



**Sudan University of Science and Technology**  
**College of Graduate studies**

**Elementary Particles Scattering on The Basis Of  
Generalized Special Relativity**

تشتت الجسيمات الأولية على أساس النسبية الخاصة المعممة

*A thesis Submitted in Fulfillment of The Requirements for the  
Degree of Doctor of Philosophy in Physics*

**By:**

**Osama Hamed Abdelwahid Mohammed**

**Supervisor:**

**Prof. Dr. Mubarak Dirar Abd Alla**

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## الآية

قال تعالى:

( اللَّهُ الَّذِي سَخَّرَ لَكُمْ الْبَحْرَ لِتَجْرِيَ الْفُلُكُ فِيهِ بِأَمْرِهِ وَلِتَبْتَغُوا مِنْ فَضْلِهِ وَلَعَلَّكُمْ تَشْكُرُونَ (12) وَسَخَّرَ لَكُمْ مَا فِي السَّمَاوَاتِ وَمَا فِي الْأَرْضِ جَمِيعًا مِنْهُ إِنَّ فِي ذَلِكَ لَآيَاتٍ لِقَوْمٍ يَتَفَكَّرُونَ (13))

سورة الجاثية

## **Dedication**

This work was dedicated to my parents, to my brothers to my sisters to my wife,  
to my uncles, to my aunts, to my teachers and all my friends.

## **Acknowledgement**

Firstly praise be to Allah for His kindness up on me to route this success. I would like to take the opportunity to thank everybody who participated in one way or other to this work. I gratefully acknowledge my supervisor professor Mubarak Dirar Abdallah, for giving me the grand opportunity to work with him, and for his invaluable advice and great support throughout my studies. Many Thanks to Sudan University of Science and Technology, department of physics for permission to do this research.

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Finally my respects and appreciative thanks go to my parents.

# **Abstract**

This study aims to study the scattering theory using the Generalized Special Relativistic and some basic quantity equations, where it was found the scattering cross-section contains a new limit in which the cross section depends on the particle mass, and this result did not appear in the scattering theory based on the Schrödinger equation , and thus this theory enables us to give us information more precisely about the scattering phenomenon, and what distinguishes this theory also, we found that it leads to the scattering theory based on the Schrödinger equation when neglecting the mass of the particle.

## المستخلص

يهدف هذا البحث إلى دراسة نظرية التثنت باستخدام النظرية النسبية الخاصة المعممة وبعض معادلات الكمية الأساسية حيث وجد أن المقطع العرضي للتثنت يحتوي على حد جديد يعتمد فيه المقطع العرضي على كتلة الجسيمات وهذه النتيجة لم تظهر في نظرية التثنت المعتمدة على معادلة شرودينجر، وبالتالي يمكننا هذه النظرية من إعطائنا معلومات أدق حول ظاهرة التثنت، وما يميز هذه النظرية أيضاً وجدنا أنها تؤول إلى نظرية التثنت المعتمدة على معادلة شرودينجر عند إهمال كتلة الجسيم.

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# Chapter One

## Introduction

### (1.1) Electromagnetic Waves:

Light is the oldest well known electromagnetic waves. It is used at that time for lighting and seeing things around. Later on light is discovered to be related to the electromagnetic waves that are electric and magnetic travelling waves perpendicular to each other [1].

The wave nature of electromagnetic waves was formulated mathematically using Maxwell's equations. This wave nature succeeded in explaining the laws of reflection and refraction beside interference and diffraction [2]. But unfortunately the spectrum of the radiation emitted by the black body seems to be too difficult to be explained using the wave nature of electromagnetic fields [3, 4]. This forces Maxplank to propose that light and electromagnetic waves behave as discrete quanta [5, 6]. This new particle (quanta) version succeeded in explaining the black body radiation beside pair production, photoelectric effect and Compton effect [7, 8].

Thus there are two versions to describe the interaction of electromagnetic waves with matter. The wave version and the particle (quanta) version [9, 10, 11]. One of the most important interactions is the scattering process [12, 13, 14].

Scattering theory is important as it underpins one of the most ubiquitous tools in physics, almost everything we know about nuclear and atomic physics has been discovered by scattering experiments, e.g. Rutherford's discovery of the nucleus, the discovery of sub-atomic particles (such as quarks), etc. In low energy physics, scattering phenomena provide the standard tool to explore solid state systems, e.g. neutron, electron, x-ray scattering, etc. [15].

Scattering is even more important, much of our information about the interaction between particles being derived from scattering experiments [16]

Scattering process takes place when the incident electromagnetic beam enter bulk matter. In this case photons collide with atoms and change their direction and energy. The scattering process leads to gain energy by the medium. This energy can be converted into heat energy or can excite atoms [17].

Almost everything we know about nuclei and elementary particles has been discovered in scattering experiments, from Rutherford's surprise at finding that atoms have their mass and positive charge concentrated in almost point-like nuclei, to the more recent discoveries, on a far smaller length scale, that protons and neutrons are themselves made up of apparently point-like quarks.

The simplest model of a scattering experiment is given by solving Schrödinger's equation for a plane wave impinging on a localized potential. A potential  $V(r)$  might represent what a fast electron encounters on striking an atom, or an alpha particle a nucleus. Obviously, representing any such system by a potential *is* only a beginning, but in certain energy ranges it is quite reasonable, and we have to start somewhere [18]

The theoretical investigation and description of scattering (collision) processes of atomic particles represents an important field of application of Quantum Mechanics. One can gain therewith valuable information about particle interactions (e.g., nuclear forces), about elementary interaction potentials, about the structure of matter (e.g., crystal structures), and so on. The energetic structure of atoms and molecules, however, is spectroscopic ally investigated, where by any kind of energy supply the particle is transferred from its ground state into an excited state. The energy, which is emitted with the return into the ground state, e.g. in form of a photon, is analyzed. Initial and final state of the process stem from the discrete spectrum of the Hamilton

operator (bound states). In contrast, it is typical for scattering processes that the initial and final state of the considered system both lie in the continuous part of the eigen-value spectrum. The scattered particle comes from infinity into the sphere of action of the scattered, in order to be detected after the collision again asymptotically at infinity. The particle is therefore not in a bound state. An example of how one can draw conclusions from scattering processes about the physical properties of atomic and subatomic particles, we have already got to know in connection with the classical Rutherford scattering. Its analysis led to a first, already rather realistic nuclear model. We had seen there that in Classical Physics the collision between two particles can uniquely be described by their velocities and the impact parameter. Although the latter could not be precisely given, so that we were forced to revert to means of Statistics, nevertheless the total classical process remained of course in principle deterministic. That is now different, though, in Quantum Mechanics, since concepts like path, impact parameter have lost their meaning. Accordingly, quantum-mechanically, for a scattering process, only probability statements are possible. In the following, we will have to concentrate ourselves on the question, with which probability particles are deflected (scattered) at the angle  $(\vartheta, \phi)$  relative to the original direction of motion, as a consequence of their interaction with collision partners [19]

### **(1.2) Research Problem:**

Elementary particles behavior cannot fully explained by using ordinary quantum field theory. For example the number of neutrinos with different masses is difficult to be explained. There are many interactions of elementary particles that cannot be explained using the ordinary scattering theories.

### **(1.3) Aim of The Work:**

The aim of this work is to construct new quantum field theory based on generalized special relativity (GSR) to explain scattering of elementary particles

### **(1.4) Thesis Layout:**

The thesis consists 4 chapters.

Chapters one and two are concerned with the introduction and theoretical background. Chapter three and four are devoted for the literature review and the model.

# Chapter Two

## Theoretical background

### (2.1) Introduction:

The scattering quantum theory is based on quantum equations. These equations are presented here.

### (2.2) A brief History:

1900 (Planck): Max Planck proposed that light with frequency  $\nu$  is emitted in quantized lumps of energy that come in integral multiples of the quantity,

$$E = hf = \hbar\omega \quad (2.2.1)$$

Where  $h = 6.63 \times 10^{-34} J \cdot s$  is *Planck's constant*, and

$$\hbar = h/2\pi = 1.06 \times 10^{-34} J \cdot s \quad (2.2.2).$$

The frequency  $\nu$  of light is generally very large (on the order of  $10^{15} s^{-1}$  for the visible spectrum), but the smallness of  $h$  wins out, so the  $hf$  unit of energy is very small (at least on an everyday energy scale). The energy is therefore essentially continuous for most purposes.

However, a puzzle in late 19th-century physics was the blackbody radiation problem. In a nutshell, the issue was that the classical (continuous) theory of light predicted that certain objects would radiate an infinite amount of energy, which of course can't be correct. Planck's hypothesis of quantized radiation not only got rid of the problem of the infinity, but also correctly predicted the shape of the power curve as a function of temperature.

Planck's hypothesis simply adds the information of how many lumps of energy a wave contains. Although strictly speaking, Planck initially thought that the quantization was only a function of the emission process and not inherent to the light itself.

1905 (Einstein): Albert Einstein stated that the quantization was in fact inherent to the light, and that the lumps can be interpreted as particles, which we now call “photons.” This proposal was a result of his work on the photoelectric effect, which deals with the absorption of light and the emission of electrons from a material. That  $E = pc$  for a light wave. (This relation also follows from Einstein's 1905 work on relativity, where he showed that  $E = pc$  for any massless particle, an example of which is a photon.) And we also know that  $w = ck$  for a light wave.

$$E = \hbar w \quad (2.2.3)$$

$$p = \hbar k \quad (2.2.4)$$

This result relates the momentum of a photon to the wavenumber of the wave it is associated with.

1913 (Bohr): Neil's Bohr stated that electrons in atoms have wavelike properties. This correctly explained a few things about hydrogen, in particular the quantized energy levels that were known.

1924 (de Broglie): Louis de Broglie proposed that all particles are associated with waves, where the frequency and wavenumber of the wave are given by the same relations we found above for photons, namely  $E = \hbar w$  and  $p = \hbar k$ . The larger  $E$  and  $p$  are, the larger  $w$  and  $k$  are. Even for small  $E$  and  $p$  that are typical of a photon,  $w$  and  $k$  are very large because  $\hbar$  is so small. So any everyday-sized particle with large (in comparison) energy and momentum values will have extremely large  $w$  and  $k$  values. This (among other reasons) makes it virtually impossible to observe the wave nature of macroscopic amounts of matter.

This proposal (that  $E = \hbar w$  and  $p = \hbar k$  also hold for massive particles) was a big step, because many things that are true for photons are *not* true for massive (and nonrelativistic) particles. For example,  $E = pc$  (and hence  $w = ck$ ) holds only for massless particles (we'll see below how  $w$  and  $k$  are related for massive particles).



But the proposal was a reasonable one to try. And it turned out to be correct, in view of the fact that the resulting predictions agree with experiments.

The fact that any particle has a wave associated with it leads to the so-called wave-particle duality. Are things particles, or waves, or both? Well, it depends what you're doing with them. Sometimes things behave like waves, sometimes they behave like particles. A vaguely true statement is that things behave like waves until a measurement takes place, at which point they behave like particles. However, approximately one million things are left unaddressed in that sentence. The wave-particle duality is one of the things that few people, if any, understand about quantum mechanics.

1925 (Heisenberg): Werner Heisenberg formulated a version of quantum mechanics that made use of matrix mechanics. We won't deal with this matrix formulation (it's rather difficult), but instead with the following wave formulation due to Schrodinger (this is a waves book, after all).

1926 (Schrodinger): Erwin Schrodinger formulated a version of quantum mechanics that was based on waves. He wrote down a wave equation (the so-called Schrodinger equation) that governs how the waves evolve in space and time. We'll deal with this equation in depth below. Even though the equation is correct, the correct interpretation of what the wave actually meant was still missing. Initially Schrodinger thought (incorrectly) that the wave represented the charge density.

1926 (Born): Max Born correctly interpreted Schrodinger's wave as a probability amplitude. By "amplitude" we mean that the wave must be squared to obtain the desired probability. More precisely, since the wave (as we'll see) is in general complex, we need to square its absolute value. This yields the probability of finding a particle at a given location (assuming that the wave is written as a function of  $x$ ). This probability isn't a consequence of ignorance, as is the case with virtually every other example of probability you're familiar with. For example, in a coin toss, if you

know everything about the initial motion of the coin (velocity, angular velocity), along with all external influences (air currents, nature of the floor it lands on, etc.), then you can predict which side will land facing up. Quantum mechanical probabilities aren't like this. They aren't a consequence of missing information. The probabilities are truly random, and there is no further information (so-called "hidden variables") that will make things unrandom. The topic of hidden variables includes various theorems (such as Bell's theorem)

And experimental results that you will learn about in a quantum mechanics course. 1926 (Dirac): Paul Dirac showed that Heisenberg's and Schrodinger's versions of quantum mechanics were equivalent, in that they could both be derived from a more general version of quantum mechanics.

### 2.3 De Broglie Matter Waves:

The possibility that particles of matter like electrons could be both particle-like and wave-like was first proposed by Louis de Broglie in 1923. Specifically he proposed that a particle of matter with momentum  $p$  could act as a wave with wavelength [20]

$$\lambda = \frac{h}{p} \quad (2.3.1)$$

From the relativistic equation for total energy:

$$E^2 = c^2p^2 + m^2c^4 \quad (2.3.2)$$

With zero photon mass, we get that

$$E^2 = c^2p^2 \quad \Rightarrow E = cp \quad (2.3.3)$$

$$P = \frac{E}{c} = hf/c = h/\lambda \quad (2.3.4)$$

When dealing with sinusoidal functions of space and time

$$\psi = [\sin(kx - \omega t)] \quad (2.3.5)$$

We usually use

$$\omega = 2\pi\nu \quad \text{and} \quad k = \frac{2\pi}{\lambda} \quad (2.3.6),$$

The angular frequency and wave number. This gives us

$$p = \hbar k \quad , \quad E = \hbar \omega \quad \text{and} \quad \omega = ck \quad (2.3.7),$$

Where

$$\hbar = h/2\pi.$$

## 2.4 The Schrodinger Equation:

The first step in the development of a logically consistent theory of nonrelativistic quantum mechanics is to devise a wave equation which can describe the covert, wave-like behavior of a quantum particle. This equation is called the Schrodinger equation. The role of the Schrodinger equation in quantum mechanics is analogous to that of Newton's Laws in classical mechanics. Both describe motion. Newton's Second Law is a differential equation which describes how a classical particle moves, whereas the Schrodinger equation is a partial differential equation which describes how the wave function representing a quantum particle ebbs and flows. In addition, both were postulated and then tested by experiment [21].

### 2.4.1 Sinusoidal Waves:

The most elegant wave is a sinusoidal travelling wave with definite wavelength  $\lambda$  and period  $\tau$ , or equivalently definite wave number,  $k = 2\pi/\lambda$  and angular frequency  $\omega = 2\pi/\tau$ . Such a wave may be represented by the mathematical function

$$\psi(x, t) = A \cos(kx - \omega t) \quad (2.4.1.1)$$

Where  $A$  is a constant. At each point  $x$ , the function  $\psi(x, t)$  oscillates with Amplitude  $A$  and period  $2\pi/\omega$ . At each time  $t$ , the function  $\psi(x, t)$  undulates with amplitude  $A$  and wavelength  $2\pi/k$ . Moreover, these undulations move, like a Mexican wave, in the direction of increasing  $x$  with velocity  $\omega/k$ ; for example, the maximum of  $\psi(x, t)$  corresponding to

$$kx - \omega t = 0 \quad (2.4.1.2)$$

Occurs at the position

$$x = \frac{\omega t}{k} \quad (2.4.1.3),$$

And the minimum corresponding to

$$kx - \omega t = \pi \quad (2.4.1.4)$$

Occurs at the position

$$x = \frac{\lambda}{2} + \frac{\omega t}{k} \quad (2.4.1.5);$$

In both cases the position moves with velocity  $\omega/k$ .

The function  $\sin(kx - \omega t)$ , like  $\cos(kx - \omega t)$ , also represents a sinusoidal Travelling wave with wave number  $k$  and angular frequency  $\omega$ . Because

$$\sin(kx - \omega t) = \cos(kx - \omega t - \pi/2) \quad (2.4.1.6),$$

The undulations and oscillations of  $\sin(kx - \omega t)$  are out of step with those of  $\cos(kx - \omega t)$ ; the waves  $\sin(kx - \omega t)$  and  $\cos(kx - \omega t)$  are said to have a phase difference of  $\pi/2$ . The most general sinusoidal travelling wave with wave number  $k$  and angular frequency  $\omega$  is the linear superposition

$$\psi(x, t) = A \cos(kx - \omega t) + B \sin(kx - \omega t) \quad (2.4.1.7)$$

Where  $A$  and  $B$  are arbitrary constants.

Very often in classical physics, and invariably in quantum physics, sinusoidal travelling waves are represented by complex exponential functions of the form

$$\psi(x, t) = A e^{i(kx - \omega t)} \quad (2.4.1.8)$$

## 2.4.2 Particle Wave Equations:

In classical physics, fundamental laws of physics are used to derive the wave equations which describe wave-like phenomena; for example, Maxwell's laws of electromagnetism can be used to derive the classical wave equation which governs electromagnetic waves in the vacuum. In contrast, we shall view the wave equation governing the wave-like properties of a quantum particle as a fundamental equation which cannot be derived from underlying basic physical principles. We, like the

inventors of quantum theory, can only guess the form of this wave equation and then test for consistency and agreement with experiment [22].

### 2.4.3 A wave Equation For a Free Particle:

We shall construct a possible wave equation for a freely moving non-relativistic Particle by considering the properties of the de Broglie waves describing the particle.

According to  $\lambda = h/p$  a particle with momentum  $p$  has a de Broglie wavelength given by  $\lambda = h/p$ . This implies that a de Broglie wave with wave number

$$k = \frac{2\pi}{\lambda} \quad (2.4.3.1)$$

Describes a particle with momentum

$$p = \hbar k \quad (2.4.3.2)$$

We shall extend this idea by assuming that a de Broglie wave packet with a range of wave numbers between  $k - \Delta k$  and  $k + \Delta k$  describes a particle with an uncertain momentum

$$\Delta p \approx \hbar \Delta k \quad (2.4.3.3)$$

We shall also assume that the length of this wave packet is a measure of  $\Delta x$ , the uncertainty in the position of the particle.

$$\Delta x \Delta p \approx h \quad (2.4.3.4)$$

Thus, a DE Broglie wave packet can account for the uncertainties in the position and momentum of a quantum particle.

