dx} j_\ell(x)$ and similarly for $n'_\ell(x)$.

Hard Sphere Potential

The simplest case is the scattering at a hard sphere potential:

$$v_\circ(r) = \infty \quad \text{for} \quad r < R_\circ \qquad \text{and} \qquad v_\circ(r) = 0 \quad \text{for} \quad r \geq R_\circ\,. \tag{92}$$

Since then the wave function at the boundary $r = R_\circ$ vanishes, it follows that $L_\ell(v_\circ \to \infty) \to \infty$, and the phase shift reduces to

$$\tan\delta_\ell(k) = -\frac{j_\ell(kR_\circ)}{n_\ell(kR_\circ)} \qquad s\text{-wave}: \quad \tan\delta_0(k) = -\frac{(\sin kR_\circ)/kR_\circ}{(\cos kR_\circ)/kR_\circ} = -\tan kR_\circ \tag{93}$$

so that $\delta_0(k) = kR_\circ$. Thus, the s-wave radial wave function for $r > R_\circ$ takes the form

$$R'_0(r) = e^{-ikR_\circ}\left(\cos kR_\circ \frac{\sin kr}{kr} - \sin kR_\circ \frac{\cos kr}{kr}\right) = e^{-ikR_\circ}\frac{1}{kr}\sin k(r - R_\circ). \tag{94}$$

The corresponding radial wave-function for the incident wave takes the form $R_0(r) = \frac{1}{kr}\sin kr$. It is clear that the actual $\ell = 0$ radial wave function is similar to the incident wave function, except that it is phase-shifted by $kR_\circ$. According to (86) the total s-wave cross-section of the hard wall potential yields then $\sigma^\infty_{\ell=0} = 4\pi R_\circ^2$, four times the geometric cross-section $\sigma_{\rm geo} = \pi R_\circ^2$ (i.e., the cross-section for classical particles bouncing off a hard sphere of radius $R_\circ$). However, low energy scattering implies relatively long wave-lengths, so we do not necessarily expect to obtain the classical result in this limit. Recall that the s-wave scattering is a good approximation to the low-energy scattering.
Consider the high energy limit $kR_\circ \gg 1$. At high energies, all partial waves up to $\ell_{\max} = kR_\circ$ contribute significantly to the scattering cross-section. With so many ℓ values contributing, it is legitimate to replace $\sin^2\delta_\ell$ in the expression (70) for the partial wave cross section by its average value $1/2$ and thus (for comparison we include also the low energy result, i.e. $kR_\circ \ll 1$)

$$\sigma^\infty_{\rm tot}(kR_\circ \ll 1) \simeq \sigma^\infty_{\ell=0} = 4\pi R_\circ^2 \qquad \text{and} \qquad \sigma^\infty_{\rm tot}(kR_\circ \gg 1) \simeq 2\pi R_\circ^2\,. \tag{95}$$

This is twice the classical result $\sigma_{\rm geo} = \pi R_\circ^2$, which is somewhat surprising, since we might expect to obtain the classical result in the short wave-length limit. For hard sphere scattering, incident waves with impact parameters less than $R_\circ$ must be deflected. However, in order to produce a "shadow" behind the sphere, there must be scattering in the forward direction (recall the optical theorem) to produce destructive interference with the incident plane-wave. In fact, the interference is not completely destructive, and the shadow has a bright spot in the forward direction. The effective cross-section associated with this bright spot is $\pi R_\circ^2$ which, when combined with the cross-section for classical reflection, $\pi R_\circ^2$, gives the actual cross-section of $2\sigma_{\rm geo}$.