However, we note that a de Broglie wave must be transformed by a measurement. If a precise measurement of the position is made, the new wave packet describing the particle must be very short, a superposition of sinusoidal waves with a very wide range of wavelengths. Similarly, if a precise measurement of the momentum is made, the new wave packet is very long with a sharply defined wavelength. This

implies that the wave packet is a fragile entity which is transformed by a measurement. No one knows how this happens.

We shall now impose the condition that the wave packet represents a moving quantum particle. Specifically, we shall require that the group velocity of the packet is equal to the velocity of a particle with mass  $m$  and momentum  $p = \hbar k$ ; we shall require that

$$\frac{d\omega}{dk} = \frac{\hbar k}{m} \quad (2.4.3.5)$$

This equation may be integrated to give the following dispersion relation for the de Broglie waves describing a freely moving quantum particle of mass  $m$ :

$$\omega = \frac{\hbar k^2}{2m} \quad (2.4.3.6)$$

In obtaining this relation we have set the constant of integration to zero because this constant gives rise to no observable consequences in non-relativistic quantum mechanics.

Our task is to find a wave equation which has sinusoidal solutions which obey this dispersion relation. The simplest such wave equation is called the Schrodinger equation. For a free particle moving in one dimension, it has the form

$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} \quad (2.4.3.7)$$

It is easy to verify that the complex exponential

$$\psi(x, t) = A e^{i(kx - \omega t)} \quad (2.4.3.8)$$

Thus

$$i\hbar \frac{\partial \psi}{\partial t} = i\hbar(-i\omega)Ae^{i(kx - \omega t)} = \hbar\omega Ae^{i(kx - \omega t)} \quad (2.4.3.9)$$

$$-\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} = \frac{\hbar^2 k^2}{2m} Ae^{i(kx - \omega t)} \quad (2.4.3.10)$$

And we have a solution provided

$$\hbar\omega = \hbar^2 k^2 / 2m \quad (2.4.3.11) .$$

Because the sinusoidal solution equation (2.4.3.10), describes a wave moving in the  $x$  direction with wave number  $k$  and angular velocity  $\omega$ , we shall assume that it represents a free particle moving in the  $x$  direction with a sharply defined momentum  $p = \hbar k$  and energy

$$E = p^2 / 2m = \hbar\omega \quad (2.4.3.12) .$$

There are, of course, many other solutions of the Schrodinger equation which represent other states of motion of the particle.

We emphasize that in order to accommodate the dispersion relation for de Broglie waves, we have arrived at a wave equation, the free particle Schrodinger equation (2.4.3.7), whose solutions are necessarily complex functions of space and time. These complex functions are called wave functions. We recall that classical waves are often represented by complex functions, but this representation is purely a matter of mathematical convenience; classical waves are real functions of space and time. In contrast, Schrodinger wave functions are not real functions of space and time. They are complex functions which describe the covert wave-like behaviour of a quantum particle.

So far we have only considered sinusoidal solutions of the Schrodinger equation, but given these solutions we can construct other types of solutions. Because each term in the Schrodinger equation is linear in the wave function  $\psi$ , a superposition of solutions is also a solution [23].

#### **2.4.4 Wave Equation For A particle in A potential Energy Field:**

The interactions of a non-relativistic particle can usually be described in terms of a potential energy field. For example, an electron in a hydrogen atom can be thought of as moving in the potential energy field

$$V(r) = -e^2/4\pi\epsilon_0 r^2 \quad (2.4.4.1)$$

Of nucleus. In classical mechanics, this field implies that an electron at a distance  $r$  from the nucleus experiences an attractive force of magnitude  $-e^2/4\pi\epsilon_0 r^2$ . In quantum mechanics, it implies that the wave equation for the electron is not the simple free-particle wave equation given by equation (2.4.3.7).

In 1926, Erwin Schrodinger invented a wave equation for a quantum particle in a potential energy field which led to a successful description of atoms and other microscopic systems. It is a generalization of the wave equation for a free particle given by equation (2.4.3.7). The Schrodinger equation for a particle moving in the three-dimensional potential energy field  $V(r)$  is

$$i\hbar \frac{\partial \psi}{\partial t} = \left[ -\frac{\hbar^2}{2m} \nabla^2 + V(x) \right] \psi \quad (2.4.4.2)$$

When the particle moves in a one-dimensional potential  $V(x)$  the Schrodinger equation simplifies to

$$i\hbar \frac{\partial \psi}{\partial t} = \left[ -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x) \right] \psi \quad (2.4.4.3)$$

It is easy to find solutions of the Schrodinger equation when the potential energy is a constant. For example, when a particle moves along the  $x$  axis with constant potential energy  $V_0$ , the wave function

$$\psi(x, t) = A e^{i(kx - \omega t)} \quad (2.4.4.4)$$

Is a solution of equation (2.4.4.3) provided

$$\hbar\omega = \frac{\hbar^2 k^2}{2m} + V_0 \quad (2.4.4.5)$$

This wave function represents a particle with sharply defined total energy  $E$  and momentum  $p$  given by



$$E = \frac{p^2}{2m} + V_0 \quad \text{and} \quad p = \hbar k \quad (2.4.4.6)$$

### 2.4.5 Particle Flux and Probability Density:

The Schrodinger wave equation

$$i\hbar \frac{\partial \psi}{\partial t} = \left[ -\frac{\hbar^2}{2m} \nabla^2 + V(x) \right] \psi \quad (2.4.5.1)$$

Where  $\psi(r, t)$  is the wave function which is interpreted as the amplitude of probability of finding the particle at position  $r$  at time  $t$ . The complex conjugate of Schrodinger wave equation is

$$-i\hbar \frac{\partial \psi^*(r, t)}{\partial t} = \left[ -\frac{\hbar^2}{2m} \nabla^2 + V(x) \right] \psi^*(r, t) \quad (2.4.5.2)$$

Multiplying equation (2.4.5.1) by  $\psi^*$  on the left and equation (2.4.5.2) by  $\psi$  on the right and subtracting the latter from the former, we get

$$-\frac{\hbar^2}{2m} \{\psi^* \nabla^2 \psi - \psi \nabla^2 \psi^*\} = i\hbar \left( \psi^* \frac{\partial \psi}{\partial t} + \frac{\partial \psi^*}{\partial t} \psi \right) \quad (2.4.5.3)$$

$$-\frac{\hbar^2}{2m} \nabla \cdot \{\psi^* \nabla \psi - \psi \nabla \psi^*\} = i\hbar \frac{\partial}{\partial t} (\psi^* \psi) \quad (2.4.5.4)$$

Defining the probability current density  $J$  and the probability density  $\rho$ ,

$$J = \frac{\hbar}{2mi} \{\psi^* \nabla \psi - \psi \nabla \psi^*\} \quad \text{and} \quad \rho = \psi^* \psi \quad (2.4.5.5)$$

We obtain the continuity equation,

$$\frac{\partial \rho}{\partial t} + \nabla \cdot J = 0 \quad (2.4.5.6)$$

Equation (2.4.5.6) is the continuity equation, expressing the conservation law that the rate of change of particle density in a given region is equivalent to the particle flux through the surface enclosing the region. Please note that the probability density  $\rho$  is a positive definite quantity which is physically acceptable [22].

## 2.5 The Klein-Gordon Equation:

The Schrodinger equation was derived from the non-relativistic energy-momentum relation. It's nonlinear in  $E$  and  $p$ , which does not allow us to use a Lorentz covariant notation. We know that there is a more appropriate relativistic equation. What happens if we take [23]

$$E^2 = p^2 c^2 + m^2 c^4 \quad (2.5.1)$$

And using the usual recipe of treating the energy and momentum as differential operators we obtain the relativistic wave equation

$$-\hbar^2 \frac{\partial^2 \psi}{\partial t^2} = (-c^2 \hbar^2 \nabla^2 + m^2 c^4) \psi \quad (2.5.2)$$

Which, on rearrangement, yields

$$\left( \frac{1}{c^2} \frac{\partial^2}{\partial t^2} - \nabla^2 + \frac{m^2 c^2}{\hbar^2} \right) \psi = 0 \quad (2.5.3)$$

Equation (2.5.3) is the Klein-Gordon equation, the complex conjugate of which is given by

$$\left( \frac{1}{c^2} \frac{\partial^2}{\partial t^2} - \nabla^2 + \frac{m^2 c^2}{\hbar^2} \right) \psi^* = 0 \quad (2.5.4)$$

Multiplying equation (2.5.3) by  $\psi^*$  on the left and equation (2.5.4) by  $\psi$  on the left and subtracting, we obtain

$$\frac{1}{c^2} \left( \psi^* \frac{\partial^2 \psi}{\partial t^2} - \psi \frac{\partial^2 \psi^*}{\partial t^2} \right) - \psi^* \nabla^2 \psi + \psi \nabla^2 \psi^* = 0 \quad (2.5.5)$$

Since

$$\frac{1}{c^2} \frac{\partial}{\partial t} \left( \psi^* \frac{\partial \psi}{\partial t} - \psi \frac{\partial \psi^*}{\partial t} \right) + \nabla \cdot (\psi^* \nabla \psi - \psi \nabla \psi^*) = 0 \quad (2.5.6)$$

This is the continuity equation for the Klein-Gordon equation, can be written in the form of continuity equation

$$\frac{\partial \rho}{\partial t} + \nabla \cdot J = 0 \quad (2.5.7)$$

Choosing for the current density  $J$  the same expression

$$J = \frac{\hbar}{2mi} \{\psi^* \nabla \psi - \psi \nabla \psi^*\} \quad (2.5.8)$$

As given in equation (2.4.5.5) for the non-relativistic Schrodinger equation. In the present case, the continuity equation will be satisfied only if we choose for the probability density  $\rho$  the expression

$$\rho = \frac{i\hbar}{2mc^2} \left( \psi^* \frac{\partial \psi}{\partial t} - \psi \frac{\partial \psi^*}{\partial t} \right) \quad (2.5.9)$$

The probability density  $\rho$  as given by equation (2.4.5.6) involves both  $\psi$  and  $\frac{\partial \psi}{\partial t}$  Which can be fixed arbitrarily and hence admits both positive and negative values. Since the probability density should be a positive definite quantity, the Klein-Gordon equation was not accepted as a wave equation for several years until Pauli and Weisskopf<sup>2</sup> reinterpreted it as a field equation in the same sense as Maxwell's equation for electromagnetic field. By putting the rest mass  $m = 0$  in is the Klein-Gordon equation (2.5.3) we obtain the field equation for the electromagnetic field. The Klein-Gordon equation is a second-order differential equation in  $t$  and this has yielded the physically unacceptable negative values also for the probability density  $\rho$ . It may be observed that the Schrodinger equation is a first-order differential equation in  $t$  and hence yielded a positive definite value for the probability density. Taking this clue, Dirac attempted to linearize the relativistic relation

$$E^2 = p^2 c^2 + m^2 c^4 \quad (2.5.10)$$

Which is quadratic in both  $E$  and  $p$  and arrived at the Dirac equation.

Thus the attempts to overcome the early difficulties encountered in the formulation of Relativistic Quantum Mechanics paid rich dividends. Dirac succeeded in linearizing the relativistic relation energy-momentum which is quadratic in both energy and momentum and obtained the Dirac equation for the electron with the intrinsic properties of spin and magnetic moment. Interpretation of the Klein-Gordon equation as a field equation has sowed the seed for the development of the Quantum Field theory [22].

## 2.6 The Dirac Equation:

The Dirac equation is a relativistic quantum mechanical wave equation for spin- $1/2$  particles (e.g. electrons), which was derived by Dirac. The difficulties in finding a consistent single-particle theory from the Klein-Gordon equation led Dirac to search for an equation that

- Had a positive-definite conserved probability density and
- Was first order both in time and space.

One can show that these two conditions imply that a matrix equation is required. The reason why the Klein-Gordon equation did not yield a positive-definite probability density is connected with the second-order time derivative in this equation, which arises because the Klein-Gordon equation is related to the relativistic energy-momentum relation via the correspondence principle that includes a term  $E^2$ . Thus, a better Lorentz covariant wave equation with a positive-definite probability density should have a first-order time derivative only [24].

Starting with the relativistic relation

$$E^2 = p^2 c^2 + m^2 c^4 \quad (2.6.1)$$

Between the energy and momentum of a free particle of mass  $m$ , Dirac obtained a linear relation

$$E = c\alpha \cdot p + \beta mc^2 \quad (2.6.2)$$

Using two operators  $\alpha$  and  $\beta$  which commute with both position and momentum vectors. Squaring equation (2.6.2), we obtain

$$E^2 = c^2(\alpha \cdot p)^2 + \beta^2 m^2 c^4 + (\alpha \cdot p)\beta mc^3 + \beta(\alpha \cdot p)mc^3 \quad (2.6.3)$$

Which will reduce to the relativistic energy-momentum relation

$$E^2 = p^2 c^2 + m^2 c^4 \quad (2.6.4)$$

If the operators  $\alpha$  and  $\beta$  obey the following relations:

$$(\alpha \cdot p)^2 = p^2, \quad \beta^2 = 1, \quad \alpha\beta = -\beta\alpha \quad (2.6.5)$$

The relation

$$(\alpha \cdot p)^2 = (\alpha_x p_x + \alpha_y p_y + \alpha_z p_z)^2 = p^2 \quad (2.6.6)$$

Implies

$$\alpha_x^2 = \alpha_y^2 = \alpha_z^2 = 1; \quad (2.6.7)$$

$$\alpha_x \alpha_y = -\alpha_y \alpha_x; \quad \alpha_y \alpha_z = -\alpha_z \alpha_y; \quad \alpha_z \alpha_x = -\alpha_x \alpha_z \quad (2.6.8)$$

Using the usual recipe for the first quantization of replacing the energy and momentum by differential operators

$$E \rightarrow i\hbar \frac{\partial}{\partial t} \quad \text{and} \quad p \rightarrow -i\hbar \nabla \quad (2.6.9)$$

Hence the time-dependent Dirac equation for a free particle is obtained.

$$i\hbar \frac{\partial \psi(r, t)}{\partial t} = (-i\hbar \alpha \cdot \nabla + \beta mc^2) \psi(r, t) \quad (2.6.10)$$

The space-time dependence of the free particle Dirac wave function can be explicitly written as

$$\psi(r, t) = A e^{(i/\hbar)(p \cdot r - Et)} \quad (2.6.11)$$

This satisfies the time-dependent Dirac equation (2.6.10) for a free particle; from which we obtain the time-independent Dirac equation

$$(c\alpha \cdot p + \beta mc^2) \psi = E \psi \quad (2.6.12)$$

With a multi-component wave function  $\psi$ . If  $\alpha_x, \alpha_y, \alpha_z$  and  $\beta$  are matrices of dimension  $N \times N$ , then the Dirac wave function  $\psi$  should be a column vector with  $N$  components. In equation (2.6.12),  $p$  is the momentum vector and not an operator.

### 2.6.1 Dirac's $\alpha$ and $\beta$ Matrices:

The Dirac Hamiltonian should be Hermitian, i.e.  $H = H^*$ . Since  $p$  is Hermitian,

$$H = c(\alpha \cdot p + \beta mc); \quad H^* = c(\alpha^* \cdot p + \beta^* mc). \quad (2.6.1.1)$$

This means that  $\alpha_i$ , ( $i = x; y; z$ ); and  $\beta$  matrices are Hermitian.

$$\alpha_i^* = \alpha_i, \quad (i = x; y; z); \quad \beta^* = \beta \quad (2.6.1.2)$$

Since

$$\alpha_i^2 = 1, \quad (i = x; y; z); \quad \text{and} \quad \beta^2 = 1 \quad (2.6.1.3)$$

It follows that

$$\alpha_i = \alpha_i^{-1} \quad \text{and} \quad \beta = \beta^{-1} \quad (2.6.1.4)$$

Which means that the matrices  $\alpha_i$  and  $\beta$  are non-singular and consequently their determinant is non-zero.

$$\det(\alpha_i) \neq 0, \quad (i = x; y; z); \quad \text{and} \quad \det(\beta) \neq 0 \quad (2.6.1.5)$$

We have already seen that the Dirac matrices  $\alpha_x, \alpha_y, \alpha_z, \beta$  anticommute.

If they are of dimension  $N \times N$ , then

$$\begin{aligned} \alpha_i \beta &= -\beta \alpha_i \\ \det(\alpha_i \beta) &= \det(-1) \det(\beta \alpha_i) \\ \det(\alpha_i) \det(\beta) &= \det(-1) \det(\beta) \det(\alpha_i) \end{aligned} \quad (2.6.1.6)$$

From which, we deduce that

$$\det(-1) = (-1)^N = 1, \quad (2.6.1.7)$$

Assuming that the matrices  $\alpha_i; \beta$  are of dimensions  $N \times N$  and the condition (2.6.1.6) is satisfied if  $N$  is even.

$$N = 2, 4, 6, \dots \dots \quad (2.6.1.8)$$

We have seen that the  $(2 \times 2)$  matrices permit only three ant commuting matrices (the Pauli matrices) along with the unit matrix as independent matrices and all other matrices can be represented as a linear combination of them. Since in Dirac equation, we have four ant commuting matrices, they should be of higher dimension, at least  $(4 \times 4)$ .

Dirac's  $\alpha$  and  $\beta$  matrices are traceless. Since  $\alpha_i\beta = -\beta\alpha_i$ , it follows that

$$\begin{aligned}\alpha_i\beta\alpha_i^{-1} &= -\beta \\ \text{Trance } (\alpha_i\beta\alpha_i^{-1}) &= -\text{Trance } \beta \\ \text{Trance } (\alpha_i^{-1}\alpha_i\beta) &= -\text{Trance } \beta \\ \text{Trance } (\beta) &= -\text{Trance } \beta\end{aligned}\quad (2.6.1.9)$$

This means that  $\text{Trance } \beta = 0$ . In the above derivation, we have used the cyclic property of the Trace.

$$\text{Trace } (ABC) = \text{Trace } (CAB) \quad (2.6.1.10)$$

Similarly, it can be shown that  $\text{Trace } \alpha_i = 0$ ; ( $i = x; y; z$ ). Let us now give an explicit representation<sup>3</sup> for the Dirac matrices which satisfy all the above properties.

$$\alpha_i = \begin{bmatrix} 0 & \sigma_i \\ \sigma_i & 0 \end{bmatrix}, \quad \beta = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}, \quad (2.6.1.11)$$

Where  $\sigma_i$  denotes the familiar Pauli matrices and  $I$  denotes the  $2 \times 2$  unit matrix. Although the Dirac matrices are of dimension  $4 \times 4$ , we have written conveniently in the  $2 \times 2$  form in equation. (2.6.1.11). Explicitly,

$$\alpha_x = \begin{bmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{bmatrix}, \quad \alpha_y = \begin{bmatrix} 0 & 0 & 0 & -i \\ 0 & 0 & i & 0 \\ 0 & -i & 0 & 0 \\ i & 0 & 0 & 0 \end{bmatrix}$$

$$\alpha_z = \begin{bmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \\ 1 & 0 & 0 & 0 \\ 1 & -1 & 0 & 0 \end{bmatrix}, \quad \beta = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{bmatrix} \quad (2.6.1.12)$$

## 2.6.2 The Continuity Equation:

Multiplying the Dirac equation (2.6.10) on the left by  $\psi^*$ , we get

$$i\hbar\psi^*\frac{\partial\psi}{\partial t} = -ic\hbar\psi^*\alpha.\nabla\psi + \beta mc^2\psi^*\psi \quad (2.6.2.1)$$

Taking the Hermitian conjugate of the Dirac equation (2.6.10) and multiplying on the right by  $\psi$ , we get

$$-i\hbar\frac{\partial\psi^*}{\partial t}\psi = ic\hbar(\nabla\psi^*).\alpha^*\psi + \beta^*mc^2\psi^*\psi. \quad (2.6.2.2)$$

Remembering that  $\alpha$  and  $\beta$  are Hermitian matrices and subtracting (2.6.2.1) from (2.6.2.2), we obtain

$$i\hbar\frac{\partial}{\partial t}(\psi^*\psi) = -ic\hbar(\psi^*\alpha.\nabla\psi + (\nabla\psi^*).\alpha\psi) = -ic\hbar\nabla.(\psi^*\alpha\psi) \quad (2.6.2.3)$$

Which can be written as a continuity equation

$$\frac{\partial\rho}{\partial t} + \nabla.J = 0 \quad (2.6.2.4)$$

Since  $\psi$  is a column vector and  $\psi^*$ , a row vector as given below

$$\psi = \begin{bmatrix} a \\ b \\ c \\ d \end{bmatrix}, \quad \psi^* = [a^* \quad b^* \quad c^* \quad d^*], \quad (2.6.2.5)$$

The probability density

$$\rho = \psi^*\psi = aa^* + bb^* + cc^* + dd^* \quad (2.6.2.6)$$

Is a positive-definite quantity, overcoming the difficulty encountered in the Klein-Gordon equation. The probability current density  $J$  together with the probability density  $\rho$  obeys the continuity equation (2.6.2.4). So, the Dirac equation has become a physically acceptable relativistic wave equation [22].



## **2.7 Scattering:**

“Scattering” evokes a simple image. We begin with separate objects which are far apart and moving towards each other. After some time they collide and then travel away from each other and, eventually are far apart again. We don’t necessarily care about the details of the collision except insofar as we can predict from it where and how the objects will end up. This picture of scattering is the first one we physicists learn, In many cases the laws of conservation of momentum and energy alone can be used to obtain important results concerning the properties of various mechanical processes. It should be noted that these properties are independent of the particular type of interaction between the particles involved [25].

### **2.7.1 Tyndall Effect:**

The Tyndall effect is the scattering of light by particles in colloidal systems such as emulsion or suspensions. It is named after 19th-century Irish scientist John Tyndall. The Tyndall effect is used to find the difference between types of mixtures, namely, solution, colloidal and suspension. For example, the Tyndall effect is seen when car headlamps are used in fog. According to [26], the light of shorter wavelength scatters better. Thus the color of scattered light has a bluish tint. This is also the reason why the sky looks blue when viewed away from the sun. The blue light from the sun is scattered to a greater degree and is therefore visible far from its source .

This effect occurs because short wavelengths of light towards the blues and the spectrum hit the air molecules in the earth’s atmosphere and are reflected down to the earth surface. Longer wavelengths towards the end of the spectrum are less affected by the particles and pass on through the earth’s atmosphere. Blue light scatters more rapidly than red light at sunset, and the path length of the sun through the atmosphere is longer at any other time of the day. This is because the blue

components of the light have undergone multiple scattering events such that the intensity at such great seeing distance is minimal due to long path length.

### **2.7.2 Multiple Scattering:**

Multiple scattering is realized in accordance with the laws of single scattering at each successive act. The final result is obtained by successive adding the results of simple scatterings taking into account the statistical nature of their occurrence. The radiation scattered by a particle may be scattered by another particle, and so on [27].

### **2.7.3 Thomson Scattering:**

Thomson scattering is the type of electromagnetic scattering by charged particles in which the electric and magnetic particles components of the incident wave accelerate the particle. As it in turn emits radiation and the wave is scattered. The main cause of the acceleration of the particle is due to the electric field components of the incident wave. The particle will move in the direction of the oscillating electric field, resulting in electromagnetic dipole radiation. The moving particle radiates strongly in a direction perpendicular to its motion and that radiation will be polarized along the direction of its motion, depending on where an observer is located. The light scattered from a small volume element may be appear to be more or less polarized [28].

### **2.7.4 Compton Scattering:**

Compton scattering is the type of scattering that occur as a result of change in energy (increase in wavelength) of an X – ray or gamma ray photon when it interacts with matter. The effect is important as it demonstrates that light cannot be explained purely as a wave phenomenon. Compton experiment convinced physicists that light

can behave as a stream of particles whose energy is proportional to the frequency [29].

### **2.7.5 Brillion Scattering:**

In Brillion scattering the light in a medium (such as crystal or water) interacts with time dependent density variation and changes its frequency and path. The density variation may be as a result of acoustic modes such as phonons or temperature gradient as described in classical physics. When the medium is compressed its index of refraction changes and light path necessarily bends [28].

From a quantum point of view, Brillion scattering is an interaction of light photons with acoustic or vibration quantum (phonons), with magnetic spin waves (magnums) or with other low frequency quasi particles interacting with light.

According to Matveev (1988), the interaction consists of an inelastic scattering process in which a phonon or magnum is either created (stokes process) or annihilation (anti stokes) the energy of the scattered light is slightly changed, that is decreased for a stokes process and increase for anti- stokes process. This shift known as Brillion shift, is equal to the energy of the interacting phonon and magnum, and thus Brillion scattering can be used to measure phonon and magnum energies.

For intense beam (e. g laser light) travelling in a medium such as fiber, the variation in the electric field of the beam itself may produce acoustic vibration in the medium. The beam may undergo Brillion scattering from these vibrations, usually in opposite direction to the incoming beam .

### **2.7.6 Raman Scattering:**

Raman scattering or the Raman Effect is the type of in-elastic scattering of a photon. When light is scattered from an atom or molecule, most photon have the same energy (frequency) and wavelength as the incident photons. A small part of the scattered

light is (approximately 1 in millions photons) is scattered by an excitation, with the scattered photons having different form, and usually lower than a frequency of the incident photons. In a gas Raman scattering can occur with a change in vibration, rotational or electronic energy of a molecule [30].

### **2.7.7 Rayleigh Scattering:**

Rayleigh scattering is strongly dependent on the viewing angle with a degree of dependence in turn dependent on photon wavelength; hence the shorter the wavelength, the stronger the light scattering. The sky is blue because of Rayleigh scattering which is stronger with shorter wavelengths. Blue-violet light has a shorter wavelength than red light, so blue-violet is scattered more strongly, resulting in a blue sky. The relative size of scattering particles is defined by the ratio of its characteristic dimension and wavelength [30] where  $r$  is the radius of a spherical particle,  $\lambda$  is wavelength.

Rayleigh scattering occurs when light travels in transparent solids and liquids but is most prominently seen in gases. The amount of Rayleigh scattering that happens to a beam of light is dependent upon the size of the particles and the wavelength of the light; in particular, the scattering coefficient, and hence the intensity of the scattered light, varies for small size particles inversely with the fourth power of the wavelength. This wavelength dependence means that blue light is scattered much more than red light. In the atmosphere, the result is that blue light is scattered much more than glare at longer wavelengths, and so one sees blue light coming from all directions of the sky. At higher altitudes, high up in the mountain or an airplane, we can observe that the sky is much darker because the amount of scattering particles is much lower. When the Sun is quiet on the horizon, the sunlight must pass through a much higher air mass to reach an observer on the ground. This causes much more scattering of blue light, but a relatively little scattering of red light, and results in a

pronounced red-hued sky in the direction towards the sun, Rayleigh scattering can be defined as scattering in small size parameters regime. The amount of Rayleigh scattering that occurs to a beam of light is dependent upon the size of the particles and the wavelength of the sun in particular, and the scattering coefficient. Moreover, the intensity of the scattered light, varies for small size parameter inversely with fourth power of the wavelength, which means that the shorter wavelength of the blue light will scatter more than the longer wavelength of green and red light which gives the sky a blue appearance. However, when one looks towards the sun one sees colors that were not scattered away to longer wavelengths, such as red and yellow light. When the sun is near the horizon the volume of air through which sunlight must pass is significantly greater than when the sun is high in the sky. Accordingly, the gradient from a red-yellow sun to the blue is considerably sharper at sunrise and sunset. Rayleigh scattering was explained by Lord Rayleigh who described the details in 1871. The angular distribution of Rayleigh scattering given by the term  $(1+\cos^2\theta)$  is symmetric in the plane normal to the incident direction of the light, and so the forward scatter equals the backward scatter [30].

## **2.8 Scattering Theory:**

One of the best ways to understand the structure of particles and the forces between them is to scatter them off each other. This is particularly true at the quantum level where the systems cannot be seen in the literal sense and must be probed by indirect means. The scattering process gives us information about the projectile, the target, and the forces between them. A natural way to proceed (when possible) is to consider cases where two of these are known and learn about the third. Consider, for example, experiments at the Stanford Linear Accelerator Center in which high-energy photons were used to bombard static neutrons. The structure of the photon and its coupling to matter are well understood the photon is a point particle to an excellent

approximation and couples to electric charge in a way we have studied in some detail. It therefore serves as an excellent probe of the neutron. For instance, the very fact that the neutron, which is electrically neutral, interacts with the photon tells us that the neutron is built out of charged constituents (whose total charge add up to zero). These scattering experiments also revealed that the neutron's constituents have spin  $\frac{1}{2}$ , and fractional charges  $(\frac{2}{3}e, -\frac{1}{3})$ , a picture that had been arrived at from another independent line of reasoning. Furthermore they also indicated that the interaction between these constituents (called quarks) gets very weak as they get close. This information has allowed us to choose, from innumerable possible models of the interquark force, one that is now considered most likely to succeed, and goes by the name of quantum chromo dynamics (QCD), a subject that is being vigorously investigated by many particle physicists today [31].

Scattering theory is the study of an interacting system on a time and/or distance scale which is large compared to the scale of the actual interaction.

This is a natural phenomenon occurring in several branches of physics; optics (think of the blue sky), acoustics, x-ray, sonar, particle physics [32].

The basic idea behind scattering theory is simple: there's an object that you want to understand. So you throw something at it. By analyzing how that something bounces off, you can glean information about the object itself.

A very familiar example of scattering theory is called "looking at things". In this section we're going to explore what happens when you look at things by throwing a quantum particle at an object.

### **2.8.1 Scattering in One Dimension:**

We start by considering a quantum particle moving along a line. The maths here will be simple, but the physics is sufficiently interesting to exhibit many of the key ideas.

The object that we want to understand is some potential  $V(x)$ . Importantly, the potential is localized to some region of space which means that  $V(x) \rightarrow 0$  as  $x \rightarrow \pm\infty$ . An example is shown to the right. We will need the potential to fall-off to be suitably fast in what follows although, for now, we won't be careful about what this means [34, 35, and 36]. A quantum particle moving along the line is governed by the Schrodinger equation,

$$-\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} + V(x)\psi = E\psi \quad (2.8.1.1)$$

Solutions to this equation are energy Eigen states. They evolve in time as  $\psi(x, t) = e^{-iEt/\hbar}\psi(x)$ . For any potential, there are essentially two different kinds of states that we're interested in.

- Bound States are states that are localized in some region of space. The wave functions are normalizable and have profiles that drop off exponentially far from the potential

$$\psi(x) \sim e^{-\lambda|x|} \quad \text{as } |x| \rightarrow \infty \quad (2.8.1.2)$$

Because the potential vanishes in the asymptotic region, the Schrodinger equation relates the asymptotic fall-off to the energy of the state,

$$E = -\frac{\hbar^2 \lambda^2}{2m} \quad (2.8.1.3)$$

In particular, bound states have  $E < 0$ . Indeed, it is this property which ensures that the particle is trapped within the potential and cannot escape to infinity.

Bound states are rather special. In the absence of a potential, a solution which decays exponentially to the left will grow exponentially to the far right. But, for the state to be normalizable, the potential has to turn this behavior around, so the wave function decreases at both  $x \rightarrow -\infty$  and  $x \rightarrow +\infty$ . This will only happen for specific values of  $\lambda$ . Ultimately, this is why the spectrum of bound states is discrete, like in the hydrogen atom. It's where the name "quantum" comes from.

- Scattering States are not localized in space and, relatedly, the wave functions are not normalizable. Instead, asymptotically, far from the potential, scattering states take the form of plane waves. In one dimension, there are two possibilities

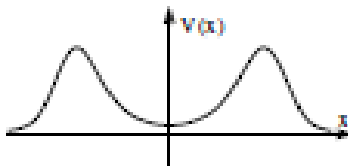
$$\begin{aligned} \text{Right moving } \psi &\sim e^{ikx} \\ \text{Left moving } \psi &\sim e^{-ikx} \end{aligned} \quad (2.8.1.4)$$

Where  $k > 0$ . To see why these are left or right moving, we need to put the time dependence back in. The wave functions then take the form  $e^{\pm ikx - iEt/\hbar}$ . The peaks and troughs of the wave move to the right with the plus sign, and to the left with the minus sign. Solving the Schrodinger equation in the asymptotic region with  $V = 0$  gives the energy

$$E = \frac{\hbar^2 k^2}{2m} \quad (2.8.1.5)$$

Scattering states have  $E > 0$ . Note that, in contrast, to bound states, nothing special has to happen to find scattering solutions. We expect to find solutions for any choice of  $k$ .

This simple classification of solutions already tells us something interesting. Suppose, for example, that the potential looks something like the one shown in the figure. You might think that we could find a localised solution that is trapped between the two peaks, with  $E > 0$ . But this can't happen because if the wave function is to be normalisable, it must have  $E < 0$ . The physical reason, of course, is quantum tunnelling which allows the would-be bound state to escape to infinity [33, 34, and 35].





### 2.8.1.1 Reflection and Transmission Amplitudes:

Suppose that we stand a long way from the potential and throw particles in. What comes out? This is answered by solving the Schrodinger equation for the scattering states. Because we have a second order differential equation, we expect that there are two independent solutions for each value of  $k$ . We can think of these solutions physically as what you get if you throw the particle in from the left or in from the right. Let's deal with each in turn [33, 34, and 35].

### 2.8.1.2 Scattering from the Left:

We throw the particle in from the left. When it hits the potential, one of two things can happen: it can bounce back, or it can pass straight through. Of course, this being quantum mechanics, it can quite happily do both at the same time. Mathematically, this means that we are looking for a solution which asymptotically takes the form

$$\psi_R(x) \sim \begin{cases} e^{ikx} + re^{-ikx} & x \rightarrow -\infty \\ te^{ikx} & x \rightarrow +\infty \end{cases} \quad (2.8.1.2.1)$$

We've labelled this state  $\psi_R$  because the ingoing wave is right-moving. This can be seen in the first term  $e^{ikx}$  which represents the particle we're throwing in from  $x \rightarrow -\infty$ . The second term  $re^{-ikx}$  represents the particle that is reflected back to  $x \rightarrow -\infty$  after hitting the potential. The coefficient  $r \in \mathbb{C}$  is called the reflection amplitude. Finally, the term  $te^{ikx}$  at  $x \rightarrow +\infty$  represents the particle passing through the potential. The coefficient  $t \in \mathbb{C}$  is called the transmission coefficient. (Note: in this formula  $t$  is a complex number that we have to determine; it is not time!) There is no term  $e^{-ikx}$  at  $x \rightarrow +\infty$  because we're not throwing in any particles from that direction. Mathematically, we have chosen the solution in which this term vanishes. Before we proceed, it's worth flagging up a conceptual point. Scattering is clearly a dynamical process: the particle goes in, and then comes out again. Yet there's no

explicit time dependence in our ansatz (2.8.1.2.1); instead, we have a solution formed of plane waves, spread throughout all of space. It's best to think of these plane waves as describing a beam of particles, with the ansatz (2.8.1.2.1) giving us the steady-state solution in the presence of the potential.

The probability for reflection  $R$  and transmission  $T$  are given by the usual quantum mechanics rule:

$$R = |r|^2 \quad \text{and} \quad T = |t|^2 \quad (2.8.1.2.2)$$

In general, both  $R$  and  $T$  will be functions of the wavenumber  $k$ . This is what we would like to calculate for a given potential and we will see an example shortly. But, before we do this, there are some observations that we can make using general statements about quantum mechanics.

Given a solution  $\psi(x)$  to the Schrodinger equation, we can construct a conserved probability current

$$J(x) = \frac{-i\hbar}{2m} \left( \psi^* \frac{\partial \psi}{\partial x} - \psi \frac{\partial \psi^*}{\partial x} \right) \quad (2.8.1.2.3)$$

Which obeys

$$\frac{dJ}{dx} = 0 \quad (2.8.1.2.4).$$

This means that  $J(x)$  is constant. (Mathematically, this is the statement that the Wronskian is constant for the two solutions to the Schrodinger equation). For our scattering solution  $\psi_R$ , with asymptotic form (2.8.1.2.1), the probability current as  $x \rightarrow -\infty$  is given by

$$J(x) = \frac{\hbar k}{2m} \left[ (e^{-ikx} + r^* e^{+ikx})(e^{ikx} - r e^{-ikx}) + (e^{ikx} + r e^{-ikx})(e^{-ikx} - r^* e^{+ikx}) \right] \quad (2.8.1.2.5)$$

$$J(x) = \frac{\hbar k}{m} (1 - |r|^2) \quad \text{as} \quad x \rightarrow -\infty \quad (2.8.1.2.6)$$

Meanwhile, as  $x \rightarrow +\infty$ , we have

$$J(x) = \frac{\hbar k}{2m} |t|^2 \quad \text{as } x \rightarrow +\infty \quad (2.8.1.2.7)$$

Equating the two gives

$$1 - |r|^2 = |t|^2 \quad \Rightarrow R + T = 1 \quad (2.8.1.2.8)$$

This should make us happy as it means that probabilities do what probabilities are supposed to do. The particle can only get reflected or transmitted and the sum of the probabilities to do these things equals one [33, 34, and 35].