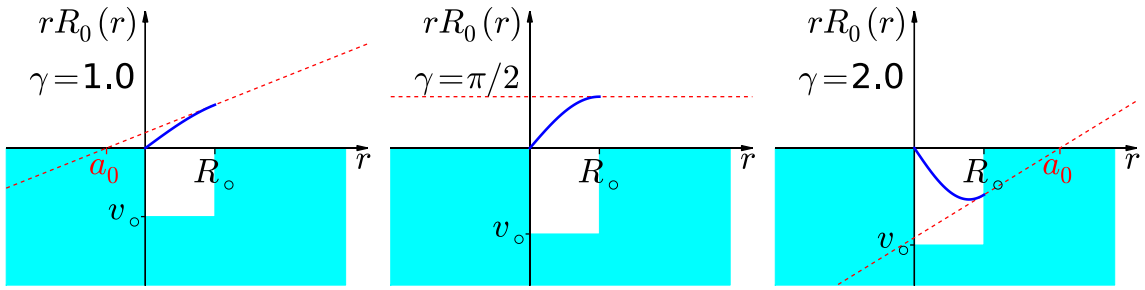


Fig. 5: *Radial scattering wave function, $rR_0(r)$, for three-dimensional square well potential of radius $R_\circ$ for $kR_\circ = 0.1$ and $\gamma = k_v R_\circ = 1$ (left), $\pi/2$ (middle) and 2 (right). Note that the scattering length, a_0 changes from negative to positive as system passes through bound state.*

Soft Sphere Potential

For a potential with finite scattering strength $V(r) = -\frac{\hbar^2}{2m} v_\circ(r)$ the logarithmic derivative of the scattering potential L_ℓ is finite. Analogously to (93) for s-wave scattering, Eq. (93) is simplified to

$$\tan\delta_0(k) = \frac{k\tan(\kappa R_\circ) - \kappa\tan(kR_\circ)}{\kappa + k\tan(kR_\circ)\tan(\kappa R_\circ)}. \tag{96}$$

Then, unless $\tan(\kappa R_\circ) = \infty$, an expansion at low energy (small k) yields $\delta_0(k) \simeq kR_\circ \times$ $\times \left(\frac{\tan(\kappa R_\circ)}{\kappa R_\circ} - 1\right)$, and the $\ell = 0$ partial cross section,

$$\sigma_{\ell=0}(k) = \frac{4\pi}{k^2}\sin^2\delta_0(k) = \frac{4\pi}{k^2}\frac{1}{1+\cot^2\delta_0(k)} \simeq \frac{4\pi}{k^2}\delta_0^2(k) = 4\pi R_\circ^2\left(\frac{\tan(\kappa R_\circ)}{\kappa R_\circ} - 1\right) \tag{97}$$

From this result we find that, when $\frac{\tan(\kappa R_\circ)}{\kappa R_\circ} = 1$, the scattering cross-section vanishes. An expansion in small k obtains,

$$k\cot\delta_0(k) = -\frac{1}{a_0} + \frac{1}{2}r_0 k^2 + \cdots, \tag{98}$$

where $a_0 = \left(1 - \frac{\tan(k_v R_\circ)}{k_v R_\circ}\right) R_\circ$, defines the scattering length a_0 or a_s, respectively, and r_0 is the effective range of the interaction that is obtained from the Taylor expansion of (96) for small $kR_\circ$. At low energies, $k \to 0$, the scattering cross section, $\sigma_0 = 4\pi a_0^2$ (see above) is fixed by the scattering length alone. If $|k_v R_\circ| \ll 1$, a_0 is negative. As $k_v R_\circ$ is increased, when $k_v R_\circ = \pi/2$, both a_0 and σ_0 diverge there is said to be a zero energy resonance. This condition corresponds to a potential well that is just able to support an s-wave bound state at zero energy. If $k_v R_\circ$ is further increased, a_0 turns positive as it would be for an effective repulsive interaction until $k_v R_\circ = \pi$ when $\sigma_0 = 0$ and the process is repeated with the appearance of a second bound state at $k_v R_\circ = 3/2$, and so on. Since the scattering state must be orthogonal to all bounded states of the potential $V(r)$, the radial wave function of the scattering state must be orthogonal to all radial wave functions of bound states at equal angular momentum ℓ.[9] Consider the situation of a potential that supports at a given energy two bound states of s character. Then the scattering

[9]The orthogonality to states of different ℓ is automatically taken care of by orthogonality conditions of the angular part of the wave function.

wave should also have two additional nodes, which moves the scattering phase δ_ℓ about 2π. This is quantitatively expressed by the *Levinson Theorem*

$$\delta_\ell(k=0) = N_\ell \pi \tag{99}$$

where N_ℓ is the number of bound states at given angular momentum ℓ. If $\delta_\ell(k)$ is increasing rapidly through an odd multiple of $\pi/2$, $\sin^2\delta_\ell = 1$ the ℓ-th partial cross-section takes its maximum value and the cross-section exhibits a narrow peak as a function of energy and there is said to be a resonance. The analysis leads to the Breit-Wigner formula that goes beyond the scope of this lecture.