### 2.8.1.3 Scattering from the Right:

This time, we throw the particle in from the right. Once again, it can bounce back off the potential or pass straight through. Mathematically, we're now looking for solutions which take the asymptotic form

$$\psi_L(x) \sim \begin{cases} t' e^{-ikx} & x \rightarrow -\infty \\ e^{-ikx} + r' e^{+ikx} & x \rightarrow +\infty \end{cases} \quad (2.8.1.2.9)$$

Where we've now labelled this state  $\psi_L$  because the ingoing wave, at  $x \rightarrow +\infty$ , is left-moving. We've called the reflection and transmission amplitudes  $r'$  and  $t'$ .

There is a simple relation between the two solutions  $R$  in (2.8.1.2.1) and  $L$  in (2.8.1.2.9).

This follows because the potential  $V(x)$  in (2.8.1.1) is a real function, so if  $\psi_R$  is a solution then so is  $\psi_R^*$ . And, by linearity, so is  $\psi_R^* - r^* \psi_R$  which is given by

$$\psi_R^*(x) - r^* \psi_R(x) \sim \psi_L(x) \sim \begin{cases} (1 - |r|^2) e^{-ikx} & x \rightarrow -\infty \\ t^* e^{-ikx} + r^* t e^{+ikx} & x \rightarrow +\infty \end{cases} \quad (2.8.1.2.1)$$

This takes the same functional form as (2.8.1.2.9) except we need to divide through by  $t^*$  to make the normalisations agree. (Recall that scattering states aren't normalized anyway so we're quite at liberty to do this.) Using  $1 - |r|^2 = |t|^2$ , this tells us that there is a solution of the form (2.8.1.2.9) with

$$t' = t \quad \text{and} \quad r' = -\frac{r^* t}{t^*} \quad (2.8.1.2.2)$$

Notice that the transition amplitudes are always the same, but the reflection amplitudes can differ by a phase. Nonetheless, this is enough to ensure that the reflection probabilities are the same whether we throw the particle from the left or right

$$R = |r|^2 = |r'|^2 \quad (2.8.1.2.3).$$

## 2.8.2 Scattering in Three Dimensions:

Our real interest in scattering is for particles moving in three spatial dimensions, with Hamiltonian

$$H = \frac{p^2}{2m} + V(r) \quad (2.8.1.2.1)$$

Recall that there are two distinct interpretations for such a Hamiltonian

- We could think of this as the motion of a single particle, moving in a fixed background potential  $V(r)$ . this would be appropriate, for example, in Rutherford's famous experiment where we fire an alpha particle at a gold nucleus.

- Alternatively, We could think of this as the relative motion of two particles, separated by distance  $r$ , interacting through the force

$$F = -\nabla V(r) \quad (2.8.1.2.2)$$

We could take  $V(r)$  to be the Coulomb force, to describe the scattering of electrons, or the Yukawa force to describe the scattering of neutrons.

In this section, we will use language appropriate to the first interpretation, but everything we say holds equally well in the second. Throughout this section, we will work with rotationally invariant (i.e. central) potentials, so that  $V(r) = V(|r|)$ .

### 2.8.2.1 The Cross-Section:

Our first goal is to decide what we want to calculate. The simple reflection and transmission coefficients of the one-dimensional problem are no longer appropriate. We need to replace them by something a little more complicated. We start by thinking of the classical situation [33, 34, and 35].

### 2.8.2.2 Classical Scattering:

Suppose that we throw in a single particle with kinetic energy  $E$ . Its initial trajectory is characterized by the impact parameter  $b$ , defined as the closest the particle would get to the scattering center at  $r = 0$  if there were no potential. The particle emerges with scattering angle  $\theta$ , which is the angle between the asymptotic incoming and outgoing trajectories, as shown in the figure. By solving the classical equations of motion, we can compute  $\theta(b; E)$  or, equivalently,  $b(\theta; E)$ .

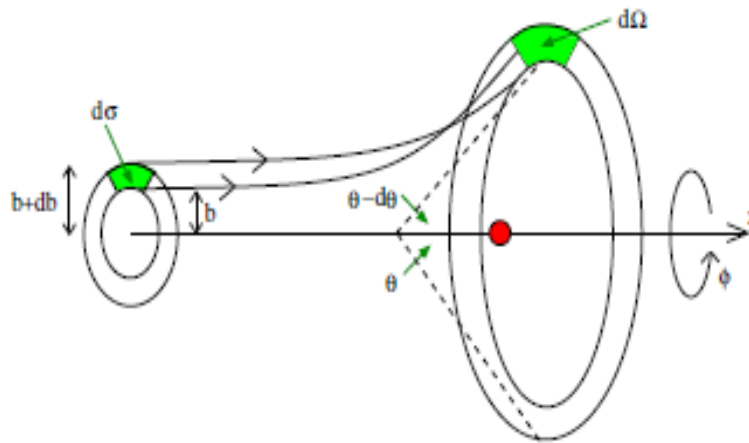


Figure: What becomes of an infinitesimal cross-sectional area after scattering.

Now consider a uniform beam of particles, each with kinetic energy  $E$ . We want to understand what becomes of this beam. Consider the cross-sectional area, denoted  $d\sigma$ . We write this as

$$d\sigma = b d\phi db \quad (2.8.2.2.1)$$

The particles within  $d\sigma$  will evolve to lie in a cone of solid angle  $d\Omega$ , given by

$$d\Omega = \sin\theta d\phi d\theta \quad (2.8.2.2.2)$$

Where, for central potentials, the infinitesimal angles  $d\phi$ , are the same in both these formulae. The differential cross-section is defined to be

$$\frac{d\sigma}{d\Omega} = \frac{b}{\sin\theta} \left| \frac{db}{d\theta} \right| \quad (2.8.2.2.3)$$

The left-hand side should really be  $|d\sigma/d\Omega|$ , but we'll usually drop the modulus. The differential cross-section is a function of incoming momentum  $k$ , together with the outgoing angle  $\theta$  [33, 34, and 35].

More colloquially, the differential cross-section can be thought of as

$$\begin{aligned} & \frac{d\sigma}{d\Omega} d\Omega \\ &= \frac{\text{Number of particles scattered into } d\Omega \text{ per unit time}}{\text{Number of incident particles per area } d\sigma \text{ per unit time}} \end{aligned} \quad (2.8.2.2.4)$$

We write this in terms of flux, defined to be the number of particles per unit area per unit time. In this language, the differential cross-section is

$$\frac{d\sigma}{d\Omega} = \frac{\text{Scattered flux}}{\text{Incident flux}} \quad (2.8.2.2.5)$$

We can also define the total cross-section

$$\sigma_T = \int d\Omega \frac{d\sigma}{d\Omega} \quad (2.8.2.2.6)$$

Both the differential cross-section and the total cross-section have units of area. The usual unit used in particle physics, nuclear physics and atomic physics is the barn, with  $1 \text{ barn} = 10^{-28} \text{ m}^2$ . The total cross-section is a crude characterisation of the scattering power of the potential. Roughly speaking, it can be thought of as the total area of the incoming beam that is scattered. The differential cross-section contains more detailed information.

### 2.8.2.3 Rutherford Scattering:

Rutherford scattering is the name given to scattering off a repulsive Coulomb potential of the form

$$V(r) = \frac{A}{r} \quad \text{with} \quad A > 0 \quad (2.8.2.3.1)$$

Where, for two particles of charge  $q_1$  and  $q_2$ , we have

$$A = \frac{q_1 q_2}{4\pi\epsilon_0} \quad (2.8.2.3.2).$$

$$2bE = A \cot \frac{\theta}{2} \quad (2.8.2.3.3)$$

This gives the differential cross-section,

$$\frac{d\sigma}{d\Omega} = \frac{b}{\sin\theta} \left| \frac{db}{d\theta} \right| = \left( \frac{A}{4E} \right)^2 \frac{1}{\sin^4(\theta/2)} \quad (2.8.2.3.4)$$

This scattering amplitude played an important role in the history of physics. Rutherford, together with Geiger and Marsden, fired alpha particles (a helium nucleus) at gold foil. They discovered that the alpha particles could be deflected by a large angle, with the cross-section given by (2.8.2.3.4). Rutherford realized that this meant the positive charge of the atom was concentrated in a tiny, nucleus.

There is, however, a puzzle here. Rutherford did his experiment long before the discovery of quantum mechanics. While his data agreed with the classical result (2.8.2.3.4), there is no reason to believe that this classical result carries over to a full quantum treatment. We'll see how this pans out later in this section.

There's a surprise when we try to calculate the total cross-section  $\sigma_T$ . We find that it's infinite! This is because the Coulomb force is long range. The potential decays to  $V(r) \rightarrow 0$  as  $r \rightarrow \infty$ , but it drops off very slowly. This will mean that we will have to be careful when applying our formalism to the Coulomb force.

### 2.8.2.4 The Scattering Amplitude:

The language of cross-sections is also very natural when we look at scattering in quantum mechanics [34, 35, and 36]. As in equation (2.8.1.1), we set up the scattering problem as a solution to the time-independent Schrodinger equation, which now reads

$$\left[ -\frac{\hbar^2}{2m} \nabla^2 + V(r) \right] \psi = E\psi \quad (2.8.2.4.1)$$

We will send in a plane wave with energy  $E$  which we choose to propagate along the  $z$ -direction. This is just

$$\psi_{incident}(r) = e^{ikz} \quad (2.8.2.4.2)$$

Where  $E = \hbar^2 k^2 / 2m$ . However, after scattering off the potential, the wave doesn't only bounce back in the  $z$  direction. Instead, it spreads out spherically, albeit with a phase and amplitude which can vary around the sphere. It's hard to take photographs of quantum wave functions, but the water waves shown on the right give a good analogy for what's going on. Asymptotically, as  $r \rightarrow \infty$ , this scattered wave takes the form

$$\psi_{scattered}(r) = f(\theta, \phi) \frac{e^{ikr}}{r} \quad (2.8.2.4.3)$$

The  $1/r$  fall-off follows from solving the free Schrodinger equation; we'll see this explicitly below. However, there is a simple intuition for this behavior which follows from thinking of  $|\psi|^2$  as a probability, spreading over a sphere which grows as  $r^2$  as  $r \rightarrow \infty$ . The  $1/r$  fall-off ensures that this probability is conserved. Our final ansatz for the asymptotic wave function is then

$$\psi(r) = \psi_{incident}(r) + \psi_{scattered}(r) \quad (2.8.2.4.4)$$

The function  $f(\theta; \phi)$  is called the scattering amplitude. For the central potentials considered here it is independent of  $\phi$ , so  $f = f(\theta)$ . It is the 3d generalisation of the reflection and transmission coefficients that we met in the previous section. Our goal is to calculate it.

The scattering amplitude is very closely related to the differential cross-section. To see this, we can look at the probability current

$$J = -i \frac{\hbar}{2m} (\psi^* \nabla \psi - \psi \nabla \psi^*) \quad (2.8.2.4.5)$$

Which obeys  $\nabla \cdot J = 0$ . For the incident wave, we have



$$J_{incident} = \frac{\hbar k}{m} \hat{z} \quad (2.8.2.4.6)$$

This is interpreted as a beam of particles with velocity  $v = \hbar k/m$  travelling in the z-direction. Meanwhile, for the scattered wave we use the fact that

$$\nabla\psi_{scattered} = ik f(\theta) \frac{e^{ikr}}{r} \hat{r} + \mathcal{O}\left(\frac{1}{r^2}\right) \quad (2.8.2.4.7)$$

$$J_{scattered} = \frac{\hbar k}{m} \frac{1}{r^2} |f(\theta)|^2 \hat{r} + \mathcal{O}\left(\frac{1}{r^3}\right) \quad (2.8.2.4.8)$$

This means that, as  $r \rightarrow \infty$ , the flux of outgoing particles crossing an area  $dA$  subtended by the solid angle  $d\Omega$

$$J_{scattered} \cdot \hat{r} dA = \frac{\hbar k}{m} |f(\theta)|^2 d\Omega \quad (2.8.2.4.9)$$

The differential cross-section is defined to be the ratio of the scattered flux through  $d\Omega$ , divided by the incident flux. In other words, it is

$$\frac{d\sigma}{d\Omega} = \frac{\hbar k |f(\theta)|^2 / m}{\hbar k / m} = |f(\theta)|^2 \quad (2.8.2.4.10)$$

This is rather nice. It means that if we can compute the scattering amplitude  $f(\theta)$ , it immediately tells us the differential cross-section. The total cross-section is defined, as before, as

$$\sigma_T = \int d\Omega |f(\theta)|^2 \quad (2.8.2.4.11)$$

### 2.8.3 Scattering off a Lattice:

There, we confidently described the various lattice structures that underlay different solids. But how do we know this? The answer, of course, is scattering. Firing a beam of particles whether neutrons, electrons or photons in the X-ray spectrum at the solid reveals a characteristic diffraction pattern. Our goal here is to understand this within the general context of scattering theory.

Our starting point is the standard asymptotic expression describing a wave scattering off a central potential, localized around the origin,

$$\psi(\mathbf{r}) \sim e^{i\mathbf{k}\cdot\mathbf{r}} + f(\mathbf{k}; \mathbf{k}') \frac{e^{ikr}}{r} \quad (2.8.3.1)$$

Here we're using the notation, introduced in earlier sections, of the scattered momentum

$$\mathbf{k}' = k\hat{\mathbf{r}} \quad (2.8.3.2)$$

The idea here is that if you sit far away in the direction  $\hat{\mathbf{r}}$ , you will effectively see a wave with momentum  $\mathbf{k}'$ . We therefore write  $f(\mathbf{k}; \mathbf{k}')$  to mean the same thing as  $f(k; \theta, \phi)$ .

Suppose now that the wave scatters off a potential which is localized at some other position,  $\mathbf{r} = \mathbf{R}$ . Then the equation (2.8.3.1) becomes

$$\psi(\mathbf{r}) \sim e^{i\mathbf{k}\cdot(\mathbf{r}-\mathbf{R})} + f(\mathbf{k}; \mathbf{k}') \frac{e^{ik|\mathbf{r}-\mathbf{R}|}}{|\mathbf{r}-\mathbf{R}|} \quad (2.8.3.3)$$

For  $r \rightarrow \infty$ , we can expand

$$|\mathbf{r}-\mathbf{R}| = \sqrt{r^2 + R^2 - 2\mathbf{r}\cdot\mathbf{R}} \approx r\sqrt{1 - 2\mathbf{r}\cdot\mathbf{R}/r^2} \approx r - \hat{\mathbf{r}}\cdot\mathbf{R} \quad (2.8.3.4)$$

We then have

$$\psi(\mathbf{r}) \sim e^{-i\mathbf{k}\cdot\mathbf{R}} \left[ e^{i\mathbf{k}\cdot\mathbf{r}} + f(\mathbf{k}; \mathbf{k}') e^{-i(\mathbf{k}'-\mathbf{k})\cdot\mathbf{R}} \frac{e^{ikr}}{r} \right] \quad (2.8.3.5)$$

The overall factor is unimportant, since our interest lies in the phase shift between the incident wave and the scattered wave. We see that we get an effective scattering amplitude

$$f_R(\mathbf{k}; \hat{\mathbf{r}}) = f(\mathbf{k}; \mathbf{k}') e^{i\mathbf{q}\cdot\mathbf{R}} \quad (2.8.3.6)$$

Where we have defined the transferred momentum

$$\mathbf{q} = \mathbf{k} - \mathbf{k}' \quad (2.8.3.7)$$

Now let's turn to a lattice of points  $\Lambda$ . Ignoring multiple scatterings, the amplitude is simply the sum of the amplitudes from each lattice point

$$f_{\Lambda}(\mathbf{k}, \mathbf{k}') = f(\mathbf{k}, \mathbf{k}') \sum_{\mathbf{R} \in \Lambda} e^{i\mathbf{q} \cdot \mathbf{R}} \quad (2.8.3.8)$$

However, we already discussed the sum

$$\Delta(\mathbf{q}) = \sum_{\mathbf{R} \in \Lambda} e^{i\mathbf{q} \cdot \mathbf{R}} \quad (2.8.3.9)$$

The sum has the nice property that it vanishes unless  $\mathbf{q}$  lies in the reciprocal lattice  $\Lambda^*$ . This is simple to see: since we have an infinite lattice it must be true that, for any vector  $\mathbf{R}_0 \in \Lambda$ ,

$$\Delta(\mathbf{q}) = \sum_{\mathbf{R} \in \Lambda} e^{i\mathbf{q} \cdot \mathbf{R}} = \sum_{\mathbf{R} \in \Lambda} e^{i\mathbf{q} \cdot (\mathbf{R} - \mathbf{R}_0)} = e^{-i\mathbf{q} \cdot \mathbf{R}_0} \Delta(\mathbf{q}) \quad (2.8.3.10)$$

This means that either  $e^{-i\mathbf{q} \cdot \mathbf{R}_0} = 1$  or  $\Delta(\mathbf{q}) = 0$ . The former result is equivalent to the statement that  $\mathbf{R} \in \Lambda^*$ . . More generally,

$$\sum_{\mathbf{R} \in \Lambda} e^{i\mathbf{q} \cdot \mathbf{R}} \equiv \Delta(\mathbf{q}) = V^* \sum_{\mathbf{Q} \in \Lambda^*} \delta(\mathbf{q} - \mathbf{Q}) \quad (2.8.3.11)$$

Where  $V^*$  is the volume of the unit cell of  $\Lambda^*$ . We see that  $\Delta(\mathbf{q})$  is very strongly (formally, infinitely) peaked on the reciprocal lattice.

The upshot of this discussion is a lovely result: there is scattering from a lattice if and only if

$$\mathbf{k} - \mathbf{k}' \in \Lambda^* \quad (2.8.3.12)$$

This is known as the Laue condition. If the scattered momentum does not satisfy this condition, then the interference between all the different scattering sites results in a vanishing wave. Only when the Laue condition is obeyed is this interference constructive [33, 34, and 35].

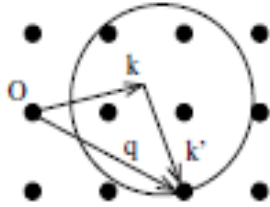


Figure 108: The Ewald sphere.

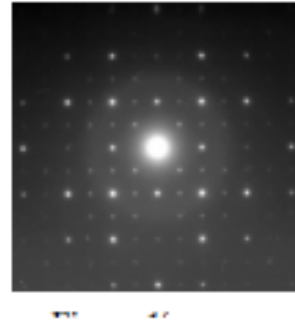


Figure 109: Salt.

Alternatively, the Laue condition can be viewed as momentum conservation, with the intuition that the lattice can only absorb momentum in  $\Lambda^*$ .

Solutions to the Laue condition are not generic. If you take a lattice with a fixed orientation and fire a beam with fixed  $\mathbf{k}$ , chances are that there are no solutions to (2.8.3.12). To see this, consider the reciprocal lattice as shown in the left-hand panel of the figure. From the tip of  $\mathbf{k}$  draw a sphere of radius  $k$ . This is sometimes known as the *Ewald sphere* and its surface gives the possible transferred momenta  $\mathbf{q} = \mathbf{k} - \mathbf{k}'$ . There is scattering only if this surface passes through a point on the reciprocal lattice.

To get scattering, we must therefore either find a wave to vary the incoming momentum  $\mathbf{k}$ , or find a way to vary the orientation of the lattice. But when this is achieved, the outgoing photons  $\mathbf{k}' = k\hat{\mathbf{r}}$  sit only at very specific positions. In this way, we get to literally take a photograph of the reciprocal lattice! The resulting diffraction pattern for salt (*NaCl*) which has a cubic lattice structure is shown in the right-hand panel. The four-fold symmetry of the reciprocal lattice is clearly visible.

### 2.8.3.1 The Bragg Condition:

There is an equivalent phrasing of the Laue condition in real space. Suppose that the momentum vectors obey

$$\mathbf{k} - \mathbf{k}' = \mathbf{Q} \in \Lambda^* \quad (2.8.3.1.1)$$

Since  $\mathbf{Q}$  is a lattice vector, so too is  $n\mathbf{Q}$  for all  $n \in \mathbf{Z}$ . Suppose that  $\mathbf{Q}$  is minimal, so that  $n\mathbf{Q}$  is not a lattice vector for any  $n < 1$ . Defining the angle  $\theta$  by  $\mathbf{k} \cdot \mathbf{k}' = k^2 \cos\theta$ , we can take the square of the equation above to get

$$2k^2(1 - \cos\theta) = 4k^2 \sin^2(\theta/2) = Q^2 \Rightarrow 2k \sin(\theta/2) = Q \quad (2.8.3.1.2)$$

We can massage this further. The vector  $\mathbf{Q} \in \Lambda^*$  defines a set of parallel planes in  $\Lambda$ . Known as Bragg planes, these are labelled by an integer  $n$  and defined by those  $\mathbf{a} \in \Lambda$  which obey  $\mathbf{a} \cdot \mathbf{Q} = 2\pi n$ . The distance between successive planes is

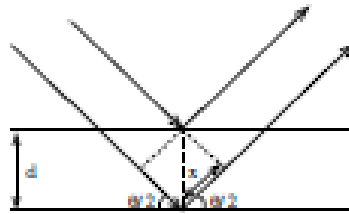
$$d = \frac{2\pi}{Q} \quad (2.8.3.1.3)$$

Furthermore, the wave vector  $k$  corresponds to a wavelength  $\lambda = 2\pi/k$ . We learn that the Laue condition written as the requirement that

$$\lambda = 2d \sin(\theta/2) \quad (2.8.3.1.4)$$

Repeating this argument for vectors  $n\mathbf{Q}$  with  $n \in \mathbf{Z}$ , we get

$$n\lambda = 2d \sin(\theta/2) \quad (2.8.3.1.5)$$



This is the Bragg condition. It has a simple interpretation. For  $n = 1$ , we assume that the wave scatters off two consecutive planes of the lattice, as shown figure. The wave which hits the lower plane travels an extra distance of  $2x = 2d \sin(\theta/2)$ . The Bragg condition requires this extra distance to coincide with the wavelength of light. In other words, it is the statement that waves reflecting off consecutive planes interfere constructively.

The Bragg condition gives us license to think about scattering of light off planes in the lattice, rather than individual lattice sites. Moreover, it tells us that the

wavelength of light should be comparable to the atomic separation in the crystal. This means x-rays. The technique of x-ray crystallography was pioneered by Max von Laue, who won the 1914 Nobel Prize. The Bragg law was developed by William Bragg, a fellow of Trinity and director of the Cavendish. He shared the 1915 Nobel Prize in physics with his father, also William Bragg, for their development of crystallographic techniques [34, 35, 36].

X-ray crystallography remains the most important technique to determine the structure of materials. Two examples of historical interest are shown in the figures. The picture on the left is something of an enigma since it has five-fold symmetry. Yet there are no Bravais lattices with this symmetry! The diffraction picture is revealing a quasi-crystal, an ordered but non-periodic crystal. The image on the right was taken by Rosalind Franklin and is known as “photograph 51”. It provided a major, and somewhat controversial, hint to Crick and Watson in their discovery of the structure of DNA.

## 2.9 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 Schrodinger equation [36]

$$\left[ -\frac{\hbar^2}{2m} \nabla^2 + V(r) \right] \psi(r) = E\psi(r) \quad V(r) = 0 \quad \text{except } r \in \text{target region T} \quad (2.9.1)$$

That is consistent with the boundary condition of an incident plane wave

$$\psi(r) = e^{ikr} \quad (2.9.2)$$

And an emanating scattered wave. The energy  $E$  is determined by the energy of the incident plane wave

$$E = \frac{\hbar^2 k^2}{2m} \quad (2.9.3)$$

By introducing the Green function  $G$

$$\left[ \frac{\hbar^2}{2m} \nabla^2 + E \right] G(r, r') = \delta(r - r') \quad (2.9.4)$$

For the potential-free Schrodinger equation, the Schrodinger equation for  $\psi(r)$ ,

$$\left[ \frac{\hbar^2}{2m} \nabla^2 + E \right] \psi(r) = V(r)\psi(r) \quad (2.9.5)$$

Can be transformed into an integral equation

$$\psi'(r) = \psi(r) + \int d^3r' G(r, r') V(r') \psi(r') \quad (2.9.6)$$

In which the formal expression  $V(r)\psi(r)$  is conceived as inhomogeneity of the differential equation (2.9.1). This integral equation is called the Lippmann-Schwinger equation. Hereby,  $\psi(r)$  is the above cited plane-wave solution of the potential-free Schrodinger equation. The index  $\mathbf{k}$  in  $\psi'$  expresses the fact that this state has evolved from one that in the remote past was a plane wave of the particular wave vector  $\mathbf{k}$ . Obviously, in the limit of zero potential,  $V(r) \rightarrow 0$ , the scattered and the incident wave are identical,

$$\psi'(r) = \psi(r) \quad (2.9.7).$$

The Green function  $G(r, r')$  is not uniquely determined by the Schrodinger equation (2.9.1).

Also here the unique solution requires a boundary condition, which is chosen such, that the solution  $\psi'(r)$  describes outgoing scattered waves. The Green function  $G(r, r')$

$$G(r, r') = -\frac{2m}{\hbar^2} \frac{1}{4\pi} \frac{e^{ik|r-r'|}}{|r-r'|} \quad \text{with} \quad k = \sqrt{\frac{2m}{\hbar^2} E} \quad (2.9.8)$$

Describes then the stationary radiation of a particle of energy  $E$  that is generated at  $r'$ , by a spherical wave outgoing from the target. In other words, the Green function  $G(r, r')$  gives the amplitude of this wave at location  $r$  due to its generation by the source at  $r'$ , under the condition that the wave is not further scattered during its propagation from  $r'$  to  $r$ . By the Lippmann-Schwinger equation, the incident wave  $\psi(r)$  is superimposed with spherical waves emitted from scattering at position  $r'$  in the target. The amplitude of these scattered waves is proportional to the interaction potential  $V(r')$  and the amplitude of the total wave field  $\psi(r')$  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  $r$  and the scattering center  $r'$  it is useful to expand the Green function  $G$  in powers of  $\frac{r'}{r} \ll 1$  assuming that the extent of  $r'$  is restricted to the space of a small target or scattering volume, respectively,  $r' \in T$ . Approximating for  $r' \ll r$

$$\frac{1}{|r - r'|} = \frac{1}{r} + \mathcal{O}\left(\frac{1}{r^2}\right) \quad \text{and} \quad |r - r'| \approx r - \hat{r} \cdot r' \quad \text{with} \quad \hat{r} = \frac{\mathbf{r}}{r} \quad (2.9.9)$$

And inserting this into the relation (2.9.8) one obtains the asymptotic form, or far-field limit, respectively, of the Green function  $G$ ,

$$G(r, r') = -\frac{2m}{\hbar^2} \frac{1}{4\pi} \frac{e^{ikr}}{r} e^{-ik\hat{r} \cdot r'} + \mathcal{O}\left(\frac{1}{r^2}\right) \quad (2.9.10)$$

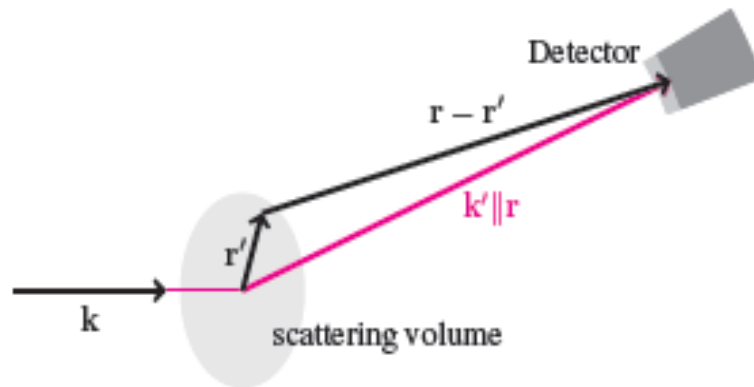
Inserting this expression into the Lippmann-Schwinger equation (2.9.6) one obtains the asymptotic solution of the wave function  $\psi(r)$  for large distances  $r$

$$\psi(\mathbf{r}) \sim e^{i\mathbf{k} \cdot \mathbf{r}} + f(\hat{r}) \frac{e^{ikr}}{r} \quad (2.9.11)$$

Which is exactly the boundary condition (2.9.11) we conjectured from Huygens' Principle, whereas the scattering amplitude  $f(\hat{r}) = f(\theta, \phi)$  is given by the integral,



That can be interpreted as a transition-matrix element from the scattering state described by  $\psi'(r')$  to the scattered state at far distances, which is a plane-wave state described by  $\mathbf{k}' = k \hat{r}$ , the wave vector of the scattered wave in the direction of the detector, which is known in the experiment.  $T(k'; k)$  is referred to as the  $T$  matrix or transition amplitude, a quantity proportional to the scattering amplitude. Due to the far-field approximation (2.9.9) the scattering pattern  $f(\hat{r})$  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 (2.9.10) is also referred to as the Fraunhofer approximation of the Green function.



Scattering geometry for the calculation of the far-field limit at the detector. In the Fraunhofer approximation, we assume that  $|r| \gg |r'|$ .

# Chapter Three

## Literature Review

### 3.1 Introduction:

Some of the attempts made to improve scattering theory to agree with observations are presented here.

Some of the researches done to use GSR and PDSR are also presented.

### 3.2 Solving the Quantum Scattering Problem for Systems of Two and Three Charged Particles:

A rigorous formalism for solving the Coulomb scattering problem has been done in this work. The approach is based on splitting the interaction potential into a finite-range part and a long-range tail part. The scattering problem can be reformulated by applying exterior complex scaling. The scaled problem has zero boundary conditions at infinity and can be implemented numerically for finding scattering amplitudes. The systems under consideration may consist of two or three charged particles [37].

The technique presented in is first developed for the case of a two body single channel Coulomb scattering problem.

The partial wave results are summed up to obtain the scattering amplitude for the three dimensional scattering problem. The approach is generalized to allow the two body multichannel scattering problem to be solved.

The potential splitting technique is further developed and validated for the three-body Coulomb scattering problem. It is shown that only a part of the total interaction potential should be split to obtain the inhomogeneous equation required such that the method of exterior complex scaling can be applied. The final six-dimensional

equation is reduced to a system of three-dimensional equations using the full angular momentum representation. Such a system can be numerically implemented using the existing full angular momentum complex exterior scaling code (FAMCES).

The total scattering amplitude is expressed as the sum of the partial wave scattering amplitudes. Then generalize this single-channel theory to a two-body multi-channel theory.

The potential division technique developed in the thesis is generalized so to describe quantum mechanical scattering of three charged particles in the sense that a third particle collides with two bound to each other particles. It is shown that only the part of the total potential which describes the interaction between the two bound particles is included in the so-called driven Schrödinger equation that describes the process. So it is only on this potential as the potential sharing technique combined with external complex scaling must be applied. This leads to a six-dimensional inhomogeneous equation which reduces to a system of three-dimensional equations in a complete angular momentum representation. This one formalism has been implemented in an existing computational computer program of resonance states in three-body systems (FAMCES) to now, in addition, calculate quantum mechanical three-body scattering.

The single channel two body scattering problem is considered in the framework of partial wave decomposition. The potential splitting approach is suggested to extent the exterior complex scaling approach first applied by Rescigno *et al* to the Coulomb scattering problem. The driven Schrödinger equation with zero boundary conditions is obtained and mathematically validated.

The integral representation for the scattering amplitude is derived using the Green's function formalism. It is shown that the scattering amplitude is completely defined by the solution of the driven equation in the inner region.

Therefore, the driven Schrödinger equation with zero boundary conditions can be used to solve the scattering problem. The local representation for the scattering amplitude is also obtained. For large values of the splitting parameter,  $R$ , the formulation of the problem and the representations for the scattering amplitudes do not include the Coulomb functions. The Coulomb potential tail is taken into account by using the factor  $\exp[ih \log 2kR]$  in the representations for the scattering amplitude. The theoretical results are tested on the example of the purely Coulomb interaction,  $V(r) = 2r^{-1}$ , and the Coulomb interaction plus the short-range term,  $V(r) = 2r^{-1} + 15r^2 \exp[-r]$ . The numerical implementation of the theory shows that the desired accuracy of the calculated data can be achieved by an appropriate choice of the splitting parameter,  $R$ . It is also shown that the integral representation for the scattering amplitude provides the better convergence as  $R$  grows as compared with the local representation [37, 38].

### **3.3 Investigations on Cement Pastes by Small-Angle X-ray Scattering and BET: the Relevance of Fractal Geometry:**

The microstructural properties of Portland cement (PC) were studied and compared by small-angle X-ray scattering (SAXS) and the Brunauer-Emmett-Teller (BET) method. SAXS measurements have shown that the microstructure of PC samples cannot be described in terms of a classical porous medium with a well-defined specific inner surface, but rather obeys the formalism of fractal geometry. Measurements have been taken on powdered and size-fractionated cement samples with different water-cement ratios (w/c) and different amounts of added chloride salts, and on different types of cements. The analysis of the data obtained by SAXS showed that inner surface and volume structure are fractal; however, only the mass fractal dimension  $D_m$  (2.3-3.0) could be evaluated with sufficient precision and reproducibility. By comparing these  $D_m$  values and the specific surface areas

obtained by BET (40-70 m<sup>2</sup>/g), a correlation between  $D_m$  and BET surface was found when only one parameter ( $w/c$ ) was varied [39].

The SAXS measurements showed that drying procedures (which are necessary for BET measurements) give rise to a different microstructure of the cement samples, as revealed by different  $D_m$  values for these samples.

Both methods BET gas adsorption and SAXS yield microstructural parameters: the specific inner-surface by BET on the one hand and the mass-fractal dimension  $D_m$  obtained from SAXS on the other. The latter combines structural properties such as spatial scale invariance, degree of porosity, branching, roughness and connectivity in one quantitative parameter for the microstructure in the nm range. When the results from the same samples were compared, a linear correlation was found at different  $w/c$  values, whereas in all other cases - where the type of cement or the amount of added chloride salts (at constant  $w/c$ ) was varied - no such correlation (either linear or inverse) between the values from the two methods could be obtained. This might be because each method accesses a different length scale in the submicroscopic range. On the other hand, there need not be a dependency between the *mass* fractal dimension  $D_m$  and the specific *surface* as obtained by BET. A comparison of the *surface* fractal dimension  $D_s$  and the BET *surface* in the case of our cement samples the scattering was largely dominated by  $D_m$  and therefore  $D_s$  was not measurable with sufficient precision.

Generally, SAXS has proved to be a suitable complementary method the results obtained with SAXS shows (where no  $S_j$  was definable) that the concept of a 'specific inner surface' is largely method-dependent, the ease and speed of modern SAXS measurements, which also reflect properties of inner structure of cement, and the fact that no pretreatment such as drying is required make this an interesting analytical tool in this field.

### **3.4 Light Scattering by Polymers:**

This work describes two light-scattering experiments that have recently been introduced into the physical chemistry teaching laboratory [40].

The first experiment involves the measurement of the mass-average molar mass and degree of coiling of polystyrene and is interpreted by the full mathematical theory of light scattering. The second experiment concerns the study of transitions in gelatin. The primary structure of a polymer is determined by the type and number of atoms in a polymer chain, the secondary structure by the mode and degree of chain coiling, and the quaternary structure by the way in which neighboring chains interact. The two experiments together illustrate the elucidation of these three levels of structure.

The results obtained shows that the scattering intensities pass through a maximum as the solutions melt but that this effect is suppressed at higher concentrations (solution 3). There is also an overall inversion in light-scattering intensity as the concentration is increased from solution

1 to 2 to 3. finally there is a decrease in intensity from solution 4 (pH 5) to solution 5 (pH 8), and a similar change can be seen with solutions made up in sodium chloride solution. All these effects can be interpreted by the students through thoughtful application of the theory described earlier.