5.4 Nuclear Scattering Length

Two fundamental interactions govern the scattering of neutrons by an atomic system and define the neutron scattering cross-section measured in an experiment. The residual strong interaction, also known as the nuclear force, gives rise to scattering by the atomic nuclei (nuclear scattering). The electromagnetic interaction of the neutron's magnetic moment with the sample's internal magnetic fields gives rise to magnetic scattering. The latter is neglected in this chapter. The nuclear force is not weak as it is responsible for holding together protons and neutrons in the nucleus. However, it has extremely short range, 10^{-13} cm to 10^{-12} cm, comparable with the size of the nuclei, and much smaller than the typical distances in solids and much smaller than the typical neutron's wavelength. Consequently, away from the conditions of the resonance neutron capture, the probability of a neutron being scattered by an individual nucleus is very small. To describe the neutron's interaction with the atomic system in which the typical distances are about 1 Å (10^{-8} cm), the nuclear scattering length operator $\mathbf{b}_\mathrm{N}$ can be effectively treated as a δ-function in the coordinate representation

$$\mathbf{b}_\mathrm{N} = b_\mathrm{N}\delta(\mathbf{r} - \mathbf{R}_\mathrm{N})\,, \tag{100}$$

where $\mathbf{r}$ is a coordinate of a neutron and $\mathbf{R}_\mathrm{N}$ is that of a nucleus. Alternatively, in the momentum representation it is just a number (for the nucleus fixed at the origin), $\mathbf{b}_\mathrm{N}(\mathbf{Q}) = b_\mathrm{N}$, independent of the incident neutron's wave vector and of the wave-vector transfer, $\mathbf{Q}$. This again indicates that the applicability of such treatment is limited to neutrons whose wavelength is large enough compared to the size of the nuclei. In the Born approximation, Eq. (100) for the scattering length would correspond to the neutron-nucleus interaction,

$$V(\mathbf{r}, \mathbf{R}_\mathrm{N}) = -4\pi\frac{\hbar^2}{2m_\mathrm{n}} b_\mathrm{N}\delta(\mathbf{r} - \mathbf{R}_\mathrm{N}) \tag{101}$$

generally known as the Fermi pseudopotential [7, 8]. In Eqs. (100) and (101), the scattering length refers to the fixed nucleus. Usually, it is treated as a phenomenological parameter that is determined experimentally [9].

6 Scattering from a Collection of Scatterers

Finally, after having considered so far only the scattering at a single site with the target potential $V(\mathbf{r})$ placed at position $\mathbf{R}_\tau = \mathbf{0}$, prior to closing this chapter we shall relate these derivations

to the scattering phenomena in solid state systems with the potential composed of an assembly of targets

$$V(\mathbf{r}) = \sum_\tau v_\tau(\mathbf{r} - \mathbf{R}_\tau) \tag{102}$$

centered at a collection of sites $\mathbf{R}_\tau$. Inserting this into the Lippmann-Schwinger equation (20), replacing the integration variable $\mathbf{r}'$ by a vector $\mathbf{r}'_\tau \in \mathbb{T}_\tau$ within the target τ and the center-of-gravity-vector $\mathbf{R}_\tau$, $\mathbf{r}'_\tau + \mathbf{R}_\tau$, and taking into consideration that the free-space Green function $G_\circ(\mathbf{r}, \mathbf{r}'|E)$ depends only on $\mathbf{r} - \mathbf{r}'$, the Lippmann-Schwinger equation for many potentials can be written as

$$\psi'_\mathbf{k}(\mathbf{r}) = \psi_\mathbf{k}(\mathbf{r}) + \sum_\tau \int_{\mathbb{T}_\tau} d^3r'_\tau G_\circ(\mathbf{r} - \mathbf{R}_\tau, \mathbf{r}'_\tau|E)\, V(\mathbf{r}'_\tau)\, \psi'_\mathbf{k}(\mathbf{r}'_\tau + \mathbf{R}_\tau). \tag{103}$$