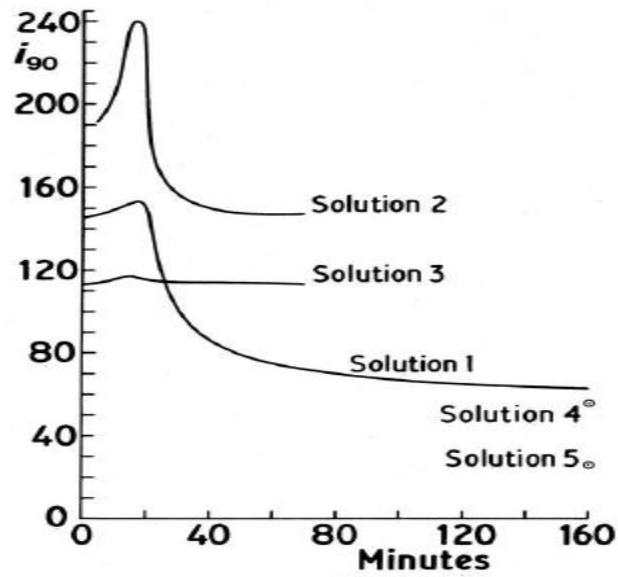


Figure. Light-scattering intensity of gelatin gels and solutions

### 3.5 Introducing Scattering Theory with a Computer:

This research presents a new way to introduce scattering theory. This new method is based on the use of a computer to calculate classical particle trajectories and then quantum mechanical phase shifts. The strategy uses a computer and general programs which, though very simple, work for any problem with a spherically symmetric potential. The strategy introduces the concepts of differential and total cross section in a classical context. It then discusses the asymptotic phase shifts between wave functions with and without the potential present and, finally, it discusses cross sections in terms of the interference between these wave functions [41].

This new way emphasizes the physical content of scattering experiments: the concept that the potential determines the number of particles scattered into various directions, and the concept that potentials change the asymptotic phase of quantum mechanical wave functions. The ideas used are easy to explain and easy to visualize, and the necessary computation can be done on even the smallest computation facilities.

### **3.6 Scattering Theory from Homogeneous and Coated Spheres:**

In this work one used computer for the Scattering of electromagnetic radiation from a sphere. This paper describes how it is possible to use the Mathematical language and structure to obtain efficient and easy scattering algorithms for homogeneous and coated spheres. The calculations are based on Mie calculation developed using Mathematical language and packages [42].

The code is based on a very easy approach taking vantage of the semantics of Mathematical. The code has been also implemented for coated sphere where the Mie coefficients are computed taking into account the new structure. The mathematical form of the scattering functions have similar form as those for homogeneous sphere. The development of our Mie scattering code by Mathematical can be considered like a tool to analyze and verify intermediate results obtained using computer codes developed using numerical approach.

### **3.7 Scattering Theory and Geometry:**

This work shows how selected geometries can be used to regularize singular potentials, and then computed scattering amplitudes for quanta incident on a static non-relativistic wormhole. Secondly, one studied selected spatial geometries that can either enhance or suppress scattering amplitudes, to produce either extremely sharp resonances and/or very strong cloaking for a specified angular momentum. One presented in detail a simple model for an impenetrable sphere surrounded by a Riemannian step geometry. Lastly, one considered the scattering of particles by a variety of geometrical holes and computed quantum scattering cross-sections for simple models where non-relativistic particles are incident on a selection of specified hole geometries in various spatial dimensions [43].

This model shows the effects of geometry on the time-independent scattering of non-relativistic particles, as described by solutions of the covariant Helmholtz equation.



Specific geometries were used to illustrate these scattering effects through the exact computation of partial wave amplitudes. One exhibited various relationships between non-relativistic quantum systems involving a potential, in flat space, and systems without a potential but defined on curved manifolds. We presented very specific examples involving  $1/r$  potentials and regularized  $1/R^4$  potentials on wormhole manifolds.

One also analyzed in detail the simple cloaked sphere geometric model to show that resonances are produced more prodigiously as the aspect ratio of the model increases, an effect somewhat similar to what happens in Mie scattering when the index of refraction is increased. One argued that such resonances tend to make it more difficult for the model to achieve stealth and invisibility to low momentum incident waves. Since the analysis is non-relativistic, one believe it may be useful as written for understanding suitably designed, nan scale quantum devices, devices one computed also scattering amplitudes for the impenetrable hyper-sphere & the foxhole geometry, and for the bottomless hyper-cylinder & the cylindrical wormhole, in  $N$  dimensions.

### **3.8 On an Evaluation of the Accuracy of the Uniform Semi Classical Approximation for Differential Elastic Scattering Cross Sections:**

The uniform approximation to the differential elastic scattering cross section is extended to allow direct comparison of approximated cross sections with cross sections computed by exact evaluation of the partial wave sum using WKB phase shifts. Results of calculations are presented and an assessment is made of the accuracy and utility of the uniform approximation [44].

This work shows that the uniform approximation offers a highly accurate method of computing differential elastic cross sections in cases where semi classical behavior is to be expected. For  $A$  greater than 50 and angles greater than  $2\pi/A$ , the cross

sections derived in this manner and those obtained by the exact evaluation of the partial wave sum are, from the point of view of experimental interpretation, indistinguishable.

The time required to compute  $\sigma_E^*$  to uniform percentage accuracy increases roughly as  $A^3$ , the calculation of  $\sigma_B^*$  is insensitive to the value of  $A$ . In fact, the computation time for  $\sigma_B^*$  decreases with increasing  $A$ , since at  $A$  values large enough that the interference term cannot be resolved experimentally its computation can be omitted, leaving only  $\sigma_{LR}^*$ . another advantage of the uniform approximation is that nearly all the computations are of classical quantities which are independent of the value of  $A$ ; if a series of cross sections for various  $A$  values is desired this fact can be used to decrease computing time still further. Typical computing time for a 200 point angular grid on the IBM 360/65 was 5-15 sec to obtain the very precise cross sections used in this work; less accurate results can be obtained in times about an order of magnitude less.

The speed of the uniform approximation, coupled with its ability to compute cross sections for large  $A$  conveniently, brings several uses immediately to mind. One of the authors (J.M.M.) has constructed a program to generate angular positions of rainbow extreme in graphical form for various three-parameter potentials. Such graphs can provide a rapid means of inferring best-fit parameters for simple potentials from differential scattering data. The analytic form of the cross section discussed here has already found use in schemes to effect an inversion of cross section data to give the point-by-point interaction potential,<sup>11-19,25</sup> and it can be anticipated that more such applications will follow.

### 3.9 Microscopic Description of Elastic and Direct Inelastic Nucleon Scattering off Spherical Nuclei:

The purpose of this study is to improve the modeling of nucleon direct inelastic scattering to the continuum using a microscopic and parameter-free approach. For the first time, direct elastic scattering, inelastic scattering to discrete excitations and to the continuum are described within a microscopic approach without adjustable parameters. Proton scattering off  $Zr^{90}$  and  $Pb^{208}$  are the reactions used as test case examples of the calculations. The model uses the Melbourne  $g$ -matrix and the Random Phase [45].

Approximation description of nuclear states, implemented with the Gogny D1S interaction. The relevant optical and transition potentials in a finite nucleus are calculated within a local density approximation.

The study is limited to incident energies above 40MeV. We first checked that this model provides an accurate account of measured cross sections for elastic scattering and inelastic scattering to discrete states. It is then applied to the direct inelastic scattering to the continuum considering all one-phonon excitations predicted within the RPA approach. This accounts for a part of the direct pre-equilibrium emission, often labeled as the one-step direct process in quantum-based approaches.

This approach provides a very accurate description of angular distributions where the one-step process dominates. The impact of collective excitations is shown to be non-negligible for energy transfer to the target up to 20MeV, decreasing as the incident energy increases. For incident energies above 80MeV, the model provides a good account of direct proton emission for an energy transfer to the target up to 30MeV. However, the proton emission we predict underestimates the measured cross sections for incident energies below 80MeV.

A fully microscopic models, based on a description of target excitations provided by the RPA nuclear structure model implemented with the Gogny force, was applied to the description of direct elastic and inelastic scattering to discrete excitations and to the continuum (pre-equilibrium emission). While previous implementation of microscopic models for pre-equilibrium emission used adjustable two body interactions, such as a Yukawa form factors, our modeling is fully based on a microscopic description of target states and a realistic two-body interaction. Furthermore, direct elastic scattering, direct excitation to collective states and pre-equilibrium emission, limited to the first step, are described within the same framework.

The Melbourne  $g$ -matrix, used as the in-medium NN interaction, and the RPA one-body ground states and transition densities matrix were used to build the relevant optical and transition potentials which are both complex, energy dependent and non-local. These ingredients were used to calculate first the elastic scattering, then the direct inelastic scattering to low energy discrete excitations in  $Zr^{90}$  and  $Pb^{208}$ , within the DWBA framework. In the 60–200MeV incident energy range, the present modeling, which does not involve any adjustment, provides a satisfactory account of measured elastic and inelastic cross sections.

These calculations demonstrate that the present modeling provides an accurate account of direct elastic scattering and inelastic scattering to discrete state processes above 60MeV. This approach was then applied to describe emission to the continuum or in other words to Pre-equilibrium emission. Calculations are limited to the one-step direct process.

From this analysis, several conclusions have been drawn. First, the collectivity described within the RPA model has a strong impact on nucleon emission up to an energy transfer to the target of 20MeV. This impact decreases as the incident energy increases. For energy transfers larger than 20MeV, calculations based on the RPA

wave function are identical to those based on uncorrelated particle-hole excitations of the HF mean field. As the Melbourne  $g$ -matrix contains two-body spin-orbit and tensor components, all transitions to non-natural parity states predicted by the RPA model are included. Comparison to data indicated that for incident energies above 120MeV, the emission is well accounted for as low emission angles and for an energy transfer up to approximately 40MeV. Inclusion of collective excitations was shown to be crucial to obtain this agreement. However, in the incident energy range 40– 80MeV, our calculations underestimate the data even at forward angles and this disagreement becomes larger for decreasing incident energies. This discrepancy is partly related the two-body interactions used in the modeling.

Various approximations that were used in the derivation of the Melbourne  $g$ -matrix were removed and provided more accurate solutions to the Bruckner-Bethe-Goldstone equation. Moreover, recent studies also revealed the role of di-nucleon structures at low densities which could strongly impact the description of nuclear surface sensitive reactions. These studies could help describing direct nucleon inelastic scattering within the nuclear matter approach, when the incident energy decreases. Besides, further developments are planned to improve the present analysis, such as the use of QRPA wave functions and the extension to more targets. Finally, the so-called rearrangement corrections, which accounts for the modification in the density-dependent two-body interaction which is caused by the density fluctuations during the inelastic process, are not included in the present work. In a previous study performed within the JLM folding model, this dynamical effect was shown to strongly impact the cross sections magnitude.

Rearrangement corrections were shown to strongly depend on the incident energy, the projectile disposing and the transition multipolarity. These corrections should be implemented in the framework of the  $g$ -matrix full folding model to assess its impact

on calculated cross sections for direct inelastic to both discrete states and to the continuum.

Those developments will ensure to accurately predict the one-step contribution to pre-equilibrium emission. More work is still needed to extend our modeling to account for emission mechanisms beyond the one-step process.

### **3.10 Energy Quantization of Electrons for Spherically Symmetric Atoms and Nano Particles According to Schrödinger Equation:**

Schrödinger Equation for spherical atoms and nano particles was used to describe the behavior of electrons and phonons by treating them as strings oscillating thermally and under the action of external force. The solution shows that for thermally excited phonons and electrons the energy and frequency are quantized. For electrons excited by external force the energy and frequency are also quantized. The energy in both cases resembles the zero point energy for harmonic oscillator of the quantum system. The solution also describes free as well as bounded electrons. The results obtained agree with previous models and observations [46].

For spherically symmetric atoms or nano particles the string model shows that the electrons are regularly distributed inside them. The energy is quantized and is imaginary for thermally oscillating strings and is also quantized and resembles that of ordinary harmonic quantum oscillator when the external force acts only. The energy is positive or negative describing either free or bounded electrons.

### **3.11 Harmonic Oscillator Solution for Free and Time Independent Potential String within the Framework of Dirac Special Relativistic Equation:**

It is well known that Dirac relativistic equation describes the relativistic particle which is either free or move in any potential field. Even if one utilized the electromagnetic Hamiltonian which recognizes the effect of electromagnetic

potential, the time dependent part of Dirac equation gives the same form which is free from the potential term if the potential is time independent. In this case the time dependent part gives a sine or cosine solution describing quantized string energy like that of harmonic oscillator but with no zero point energy. However if one follows De Broglie hypothesis and assumes that the string oscillator is in the form of a highly localized wave packet the time dependent part gives cosine solution with energy expression typical to that of Schrodinger equation which recognizes the existence of zero point energy. This means that when the wave packet is localized in the form of a particle it has a rest mass energy corresponding to the zero point energy [47].

The solution of the Klein Gordon equation shows that the energy is quantized by applying periodicity conditions and assuming the particles as continuous wave trains and as a localized wave group. Strikingly the solutions show that all particles behave as strings no matter what the potential is. When one consider strings to be highly.

### **3.12 Time Independent Generalized Special Relativity Quantum Equation and Travelling Wave Solution:**

The generalized special relativity, which accounts for the effect of fields through the potential, is used to derive a new Dirac relativistic quantum equation. This new quantum equation consists of a potential term which emerged naturally from the relativistic energy expression. The solution of this equation predicts the propagation of travelling wave inside fields without attenuation. Thus it can describe the electromagnetic wave propagation inside bulk matter. It also predicts the existence of bio photons as stationary waves that spreads themselves, instantaneously through the surrounding media. It also shows that particles behave as harmonic oscillator inside atoms with rest mass energy equal to the zero point energy. These results agree with observations [48].

The linear GSR quantum equation shows that the particles sometimes acts as travelling waves with quantized harmonic oscillator energy and zero point energy. It also predicts that bio photons are stationary simultaneously distributed waves.

### **3.13 Quantum Equation for Generalized Special Relativistic Linear Hamiltonian:**

Using generalized special relativistic energy –momentum relation, a useful linear equation was obtained. The coefficients and matrixes resembles that of Dirac relativistic quantum equation .A new quantum linear relativistic equation sensitive to the potential and the effects of fields was also obtained. This equation reduces to that of Dirac in the absence of fields. The perturbed Hamiltonian consist of free energy term beside linear potential term which resembles that of ordinary perturbation theories. The travelling wave solution gives a new potential dependent energy relation, which reduces to that of Dirac in the absences of field. Move over this expression for energy can be a pure imaginary for strong potential and energetic particle, which indicates efficient energy absorption by the medium as proposed by electromagnetic theory [49].

The coefficient and matrixes of the GSR linear Dirac quantum equation resembles that of Dirac. The GSR linear relativistic equation consists of an additional term, representing potential. This equation reduces to that of ordinary Dirac in the absence of fields. The travelling wave solution gives an energy expression reduces to that of Dirac in the absence of fields.

### **(3.14) Summary and Critique:**

Most of the work done for scattering is based on computational physics which gives limited contribution as far it does not account for the scattering of fast particles beams. The GSR attempts does not applied to the scattering process. Thus one needs a new model based on GSR to account for the scattering of fast particles.



# Chapter Four

## Scattering Using Potential Dependent SR

### 4.1 Introduction:

The scattering flux and cross section which are exhibited in the standard texts cannot account for fast particles as far as it is based on Schrodinger equation which is based also on Newtonian mechanics.

Anew relativistic scattering quantum equation is exhibited here in this chapter.

### 4.2 General Scattering Theory:

In many cases the laws of conservation of momentum and energy alone can be used to obtain important results concerning the properties of various mechanical processes. It should be noted that these properties are independent of the particular type of interaction between the particles involved [25].