Approximating the Green function by its far-field asymptotic form (23) and considering that in the far-field solution $\psi'_\mathbf{k}(\mathbf{r}'_\tau + \mathbf{R}_\tau) \simeq e^{i\mathbf{k}\mathbf{R}_\tau}\psi'_\mathbf{k}(\mathbf{r}'_\tau)$, behind which is the Huygens' principle where the wave function generated at different sites share a phase relation, which becomes exact in the limit of the Born approximation, one obtains the asymptotic solution of the wave function $\psi'_\mathbf{k}(\mathbf{r})$ for large distances $\mathbf{r}$

$$\psi'_\mathbf{k}(\mathbf{r}) \simeq e^{i\mathbf{k}\mathbf{r}} + \sum_\tau \frac{1}{|\mathbf{r} - \mathbf{R}_\tau|} e^{ik|\mathbf{r}-\mathbf{R}_\tau|} e^{i\mathbf{k}\mathbf{R}_\tau} f_\mathbf{k}(\widehat{\mathbf{r} - \mathbf{R}_\tau}) \tag{104}$$

Since in the far-field approximation (22), $r \gg R_\tau$, $k|\mathbf{r} - \mathbf{R}_\tau| \simeq k(r - \hat{\mathbf{r}} \cdot \mathbf{R}_\tau) = kr - \mathbf{k}' \cdot \mathbf{R}_\tau$, we shall rewrite the asymptotic solution of the wave function for scattering at many potentials as

$$\psi'_\mathbf{k}(\mathbf{r}) \simeq e^{i\mathbf{k}\mathbf{r}} + \frac{1}{r} e^{ikr} F(\mathbf{Q}) \qquad \text{with} \qquad F(\mathbf{Q}) = \sum_\tau P_\tau(\mathbf{Q})\, f_{\tau\mathbf{k}}(\hat{\mathbf{r}}_\tau) \qquad \text{and} \qquad \mathbf{Q} = \mathbf{k}' - \mathbf{k}\,. \tag{105}$$

where the *static structure factor* (or *structure factor* for short) $F(\mathbf{Q})$ describes the way in which an incident beam is scattered by the atoms of a solid state system, taking into account the different scattering power of the elements through the term $f_{\tau\mathbf{k}}(\hat{\mathbf{r}}_\tau)$ also called *atomic form factor*

$$f_{\tau\mathbf{k}}(\hat{\mathbf{r}}_\tau) = -\frac{2m}{\hbar^2}\frac{1}{4\pi} \int_{\mathbb{T}_\tau} d^3r'_\tau\, e^{-i\mathbf{k}'\mathbf{r}'_\tau} V(\mathbf{r}'_\tau)\, \psi'_\mathbf{k}(\mathbf{r}'_\tau) \qquad \text{with} \qquad \mathbf{r}_\tau = \mathbf{r} - \mathbf{R}_\tau \tag{106}$$

that depends only on the potential and not on the position of the atom. The atomic form factor, or scattering power, of an element depends on the type of radiation considered. Since the atoms are spatially distributed, there will be a difference in phase when considering the scattered amplitude from two atoms. This phase difference is taken into account by the phase factor

$$P_\tau(\mathbf{Q}) = e^{i\mathbf{Q}\cdot\mathbf{R}_\tau}\,, \tag{107}$$

which depends only on the position of the atoms and is completely independent of the scattering potential. So in total the structure factor separates the interference effects from the scattering within an target from the interference effects arising from scattering from different targets. Thus, the scattering intensity and the differential cross section are proportional to the square of the structure factor

$$I(\mathbf{Q}) \propto \left(\frac{d\sigma}{d\Omega}\right) = |F(\mathbf{Q}|^2 = \left|\sum_\tau P_\tau(\mathbf{Q})\, f_{\tau\mathbf{k}}(\hat{\mathbf{r}}_\tau)\right|^2 . \tag{108}$$