The energy according to the GSR given by

$$E = \frac{m_0 c^2}{\sqrt{g_{00} - v^2/c^2}} \quad (4.2.1)$$

Thus

$$E^2 = \frac{m_0^2 c^4}{\frac{g_{00} m^2 c^4 - m^2 v^2 c^2}{m^2 c^4}} \quad (4.2.2)$$

But  $E = mc^2$  (4.2.3)

Inserting equation (4.2.3) in equation (4.2.2) yields

$$g_{oo}E^2 = p^2c^2 + m^2c^4 \quad (4.2.4)$$

Where  $g_{oo} = 1 + \frac{2\phi}{c^2} = 1 + \frac{2m\phi}{mc^2}$

$$g_{oo} = 1 + \frac{2V}{E} \quad (4.2.5)$$

Substituting equation (4.2.5) in equation (4.2.4) yields

$$\left(1 + \frac{2V}{E}\right)E^2 = p^2c^2 + m^2c^4 \quad (4.2.6)$$

Rearranging equation (4.2.6) gives

$$E^2 + 2VE = p^2c^2 + m^2c^4 \quad (4.2.7)$$

Multiplying both side of this equation by  $\psi$  gives

$$E^2\psi + 2VE\psi = p^2c^2\psi + m^2c^4\psi \quad (4.2.8)$$

According to the wave nature of particles

$$\psi = Ae^{\frac{i}{\hbar}(px-Et)} \quad (4.2.9)$$

Differentiating equation (4.2.9) with respect to space and time yields

$$\frac{\partial\psi}{\partial t} = \frac{-iE}{\hbar}\psi$$

$$\frac{-\hbar}{i} \frac{\partial\psi}{\partial t} = E\psi = i\hbar \frac{\partial\psi}{\partial t}$$

$$-\hbar^2 \frac{\partial^2\psi}{\partial t^2} = E^2\psi$$

$$\frac{\partial \psi}{\partial x} = \frac{ip}{\hbar} \psi \quad \text{and} \quad \frac{\partial^2 \psi}{\partial x^2} = \frac{-p^2}{\hbar^2} \psi \Rightarrow p^2 \psi = -\hbar^2 \frac{\partial^2 \psi}{\partial x^2} \quad (4.2.10)$$

Substituting equation (4.2.10) in equation (4.2.9) yields

$$-\hbar^2 \frac{\partial^2 \psi}{\partial t^2} + 2V \left( i\hbar \frac{\partial \psi}{\partial t} \right) = -\hbar^2 c^2 \nabla^2 \psi + m_0^2 c^4 \psi \quad (4.2.11)$$

From this equation by suggesting a solution

$$\psi = u(r) e^{\frac{-i}{\hbar} Et} \quad (4.2.12)$$

$$\frac{\partial \psi}{\partial t} = \frac{-iE}{\hbar} \psi \Rightarrow \frac{\partial^2 \psi}{\partial t^2} = -\frac{E^2}{\hbar^2} \psi \quad (4.2.13)$$

A direct substitution equation (4.2.13) in equation (4.2.11) yields

$$E^2 u(r) e^{\frac{-i}{\hbar} Et} + 2VEu(r) e^{\frac{-i}{\hbar} Et} = -\hbar^2 c^2 \nabla^2 \psi + m_0^2 c^4 \psi \quad (4.2.14)$$

$$E^2 \psi + 2VE\psi = -\hbar^2 c^2 \nabla^2 \psi + m_0^2 c^4 \psi \quad (4.2.15)$$

This equation can be written as

$$\nabla^2 \psi + \frac{E^2}{\hbar^2 c^2} \psi = \frac{(m_0^2 c^4 - 2EV)}{\hbar^2 c^2} \psi \quad (4.2.16)$$

Where:

$$\frac{E^2}{\hbar^2 c^2} = k^2 \quad (4.2.17)$$

$$\frac{(m_0^2 c^4 - 2EV)}{\hbar^2 c^2} = U \quad (4.2.18)$$

Substituting (4.2.17)(4.2.18) in (4.2.16) yields

$$\nabla^2 \psi + k^2 \psi = U\psi \quad (4.2.19)$$

This equation represent scattered particles equation.

$$\nabla^2(GA) + k^2(GA) = A\delta_{rr'} \quad (4.2.20)$$

Integrating both sides yields

$$\int \nabla^2(GA)dr' + k^2 \int (GA)dr' = \int A(r')\delta_{rr'} dr' = A(r) \quad (4.2.21)$$

Comparing this equation with equation (4.2.19) gives

$$A(r) = U(r)\psi(r) \quad (4.2.22)$$

$$\psi = \int (GA)dr' = \int G(r,r')A(r,r')dr' \quad (4.2.23)$$

$$\psi(r) = \int G(r,r')U(r')\psi(r')dr' \quad (4.2.24)$$

Thus the general equation to equation (4.2.19) gives:

$$\psi(r) = e^{ikr} + \int G(r,r')U(r')\psi(r')dr' \quad (4.2.25)$$

Where

$$G(r,r') = \frac{-1}{4\pi} \frac{e^{ikr}}{r} e^{-ikr'} \quad (4.2.26)$$

$$U = \frac{(m_0^2 c^4 - 2EV)}{\hbar^2 c^2} \quad (4.2.27)$$

Substituting (4.2.26) (4.2.27) in equation (4.2.25) yields

$$\psi(r) = \frac{-1}{4\pi} \frac{e^{ikr}}{r\hbar^2 c^2} \int e^{-ik.r'} \psi(r')(m_0^2 c^4 - 2EV(r'))dr' \quad (4.2.28)$$

This equation can be written as

$$\psi(r) = \frac{-1}{4\pi r \hbar^2 c^2} \left[ m_0^2 c^4 \int e^{-ik \cdot r'} \psi(r') dr' - 2E \int e^{-ik \cdot r'} \psi(r') V(r') dr' \right] \quad (4.2.29)$$

For simplification consider

$$Q(\theta, \varphi) = \frac{-m_0^2 c^2}{4\pi \hbar^2} \int e^{-ikr' \cos \alpha} \psi(r') dr' \quad (4.2.30)$$

$$f(\theta, \varphi) = \frac{E}{2\pi \hbar^2 c^2} \int e^{-ikr' \cos \alpha} \psi(r') V(r') dr' \quad (4.2.31)$$

Thus equation (4.2.25) becomes

$$\psi(r) = e^{ikr} + Q(\theta, \varphi) \frac{e^{ikr}}{r} + f(\theta, \varphi) \frac{e^{ikr}}{r} \quad (4.2.32)$$

Where

$$\psi_{in}(r) = e^{ikr} \quad (4.2.33)$$

$$\psi_{sc}(r) = \frac{e^{ikr}}{r} (Q + f) = \frac{e^{ikr}}{r} D(\theta, \varphi) \quad (4.2.34)$$

$$\text{Where} \quad Q + f = D(\theta, \varphi) \quad (4.2.35)$$

Using the

$$S_{sc} = \frac{i\hbar}{2m} [\psi_{sc}(r) \nabla \overline{\psi_{sc}}(r) - \overline{\psi_{sc}}(r) \nabla \psi_{sc}(r)] \quad (4.2.36)$$

Where:

$$\psi_{sc}(r) = D(\theta, \varphi) \frac{e^{ikr}}{r} \quad \Rightarrow \quad \overline{\psi_{sc}}(r) = \overline{D}(\theta, \varphi) \frac{e^{-ikr}}{r} \quad (4.2.37)$$

$$\nabla \overline{\psi_{sc}}(r) = \frac{\partial \overline{\psi_{sc}}}{\partial r} = \overline{D}(\theta, \varphi) \left[ \frac{-ik}{r} - \frac{1}{r^2} \right] e^{-ikr} \quad (4.2.38)$$

$$\nabla \overline{\psi_{sc}}(r) = -\overline{D}(\theta, \varphi) \left[ \frac{ik}{r} + \frac{1}{r^2} \right] e^{-ikr} = \frac{-\overline{D}(\theta, \varphi)}{r^2} e^{-ikr} [ikr + 1]$$

$$\nabla \psi_{sc}(r) = \frac{\partial \psi_{sc}}{\partial r} = D(\theta, \varphi) \left[ \frac{ik}{r} - \frac{1}{r^2} \right] e^{ikr}$$

$$\nabla \psi_{sc}(r) = \frac{D(\theta, \varphi)}{r^2} e^{ikr} [ikr - 1] \quad (4.2.39)$$

A direct substitution equation (4.2.39) in equation (4.2.36) gives

$$S_{sc} = \frac{i\hbar}{2m} \frac{|D^2|}{r^3} [-(ikr + 1) - (ikr - 1)] \quad (4.2.40)$$

$$S_{sc} = \frac{i\hbar}{2m} \frac{|D^2|}{r^3} (-2ikr)$$

$$S_{sc} = \frac{\hbar k}{mr^2} |D^2| \quad (4.2.41)$$

but  $p = mv = \hbar k \quad (4.2.42)$

Thus the scattering flux is given by:

$$S_{sc} = \frac{mv}{mr^2} |D^2| = S_{sc} = \frac{v}{r^2} |D^2| = (4.2.43)$$

According to the definition of the scattering cross section  $S_{sc} = \frac{v}{r^2} \sigma$

Thus the scattering cross section  $\sigma$  is given by:

$$\sigma = |D^2| \quad (4.2.44)$$

Maxwell's equations describe the behavior of moving and static charges as well as electromagnetic waves (emw), the electric field intensity  $E$  for a medium with electric permittivity and conductivity is given by

$$\nabla^2 E + \epsilon\mu \frac{\partial^2 E}{\partial t^2} - \mu\sigma \frac{\partial E}{\partial t} = 0 \quad (4.2.45)$$

Consider a solution in the form

$$E = E_0 e^{i(kx - \omega t)} \quad (4.2.46)$$

Differentiating equation (4.2.46) with respect to space and time yields

$$\begin{aligned} \nabla^2 E = -k^2 E \quad , \quad \frac{\partial E}{\partial t} = -i\omega E \\ \frac{\partial^2 E}{\partial t^2} = -\omega^2 E \quad , \quad \text{and let} \quad \epsilon\mu = \frac{1}{c^2} \end{aligned} \quad (4.2.47)$$

Inserting equation (4.2.47) in (4.2.45) gives

$$-k^2 E + \frac{\omega^2}{c^2} E + i\mu\sigma\omega E = 0 \quad (4.2.48)$$

Multiplying both sides of equation (4.2.48) by  $\frac{\hbar^2 c^2}{E}$  gives

$$-\hbar^2 k^2 c^2 + \hbar^2 \omega^2 + i\mu\sigma\omega \hbar^2 c^2 = 0 \quad (4.2.49)$$

Rearranging equation (4.2.49) gives

$$\hbar^2 \omega^2 = \hbar^2 k^2 c^2 - i\mu\sigma\omega \hbar^2 c^2 \quad (4.2.50)$$

Where

$$E = \hbar\omega \quad \text{and} \quad p = \hbar k \quad (4.2.51)$$

Thus equation (4.2.50) becomes:

$$E^2 = p^2 c^2 - i\mu\sigma E\hbar c^2 \quad (4.2.52)$$

Comparing this equation with the Einstein energy momentum relation

$$E^2 = p^2 c^2 + m_0^2 c^4 \quad (4.2.53)$$

Gives:

$$m_0^2 c^4 = -i\mu\sigma E\hbar c^2 \quad (4.2.54)$$

Using the definition of the conductivity (  $\sigma = \sigma_1 + i\sigma_2$  ) thus equation (4.2.54) becomes:

$$m_0^2 c^4 = -i\mu(\sigma_1 + i\sigma_2)E\hbar c^2 \quad (4.2.55)$$

But this term ( $m_0^2 c^4$ ) represent the real part:

$$m_0^2 c^4 = \mu\sigma_2 E\hbar c^2 \quad (4.2.56)$$

To find the conductivity of a certain medium consider a particle moving with velocity  $v$  in a resistive medium of coefficient  $\gamma$  under the action of the electric field  $E$ . the equation of motion of the particle is given by:

$$m \frac{dv}{dt} = -\hbar \cdot x + \gamma v + eE \quad (4.2.57)$$

Assume the solution

$$x = x_0 e^{i\omega t} \quad (4.2.58)$$



Where:

$$v = \frac{dx}{dt} = i\omega x \quad , \quad x = \frac{v}{i\omega}$$

$$\frac{dv}{dt} = (i\omega)(i\omega x) = -\omega^2 x$$

$$\hbar\omega = m\omega^2 \tag{4.2.59}$$

Substituting (4.2.59) in (4.2.57) yields:

$$-m\omega^2 x = -m\omega_s^2 x + i\gamma\omega x + eE \tag{4.2.60}$$

Rearranging equation (4.2.60) gives:

$$eE = m(\omega_s^2 - \omega^2)x - i\gamma\omega x \tag{4.2.61}$$

Thus:

$$x = \frac{eE}{m(\omega_s^2 - \omega^2) - i\gamma\omega} \tag{4.2.62}$$

Multiplying both side of equation (4.2.62) by  $m(\omega_s^2 - \omega^2) + i\gamma\omega$  gives:

$$x = \frac{eE[m(\omega_s^2 - \omega^2) + i\gamma\omega]}{m^2(\omega_s^2 - \omega^2)^2 + \gamma^2\omega^2} \tag{4.2.63}$$

Where:

$$x = \frac{v}{i\omega} \quad \Rightarrow \quad v = i\omega x \tag{4.2.64}$$

Thus:

$$v = \frac{\omega eE[-\gamma\omega + im(\omega_s^2 - \omega^2)]}{m^2(\omega_s^2 - \omega^2)^2 + \gamma^2\omega^2} \tag{4.2.65}$$

From equation (4.2.65) one gets:

$$v = v_1 + iv_2 \quad \Rightarrow \quad \sigma = \sigma_1 + i\sigma_2 \quad (4.2.66)$$

Using the definition of current density  $j$  and the conductivity  $\sigma$  one gets:

$$j = nev = \sigma E \quad (4.2.67)$$

Substituting (4.2.65) in (4.2.67) yields:

$$\sigma = \frac{n\omega e^2[-\gamma\omega + im(\omega_0^2 - \omega^2)]}{m^2(\omega_0^2 - \omega^2)^2 + \gamma^2\omega^2} \quad (4.2.68)$$

Thus the real part  $\sigma_1$  and the imaginary part  $\sigma_2$  of the conductivity are given by:

$$\sigma_1 = \frac{n\omega e^2[-\gamma\omega]}{m^2(\omega_0^2 - \omega^2)^2 + \gamma^2\omega^2} \quad (4.2.69)$$

$$\sigma_2 = \frac{n\omega e^2[m(\omega_0^2 - \omega^2)]}{m^2(\omega_0^2 - \omega^2)^2 + \gamma^2\omega^2} \quad (4.2.70)$$

Hence from (4.2.70) equation (4.2.56) becomes:

$$m_0^2 c^4 = \frac{n\mu e^2 E^2 c^2 m(\omega_0^2 - \omega^2)}{m^2(\omega_0^2 - \omega^2)^2 + \gamma^2\omega^2} \quad (4.2.71)$$

While the imaginary part in equation (4.2.55) represent the energy of frictional medium  $E_f$

Thus For frictional medium

$$E^2 = p^2 c^2 + m_0^2 c^4 + iE_f \quad (4.2.72)$$

From equation (4.2.55) yields  $E_f$

$$m_0^2 c^4 = -i\mu\sigma E\hbar c^2 = -i\mu E\hbar c^2(\sigma_1 + i\sigma_2) \quad (4.2.73)$$

Hence:

$$E_f = -i\mu E \hbar c^2 \sigma_1 \quad (4.2.74)$$

$$E_f = \frac{i n \mu e^2 E^2 c^2 \gamma \omega}{m^2 (\omega_s^2 - \omega^2)^2 + \gamma^2 \omega^2} \quad (4.2.75)$$

Let:

$$V = 0 \text{ [Thus see equation (4.2.31) ] } f(\theta, \varphi) = 0$$

Thus according to equation (4.2.35)

$$D(\theta, \varphi) = Q(\theta, \varphi) \quad (4.2.76)$$

Thus equation (4.2.27) becomes

$$U = \frac{m_s^2 c^4}{\hbar^2 c^2} \quad (4.2.77)$$

For simplification equation (4.2.71) consider

$$m^2 (\omega_s^2 - \omega^2)^2 \ll \gamma^2 \omega^2 \quad \text{and using } E^2 = \hbar^2 \omega^2 \quad (4.2.78)$$

Therefor equation (4.2.71) becomes:

$$m_s^2 c^4 = \frac{n \mu e^2 \hbar^2 c^2 m (\omega_s^2 - \omega^2)}{\gamma^2} \quad (4.2.79)$$

Substituting equation (4.2.79) in equation (4.2.77) yields:

$$U = \frac{n \mu e^2 m (\omega_s^2 - \omega^2)}{\gamma^2} \quad (4.2.80)$$

In this case equation (4.2.28) becomes:

$$\psi_{sc}(r) = \frac{-1}{4\pi} \frac{e^{ikr}}{r} \left[ \frac{n\mu e^2 m(\omega_s^2 - \omega^2)}{\gamma^2} \int e^{-ik \cdot r'} \psi(r') dr' \right] \quad (4.2.81)$$

$$\psi_{sc}(r) = \frac{Q(\theta, \varphi)}{4\pi} \frac{e^{ikr}}{r} \quad (4.2.82)$$

Where:

$$Q(\theta, \varphi) = \left[ -\frac{n\mu e^2 m(\omega_s^2 - \omega^2)}{\gamma^2} \int e^{-ik \cdot r'} \psi(r') dr' \right] \quad (4.2.83)$$

### 4.3 Scattering by Uniform Potential for Nearly Free Particle:

For nearly free particle the wave function is

$$\psi(r) = e^{ikr \cos \alpha} \quad (4.3.1)$$

If the potential is uniform

$$V = V_0 \quad (4.3.2)$$

According to equation (4.2.30) (4.2.31) and Substituting equations (4.3.1) (4.3.2) yields

$$Q(\theta, \varphi) = \frac{-m_s^2 c^2}{4\pi \hbar^2} \int_0^{r_0} e^{ikr' \cos \alpha} e^{-ikr' \cos \alpha} dr' \quad (4.3.3)$$

$$Q(\theta, \varphi) = \frac{-m_s^2 c^2}{4\pi \hbar^2} \int_0^{r_0} dr' = \frac{-m_s^2 c^2}{4\pi \hbar^2} [r']_0^{r_0} \quad (4.3.4)$$

$$Q(\theta, \varphi) = \frac{-m_s^2 c^2}{4\pi \hbar^2} r_0 \quad (4.3.5)$$

$$f(\theta, \varphi) = \frac{E}{2\pi \hbar^2 c^2} \int e^{-ikr' \cos \alpha} e^{ikr' \cos \alpha} V_0 dr' \quad (4.3.6)$$

$$f(\theta, \varphi) = \frac{EV_0}{2\pi\hbar^2c^2} \int_0^{r_0} dr' = \frac{EV_0}{2\pi\hbar^2c^2} [r']_0^{r_0} \quad (4.3.7)$$

$$f(\theta, \varphi) = \frac{EV_0}{2\pi\hbar^2c^2} r_0 \quad (4.3.8)$$

Using equation (4.2.35) together with equation (4.3.5) (4.3.8) one gets:

$$D(\theta, \varphi) = Q + f = \frac{-m_0^2c^2}{4\pi\hbar^2} r_0 + \frac{EV_0}{2\pi\hbar^2c^2} r_0 \quad (4.3.9)$$

Thus according to equation (4.2.43) the scattering flux is given by:

$$S_{sc} = \frac{v}{r^2} |D^2|$$

$$S_{sc} = \frac{v}{r^2} \left[ \frac{-m_0^2c^2}{4\pi\hbar^2} r_0 + \frac{EV_0}{2\pi\hbar^2c^2} r_0 \right]^2 \quad (4.3.10)$$

$$S_{sc} = \frac{v}{r^2} \frac{r_0^2}{4\pi^2\hbar^4} \left[ \frac{m_0^4c^4}{4} - m_0^2EV_0 + \frac{E^2V_0^2}{c^4} \right] \quad (4.3.11)$$

According to the definition of the scattering cross section  $\sigma$ :

$$S_{sc} = \sigma \frac{v}{r^2} \quad (4.3.12)$$

Thus from equation (4.2.43)

$$S_{sc} = \frac{v}{r^2} |D^2|$$

Comparing equation (4.3.12) with equation (4.2.43) the scattering cross section is thus given by:

$$\sigma = |D^2| \quad (4.3.13)$$

$$\sigma = |D^2| = \frac{r_0^2}{4\pi^2\hbar^4} \left[ \frac{m_0^4 c^4}{4} - m_0^2 E V_0 + \frac{E^2 V_0^2}{c^4} \right] \quad (4.3.14)$$

#### 4.4 Scattering by Spherical Nucleus for Nearly Free Particle:

If the atom has  $Z$  protons then the coulomb potential is given by:

$$V = \frac{-Ze^2}{4\pi\epsilon_0 r} \quad (4.4.1)$$

For nearly free particle the wave function is

$$\psi(r) = e^{ikr \cos\alpha} \quad (4.4.2)$$

Substituting equation (4.4.1) and (4.4.2) in equation (4.2.30) (4.2.31) one gets:

$$f(\theta, \varphi) = \frac{E}{2\pi\hbar^2 c^2} \int_{r_n}^{r_0} e^{-ikr' \cos\alpha} e^{ikr' \cos\alpha} \left( \frac{-Ze^2}{4\pi\epsilon_0 r'} \right) dr' \quad (4.4.3)$$

Where  $r_n$  is the nucleus radius

Thus:

$$f(\theta, \varphi) = \frac{-E}{8\pi^2\hbar^2 c^2} \frac{Ze^2}{\epsilon_0} \int_{r_n}^{r_0} \frac{dr'}{r'} \quad (4.4.4)$$

$$f(\theta, \varphi) = \frac{-E}{8\pi^2\hbar^2 c^2} \frac{Ze^2}{\epsilon_0} [\ln r']_{r_n}^{r_0} \quad (4.4.5)$$

$$f(\theta, \varphi) = \frac{E}{8\pi^2\hbar^2 c^2} \frac{Ze^2}{\epsilon_0} [\ln r_n - \ln r_0] \quad (4.4.6)$$

$$f(\theta, \varphi) = \frac{E}{8\pi^2\hbar^2 c^2} \frac{Ze^2}{\epsilon_0} \left[ \ln \frac{r_n}{r_0} \right] \quad (4.4.7)$$

$$Q(\theta, \varphi) = \frac{-m_0^2 c^2}{4\pi\hbar^2} \int_{r_n}^{r_0} e^{ikr' \cos\alpha} e^{-ikr' \cos\alpha} dr' \quad (4.4.8)$$

$$Q(\theta, \varphi) = \frac{m_o^2 c^2}{4\pi\hbar^2} [r_n - r_o] \quad (4.4.9)$$

Using equation (4.2.35) together with equation (4.4.7) (4.4.9) one gets:

$$D(\theta, \varphi) = Q + f = \frac{m_o^2 c^2}{4\pi\hbar^2} [r_n - r_o] + \frac{E}{8\pi^2\hbar^2 c^2} \frac{Ze^2}{\epsilon_o} \left[ \ln \frac{r_n}{r_o} \right] \quad (4.4.10)$$

Thus according to equation (4.2.43) the scattering flux in this case is given by:

$$S_{sc} = \frac{v}{r^2} |D^2|$$

$$S_{sc} = \frac{v}{r^2} \left| \left( \frac{m_o^2 c^2}{4\pi\hbar^2} [r_n - r_o] + \frac{E}{8\pi^2\hbar^2 c^2} \frac{Ze^2}{\epsilon_o} \left[ \ln \frac{r_n}{r_o} \right] \right)^2 \right| \quad (4.4.11)$$

Using equation (4.2.44) the scattering cross section takes the form:

$$\sigma = |D^2| = \left| \left( \frac{m_o^2 c^2}{4\pi\hbar^2} [r_n - r_o] + \frac{E}{8\pi^2\hbar^2 c^2} \frac{Ze^2}{\epsilon_o} \left[ \ln \frac{r_n}{r_o} \right] \right)^2 \right| \quad (4.4.12)$$

## 4.5 Scattering by Harmonic Oscillator for Nearly Free Particle:

Atoms can also be treated as harmonic oscillators, in this case the potential is given by:

$$V(r) = -\hbar r \quad (4.5.1)$$

Inserting equation (4.5.1) in equation (4.2.30) (4.2.31) together with equation (4.3.1) gives:

$$f(\theta, \varphi) = \frac{E}{2\pi\hbar^2 c^2} \int_{r_h}^{r_o} e^{-ikr' \cos\alpha} e^{ikr' \cos\alpha} (-\hbar r') dr' \quad (4.5.2)$$

$$f(\theta, \varphi) = \frac{-E\hbar}{2\pi\hbar^2 c^2} \int_{r_h}^{r_o} (r') dr' = \frac{-E\hbar}{2\pi\hbar^2 c^2} \left[ \frac{r'^2}{2} \right]_{r_h}^{r_o} \quad (4.5.3)$$

$$f(\theta, \varphi) = \frac{E\hbar}{2\pi\hbar^2c^2} \left[ \frac{r_h^2}{2} - \frac{r_o^2}{2} \right] \quad (4.5.4)$$

$$Q(\theta, \varphi) = \frac{-m_o^2c^2}{4\pi\hbar^2} \int_{r_h}^{r_o} e^{ikr' \cos\alpha} e^{-ikr' \cos\alpha} dr' \quad (4.5.5)$$

$$Q(\theta, \varphi) = \frac{-m_o^2c^2}{4\pi\hbar^2} \int_{r_h}^{r_o} dr' = \frac{-m_o^2c^2}{4\pi\hbar^2} [r_o - r_h] \quad (4.5.6)$$

$$Q(\theta, \varphi) = \frac{m_o^2c^2}{4\pi\hbar^2} [r_h - r_o] \quad (4.5.7)$$

Hence according to equation (4.2.35)

$$D(\theta, \varphi) = Q + f = \frac{m_o^2c^2}{4\pi\hbar^2} [r_h - r_o] + \frac{E\hbar}{2\pi\hbar^2c^2} \left[ \frac{r_h^2}{2} - \frac{r_o^2}{2} \right] \quad (4.5.8)$$

Thus according to equation (4.2.43) the scattering flux in this case is given by:

$$S_{sc} = \frac{v}{r^2} \left| \left( \frac{m_o^2c^2}{4\pi\hbar^2} [r_h - r_o] + \frac{E\hbar}{2\pi\hbar^2c^2} \left[ \frac{r_h^2}{2} - \frac{r_o^2}{2} \right] \right)^2 \right| \quad (4.5.9)$$

Using equation (77) the scattering cross section takes the form:

$$\sigma = |D^2| = \left| \left( \frac{m_o^2c^2}{4\pi\hbar^2} [r_h - r_o] + \frac{E\hbar}{2\pi\hbar^2c^2} \left[ \frac{r_h^2}{2} - \frac{r_o^2}{2} \right] \right)^2 \right| \quad (4.5.10)$$

## 4.6 Scattering of Ground State Harmonic Oscillator for Perpendicular Scattering:

The wave function for ground state harmonic oscillator is:

$$\psi(r) = \frac{\alpha^{1/2}}{\pi^{1/4}} e^{-\frac{\alpha^2 r^2}{2}} \quad (4.6.1)$$



The potential is given by:

$$V(r) = -\hbar r \quad (4.6.2)$$

For perpendicular scattering:

$$\alpha = 90 \quad \cos\alpha = 0 \quad (4.6.3)$$

Substituting equations (4.6.1) (4.6.2) and (4.6.3) in equation (4.2.30) (4.2.31) gives:

$$Q(\theta, \varphi) = \frac{-m_0^2 c^2}{4\pi\hbar^2} \int_{r_h}^{r_0} \left( \frac{\alpha^{1/2}}{\pi^{1/4}} \right) e^{-\frac{\alpha^2 r'^2}{2}} dr' \quad (4.6.4)$$

For  $r_0 \rightarrow \infty$  and  $r_h \rightarrow 0$  one can let:

$$x = \frac{\alpha^2 r'^2}{2} \Rightarrow \frac{dx}{dr'} = \alpha^2 r' \quad (4.6.5)$$

$$dr' = \frac{dx}{\alpha^2 r'} = \frac{\alpha dx}{\alpha^2 (2x)^{1/2}} = \frac{x^{-1/2} dx}{\sqrt{2} \alpha} \quad (4.6.6)$$

Inserting equations (4.6.5) (4.6.6) in equation (4.6.4) gives:

$$Q(\theta, \varphi) = \frac{-m_0^2 c^2}{4\sqrt{2} \hbar^2 \pi^{(5/4)} \alpha^{(1/2)}} \int_0^\infty x^{(-1/2)} e^{-x} dx \quad (4.6.7)$$

$$Q(\theta, \varphi) = \frac{-m_0^2 c^2 \Gamma(1/2)}{4\sqrt{2} \hbar^2 \pi^{(5/4)} \alpha^{(1/2)}} = \frac{-m_0^2 c^2 \sqrt{\pi}}{4\sqrt{2} \hbar^2 \pi^{(5/4)} \alpha^{(1/2)}} \quad (4.6.8)$$

$$Q(\theta, \varphi) = \frac{-m_0^2 c^2}{4\sqrt{2} \hbar^2 \pi^{(3/4)} \alpha^{(1/2)}} \quad (4.6.9)$$

$$f(\theta, \varphi) = \frac{E}{2\pi\hbar^2 c^2} \int_{r_h}^{r_0} \left( \frac{\alpha^{1/2}}{\pi^{1/4}} e^{-\frac{\alpha^2 r'^2}{2}} \right) (-\hbar r') dr' \quad (4.6.10)$$

$$f(\theta, \varphi) = \left( \frac{E}{2\pi\hbar^2 c^2} \right) \left( \frac{-\hbar \alpha^{1/2}}{\pi^{1/4}} \right) \int_{r_h}^{r_0} e^{-\frac{\alpha^2 r'^2}{2}} r' dr' \quad (4.6.11)$$

Put

$$y = -\frac{\alpha^2 r'^2}{2} \Rightarrow \frac{dy}{dr'} = -\alpha^2 r' \quad (4.6.12)$$

$$r' dr' = \frac{dy}{-\alpha^2} \quad (4.6.13)$$

Thus equation (4.6.11) become:

$$f(\theta, \varphi) = \left( \frac{E}{2\pi\hbar^2 c^2} \right) \left( \frac{-\hbar \alpha^{1/2}}{-\alpha^2 \pi^{1/4}} \right) \int_{r_h}^{r_0} e^y dy \quad (4.6.14)$$

$$\begin{aligned} f(\theta, \varphi) &= \frac{\hbar E}{2\pi^{(5/4)} \alpha^{(3/2)} \hbar^2 c^2} [e^y]_{r_h}^{r_0} \\ &= \frac{\hbar E}{2\pi^{(5/4)} \alpha^{(3/2)} \hbar^2 c^2} \left[ e^{-\frac{\alpha^2 r'^2}{2}} \right]_{r_h}^{r_0} \end{aligned} \quad (4.6.15)$$

$$f(\theta, \varphi) = \frac{\hbar E}{2\pi^{(5/4)} \alpha^{(3/2)} \hbar^2 c^2} \left[ e^{-\frac{\alpha^2 r_0^2}{2}} - e^{-\frac{\alpha^2 r_h^2}{2}} \right] \quad (4.6.16)$$

According to equation (4.2.35) and substituting equations (4.6.9) (4.6.16) yields:

$$\begin{aligned} D(\theta, \varphi) &= \frac{-m_0^2 c^2}{4\sqrt{2} \hbar^2 \pi^{(3/4)} \alpha^{(1/2)}} \\ &\quad + \frac{\hbar E}{2\pi^{(5/4)} \alpha^{(3/2)} \hbar^2 c^2} \left[ e^{-\frac{\alpha^2 r_0^2}{2}} - e^{-\frac{\alpha^2 r_h^2}{2}} \right] \end{aligned} \quad (4.6.17)$$

Thus according to equation (4.2.43) the scattering flux in this case:

$$S_{sc} = \frac{v}{r^2} \left| \left( \frac{-m_0^2 c^2}{4\sqrt{2} \hbar^2 \pi^{(3/4)} \alpha^{(1/2)}} + \frac{\hbar E}{2\pi^{(5/4)} \alpha^{(3/2)} \hbar^2 c^2} \left[ e^{-\frac{\alpha^2 r_0^2}{2}} - e^{-\frac{\alpha^2 r h^2}{2}} \right] \right)^2 \right| \quad (4.6.18)$$

Using equation (4.2.44) the scattering cross section in this case:

$$\sigma = \left| \left( \frac{-m_0^2 c^2}{4\sqrt{2} \hbar^2 \pi^{(3/4)} \alpha^{(1/2)}} + \frac{\hbar E}{2\pi^{(5/4)} \alpha^{(3/2)} \hbar^2 c^2} \left[ e^{-\frac{\alpha^2 r_0^2}{2}} - e^{-\frac{\alpha^2 r h^2}{2}} \right] \right)^2 \right| \quad (4.6.19)$$

#### 4.7 Scattering of Nearly Free Particle by Electric Dipole Molecules:

When the molecules of the bulk matter are in the form of electric dipole having charge ( $q$ ) such that the distance between the poles are  $d$ . in this case the potential is given by:

$$V = \frac{qd}{4\pi\epsilon_0 r^2} \quad (4.7.1)$$

For nearly free particle the wave function is

$$\psi(r) = e^{ikr \cos\alpha} \quad (4.7.2)$$

Thus according to equation (4.2.30) (4.2.31) and substituting (4.7.1) (4.7.2)

$$Q(\theta, \varphi) = \frac{-m_0^2 c^2}{4\pi \hbar^2} \int_d^{r_0} dr' \quad (4.7.3)$$

$$Q(\theta, \varphi) = \frac{m_0^2 c^2}{4\pi \hbar^2} [d - r_0] \quad (4.7.4)$$

$$f(\theta, \varphi) = \frac{E}{2\pi\hbar^2 c^2} \int_d^{r_0} \left( \frac{qd}{4\pi\epsilon_0 r'^2} \right) dr' \quad (4.7.5)$$

$$f(\theta, \varphi) = \frac{Eqd}{8\pi^2\hbar^2 c^2 \epsilon_0} \int_d^{r_0} \frac{dr'}{r'^2} \quad (4.7.6)$$

$$f(\theta, \varphi) = \frac{Eqd}{8\pi^2\hbar^2 c^2 \epsilon_0} \left[ \frac{-1}{r'} \right]_d^{r_0} \quad (4.7.7)$$

$$f(\theta, \varphi) = \frac{Eqd}{8\pi^2\hbar^2 c^2 \epsilon_0} \left[ \frac{1}{d} - \frac{1}{r_0} \right] \quad (4.7.8)$$

Hence from equation (4.2.35):

$$D(\theta, \varphi) = Q + f = \frac{m_0^2 c^2}{4\pi\hbar^2} [d - r_0] + \frac{Eqd}{8\pi^2\hbar^2 c^2 \epsilon_0} \left[ \frac{1}{d} - \frac{1}{r_0} \right] \quad (4.7.9)$$

Thus the scattering flux in this case is given according to equation (4.2.43) by:

$$S_{sc} = \frac{v}{r^2} |D^2| = S_{sc} = \frac{v}{r^2} \left| \left( \frac{m_0^2 c^2}{4\pi\hbar^2} [d - r_0] + \frac{Eqd}{8\pi^2\hbar^2 c^2 \epsilon_0} \left[ \frac{1}{d} - \frac{1}{r_0} \right] \right)^2 \right| \quad (4.7.10)$$

The scattering cross section is given according to equation (4.2.44):

$$\sigma = |D^2| = \left| \left( \frac{m_0^2 c^2}{4\pi\hbar^2} [d - r_0] + \frac{Eqd}{8\pi^2\hbar^2 c^2 \epsilon_0} \left[ \frac{1}{d} - \frac{1}{r_0} \right] \right)^2 \right| \quad (4.7.11)$$

## 4.8 Discussion:

Using the GSR and PDSR a useful expression relating energy, momentum and potential energy has been found in equation (4.2.7) with the aid of the wave equation (4.2.9) a new PDSR and GSR quantum was found in equation (4.2.11).

For time independent potential  $V(r)$  a time dependent solution was suggested in equation (4.2.12) the new quantum equation which depend on the potential  $V$ ,

energy  $E$  and the spatial variation of the wave function  $\psi$ , has been exhibited in equations (4.2.16) and (4.2.19).

Green's equation and function in equation (4.2.20)(4.2.26) and (4.2.27) was used to solve the quantum equation (4.2.19) as shown by equations (4.2.28) and (4.2.32). According to equations (4.2.30) (4.2.31) (4.2.32) (4.2.34) and (4.2.44) the scattering cross section  $\sigma$  consists of two terms  $f$  and  $Q$ . The term  $f$  is the ordinary well known term, while the new term  $Q$  consists of rest mass energy  $m_0c^2$  instead of the potential  $V$ . Using Maxwell's equation (4.2.45), beside Max Planck and De Broglie hypothesis a relativistic energy – momentum relation consisting of an imaginary term dependent on the conductivity  $\sigma$  was found as shown by equation (4.2.52). This term is related to the rest mass  $m_0$  according to equation (4.2.54), when comparing (4.2.52) with the ordinary SR energy – momentum relation (4.2.53). Considering  $\sigma$  in a complex form (see equation (4.2.55)) an additional imaginary term standing for friction as shown by equation (4.2.74). Using the equation (4.2.57), which describes the freely vibrating particle moving in a frictional medium under the action of a travelling electromagnetic field, a useful expression for conductivity was found in equations (4.2.69) and (4.2.70). This enables expressing the rest mass term in terms of electromagnetic wave frequency  $\omega$ . This enables describing the scattering processes of electromagnetic waves which propagate inside a medium in which particles vibrate with natural frequency  $\omega_0$ .

Restricting ourselves to high resistive medium as shown by equation (4.2.78) the scattering cross section  $\sigma = Q(\theta, \varphi)$  is frequency dependent as shown by equation (4.2.83). According to plank theory  $E = \hbar\omega$  the scattering cross section depends on particles energy which agrees with observations.

In section (4.3) the scattering by uniform potential indicates that the scattering cross section depends on the rest mass, thus depends on the frequency as shown by equations (4.3.14) and (4.2.79). The scattering by spherical nucleus by nearly free particle, also indicates frequency and rest mass dependence of the scattering cross section, with additional terms representing the nucleus radius and the particle size as shown by equation (4.4.12). The scattering by harmonic oscillator and electric dipoles indicate the same dependence of the scattering cross sections as shown by equations (4.5.10) (4.6.19) and (4.7.11).

#### **4.9 Conclusion:**

The new quantum PDSR (GSR) equation for scattering process shows some interesting results. It indicates that the scattering cross section and flux reduces to the ordinary one. It consists also of an additional term standing for rest mass energy and is frequency dependent.

#### **4.10 Future Work:**

This new equation need to be verified experimentally to see how the additional term can correct calculations for the scattering flux and cross section. The new model need to be examined for fast particles where SR is applicable.

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