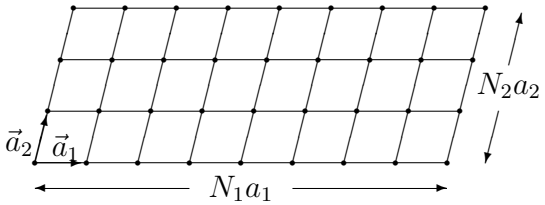
If we ignore spin degrees of freedom, so that we do not have to worry whether an electron does or does not flip its spin during the scattering process, then at low energies the scattering amplitude $f(\theta)$ of particles from a cluster of atoms or a crystal becomes independent of angle (s-wave) and maybe described by the scattering length b_τ for atom τ, i.e. $f_{\tau\mathbf{k}}(\hat{\mathbf{r}}_\tau) = b_\tau$. Then, the differential cross section simplifies to

$$\left(\frac{d\sigma}{d\Omega}\right) = \left|\sum_\tau P_\tau(\mathbf{Q})\, b_\tau\right|^2 . \tag{109}$$

If we consider scattering from a periodic crystal lattice, all atoms are same, i.e. have the same nuclear number (and we consider here also all nuclei as identical), thus $b_\tau = b$ for all atoms τ. Then, we are left with the differential cross section

$$\left(\frac{d\sigma}{d\Omega}\right) = N|b|^2 S(\mathbf{Q}) \qquad \text{with} \qquad S(\mathbf{Q}) = \frac{1}{N}\left|\sum_\tau e^{i\mathbf{Q}\mathbf{R}_\tau}\right|^2 . \tag{110}$$

$S(\mathbf{Q})$ is the form factor of the lattice, a quantity closely related to the pair density of a solid. For simplicity we consider scattering at a finite Bravais lattice. The lattice points are spanned by the lattice vector $\mathbf{R}_\tau = \mathbf{R}_\mathbf{m} = \boldsymbol{A}\mathbf{m}$, where $\boldsymbol{A}$ is the Bravais matrix consistent with the primitive vectors $(\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3)$ of the three dimensional lattice, and $\mathbf{m} = (m_1, m_2, m_3) \in \mathbb{N}^3$ with $0 \le m_i \le (N_i - 1)$. The reciprocal lattice is defined by the matrix $\boldsymbol{B}$, that is orthogonal to $\boldsymbol{A}$, $\boldsymbol{B}^T\boldsymbol{A} = 2\pi\mathbf{1}$. The reciprocal lattice vectors are given as $\mathbf{G}_\mathbf{h} = \boldsymbol{B}\mathbf{h}$ with $\mathbf{h} = (h_1, h_2, h_3) \in \mathbb{Z}^3$. The transfer of scattering momentum vector is expressed by $\mathbf{Q} = (\mathbf{Q}_1, \mathbf{Q}_2, \mathbf{Q}_3) = \boldsymbol{B}\kappa$, with $\kappa = (\kappa_1, \kappa_2, \kappa_3) \in \mathbb{R}^3$. The scattering amplitude is calculated analytically summing up the geometrical series



$$\begin{aligned}
\sum_\mathbf{m} e^{i\mathbf{Q}\mathbf{R}_\mathbf{m}} &= \sum_\mathbf{m} e^{i2\pi\kappa\mathbf{m}} = \sum_{m_1=0}^{N_1-1}\sum_{m_2=0}^{N_2-1}\sum_{m_3=0}^{N_3-1} e^{i2\pi\kappa_1 m_1} e^{i2\pi\kappa_2 m_2} e^{i2\pi\kappa_3 m_3} \\
&= \frac{1-e^{i2\pi\kappa_1 N_1}}{1-e^{i2\pi\kappa_1}} \cdot \frac{1-e^{i2\pi\kappa_2 N_2}}{1-e^{i2\pi\kappa_2}} \cdot \frac{1-e^{i2\pi\kappa_3 N_3}}{1-e^{i2\pi\kappa_3}} \\
&= e^{i2\pi(\kappa_1(N_1-1)/2+\kappa_2(N_2-1)/2+\kappa_3(N_3-1)/2)} \cdot \frac{\sin N_1\pi\kappa_1}{\sin\pi\kappa_1} \cdot \frac{\sin N_2\pi\kappa_2}{\sin\pi\kappa_2} \cdot \frac{\sin N_3\pi\kappa_3}{\sin\pi\kappa_3}
\end{aligned}$$

giving the scattered intensity

$$I(\mathbf{Q}) \propto \left(\frac{d\sigma}{d\Omega}\right) = |b|^2 \frac{\sin^2\frac{1}{2}N_1\mathbf{Q}_1\mathbf{a}_1}{\sin^2\frac{1}{2}\mathbf{Q}_1\mathbf{a}_1} \cdot \frac{\sin^2\frac{1}{2}N_2\mathbf{Q}_2\mathbf{a}_2}{\sin^2\frac{1}{2}\mathbf{Q}_2\mathbf{a}_2} \cdot \frac{\sin^2\frac{1}{2}N_3\mathbf{Q}_3\mathbf{a}_3}{\sin^2\frac{1}{2}\mathbf{Q}_3\mathbf{a}_3} . \tag{111}$$

taking into account that $2\pi\kappa_i = \mathbf{Q}_i\mathbf{a}_i$, for $i = 1, 2, 3$. The dependence of the scattering intensity on the scattering vector $\mathbf{Q}$ is given by the so-called *Laue function*, which separates according to the three Bravais vectors. One factor along one lattice direction a is plotted in Fig. 6.
The main peaks are the *Bragg reflections*. They occur at integer κ, $\kappa = (\kappa_1, \kappa_2, \kappa_3) \in \mathbb{Z}^3$, i.e. at reciprocal lattice vectors $\mathbf{Q} = \mathbf{G}_\mathbf{n}$. At points of Bragg reflection the coherent interference of scattering waves of all atoms add up constructively so that the maximum intensity scales

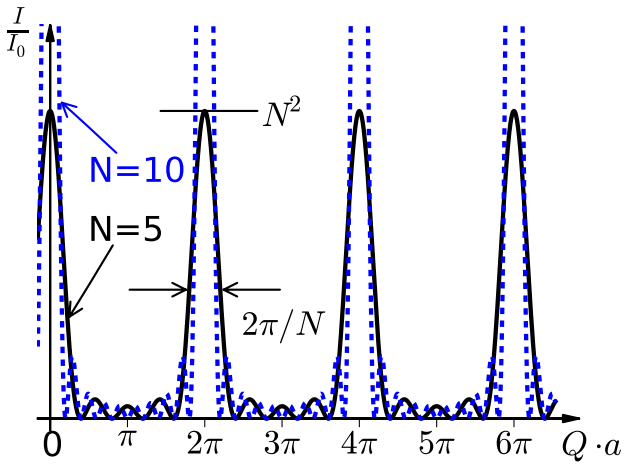


Fig. 6: *Laue function along the lattice direction a for a lattice with $N = 5$ and $N = 10$ periods.*

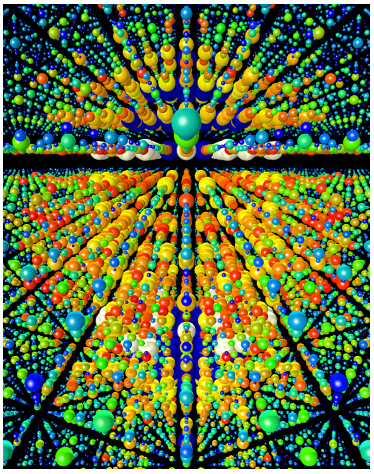


Fig. 7: *Three-dimensional rendering of x-ray diffraction data obtained from over 15 000 single nanocrystal diffraction snapshots of a protein complex [10].*

with the square of the number of periods N^2. This high intensity is the reason why the Born approximation can in general not be used to describe the scattering at Bragg peaks. At small deviations $\Delta\kappa$ from the exact Bragg condition the intensity drops fast,[10] so that the total intensity integrated over a small $\Delta\kappa$ region, $\Delta\kappa \simeq 1/N$, varies only $\simeq N$. The half width is given approximately by $\Delta Q = \frac{2\pi}{a}\frac{1}{N}$. The more periods contribute to coherent scattering, the sharper and higher are the main peaks. Between the main peaks, there are $N-2$ side maxima. With increasing number of periods N, their intensity becomes rapidly negligible compared to the intensity of the main peaks. From the position of these Bragg peaks in momentum space, the metric of the unit cell can be deduced (lattice constants a_1, a_2, a_3 in the three Bravais vector directions and unit cell angles α, β, γ). The width of the Bragg peaks is determined by the size of the coherently scattering volume $N = N_1N_2N_3$ and experimental factors (resolution) as well as details of the sample (size of crystallite, mosaic distribution, internal strains, etc.). For large N the form factor approaches a δ-function

$$\left(\frac{d\sigma}{d\Omega}\right) = N|b|^2 V_{\rm BZ}\sum_{\mathbf{h}}\delta(\mathbf{Q}-\mathbf{G_h})\,, \tag{112}$$

where $V_{\rm BZ}$ is the Brillouin-zone volume.

I shall conclude this chapter by mentioning that in 1914 the Nobel Prize in Physics was awarded to Max von Laue "for his discovery of the diffraction of x-rays by crystals" and in 1915 the Nobel Prize in Physics was awarded to Sir William Henry Bragg and William Lawrence Bragg "for their services in the analysis of crystal structure by means of x-rays". Since the pioneering

[10] For $\kappa \ll 1$ it follows that $\frac{\sin^2 N\pi\kappa}{\sin^2\pi\kappa} \approx \frac{\sin^2 N\pi\kappa}{\pi^2\kappa^2} \Longrightarrow \int\limits_{-\infty}^{\infty} d\kappa\,\frac{\sin^2 N\pi\kappa}{\sin^2\pi\kappa} \approx \frac{N}{\pi}\int\limits_{-\infty}^{\infty} dx\,\frac{\sin^2 x}{x^2} = N \Longrightarrow \bar{\kappa} \simeq 1/N.$

days of von Laue, Ewald, Knipping, Friedrich, the Bragg's, Compton, etc., diffraction experiments went a long way deciphering today the atomic arrangement of noncrystalline solids such as viruses as shown in a recent experiment [10] carried out at the Linac Coherent Light Source (LCLS), at SLAC National Accelerator Laboratory in California, USA) as shown in the diffraction image Fig. 7. Physical principles established 100 years ago and subsequent theoretical and experimental methods developed, reinvented and constantly brought to perfection contribute to day and will contribute in the future to the welfare of mankind.

Acknowledgements

I thank Dr. Phivos Mavropoulos and Prof. Peter Dederichs for discussions and Benedikt Schweflinghaus for his assistance in preparing the figures.

References

[1] J.J. Sakurai, *Modern Quantum Theory*, (Addison Wesley, 1984).

[2] Wu and Ohmura, *Quantum Theory of Scattering*, (Prentice Hall, 1962).

[3] A. S. Davidov, *Quantum Mechanics*, (Pergamon Press, 1991)

[4] N. W. Ashcroft and N. D. Mermin, *Solid State Physics*, (Brooks Cole, 1976)

[5] Chr. Huygens, Trait de la Lumiere (completed in 1678, published in Leyden in 1690)

[6] Sabrina Disch, Erik Wetterskog, Raphaël P. Hermann, German Salazar-Alvarez, Peter Busch, Thomas Brückel, Lennart Bergström, and Saeed Kamali, Nano Lett. **11**, 1651 (2011).

[7] G. L. Squires, *Introduction to the theory of thermal neutron scattering*, (Cambridge: Cambridge University Press, 1978); (New York: Dover Publications, 1996).

[8] E. Fermi, Ric. Sci. **7**, 13 (1936).

[9] E. Fermi, and L. Marshall, Phys. Rev. **71**, 666 (1947); Phys. Rev. **72**, 408 (1947).

[10] Henry N. Chapman *et al.*, Nature **470**, 73 (2011).