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Scattering of Quantum Particles by Time-Independent Scalar Fields

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Abstract:

In the context of relativistic quantum mechanics, our work has been organized into two main parts.

In the first part, we first proposed the formalism of the spin-s ($s = 0,1/2$) relativistic wave equation. Then, based on the stationary scattering states of a relativistic particle governed by the spin-s relativistic wave equation in the presence of a localized electromagnetic field $A_{\mu}(x,t) = \left(A_0(x,t), \vec{A}(x,t)\right)$, we constructed the formalism of the one-dimensional scattering matrix $\hat{S}_{-s}$.

In the second part, as an application, we studied the scattering of relativistic spin-s particles interacting with certain scalar potentials with some symmetry and range properties (Woods-Saxon potential, barrier potential, and periodic potential). For these potentials, the spin-s relativistic wave equation was first solved analytically. From the asymptotic behavior, we derived the scattering matrix. Then, using the scattering matrix formalism, we calculated even and odd wave phase shifts, scattering amplitudes, transmission and reflection coefficients, and the total effective cross-section.

Keywords: Relativistic spin-s wave equation ($s = 0,1/2$), Scattering matrix formalism, Woods-Saxon potential, Periodic potential.

الملخص :

في سياق ميكانيكا الكم النسبية، ينقسم عملنا إلى جزأين رئيسيين .

في الجزء الأول، اقترحنا أولاً شكلية المعادلة الموجية النسبية المغزلية ($s = 0,1/2$)، ثم استنادًا إلى حالات التشتت الثابتة لجسيم نسبي تحكمه المعادلة الموجية النسبية المغزلية-s في وجود مجال كهرومغناطيسي موضعي $A_{\mu}(x,t) = \left(A_0(x,t), \vec{A}(x,t)\right)$ قمنا ببناء شكلية مصفوفة التشتت أحادية البعد $\hat{S}_{-s}$.

في الجزء الثاني، كتطبيق، درسنا تشتت الجسيمات النسبية المغزلية التي تتفاعل مع بعض الكمونات السلمية التي لها بعض خصائص التماثل والمدى (كمون وودز-ساكسون، كمون الحاجز والكمون الدوري) . بالنسبة لهذه الكمونات، تم أولاً حل المعادلة الموجية النسبية المغزلية تحليلياً. ومن السلوك التقاربي، استنتجنا مصفوفة التشتت، ثم باستخدام شكلية مصفوفة التشتت، قمنا بحساب الإزاحة الطورية للموجات الزوجية والفردية، وسعات التشتت، ومعاملات النفاذ والانعكاس، والمقطع العرضي الكلي.

الكلمات الرئيسية: المعادلة الموجية النسبية المغزلية ($s = 0,1/2$)، شكلية مصفوفة التشتت، كمون وودز-ساكسون، الكمون الدوري.

Résumé :

Dans le contexte de la mécanique quantique relativiste, notre travail s'est articulé autour de deux grandes parties.

Dans la première partie, nous avons tout abord proposé le formalisme de l'équation d'onde relativiste spin-s ($s = 0,1/2$). Ensuite, en se basant sur les états stationnaires de diffusion d'une particule relativiste gouvernée par l'équation d'onde relativiste de spin-s en présence d'un champ électromagnétique localisé $A_\mu(x,t) = \left(A_0(x,t), \vec{A}(x,t)\right)$, nous avons construit le formalisme de la matrice de diffusion $\hat{S}_{-s}$ à une dimension.

Dans la deuxième partie, comme application, nous avons étudier la diffusion des particules relativistes de spin-s en interaction avec certains potentiels scalaires ayant quelques propriétés de symétrie et de portée (potentiel de Woods-Saxon, potentiel barrière et potentiel périodique). Pour ces potentiels, l'équation d'onde relativiste de spin-s a été d'abord résolue analytiquement. Du Comportement asymptotique, nous avons tiré la matrice de diffusion. Par la suite, en utilisons le formalisme de la matrice de diffusion, nous avons calculer les déphasages des ondes paires et impaires, les amplitudes de diffusion, les coefficients de transmission et de réflexion, ainsi que la section efficace totale.

Mots clés : Équation d'onde relativiste de spin-s ($s = 0,1/2$), Formalisme de la matrice de diffusion, Potentiel de Woods-Saxon, Potentiel périodique

Contents

Introduction

Classical mechanics gives a good account of reality as we observe it on a daily basis. It distinguishes two types of objects: matter and radiation. Matter follows Newton's laws of rational mechanics and radiation follows Maxwell's laws of electromagnetism. After the emergence of theories such as Newton's classical mechanics, thermodynamics, electromagnetism and statistical mechanics, it is believed that all the laws of physics have been found and all that remains is to refine the precision of measurements. However, there are still many unanswered questions. Towards the end of the 19th century, certain new phenomena (black body radiation, the photoelectric effect, the Compton effect, wave-particle duality, the atomic spectrum, invariance of the speed of light, etc) were unable to be explained by classical physics. This led to the appearance of new concepts radically different from those of classical physics. For example, we had to abandon the notion of trajectory and consider that microscopic particles sometimes behave similary to a wave. All of these new concepts gave birth to a new physics, "quantum physics." In this physics, the trajectory no longer has any meaning and we speak of the probability of presence. In fact, an elementary particle manifests itself in space as a wave represented by a wave function $\Psi\left(\overrightarrow{r},t\right)$, where $\overrightarrow{r}$ is the position of the particle in space and t is time. As with any wave, $\Psi\left(\overrightarrow{r},t\right)$ must satisfy a wave equation. This is the Schrödinger equation [1, 2, 3], designed by the Austrian physicist Erwin Schrödinger in 1926, which is a fundamental equation in nonrelativistic quantum physics. It describes the evolution over time of a massive non-relativistic particle, and thus fulfills the same role as the fundamental relation of dynamics in classical mechanics.

However, quantum mechanics did not satisfy the principles of Einstein's special relativity [4, 5], a principle stated at the beginning of the century. It was therefore necessary to take another step towards a more general and more complete physics that would obey all experimental evidence. Therefore, to satisfy covariance, a principle arising from Einstein's special relativity, physicists have developed new theories. Relativistic quantum mechanics thus began with the arrival of the Klein-Gordon equation (1926), which allows us to describe the dynamics of relativistic particles of mass m having a spin-0, with or without charge [6, 7, 8]. Unfortunately, this equation presents serious difficulties of interpretation within the framework of original quantum mechanics, a theory supposed to describe a single particle. The relay taken by the Dirac equation has succeeded in re-establishing this defect. However, it does so at the cost of adding a sea of particles which gives rise to the antiparticle (particle having a mass, a spin, and an average life identical to that of the particle, located in the same state of momentum, position, but opposite charges: electric charge, weak, and other quantum numbers), but it can only describe phenomena where the number of particles does not vary. It cannot describe processes in which particles appear or disappear, for example, matter-antimatter annihilation [6, 8, 9].

In 1948, research continued through important work performed by Julian Schwinger and Tomonaga, as well as Richard P. Feynman who established a formalism where relativistic covariance was highlighted, which made it possible to separate the contributions of vacuum fluctuations into divergent parts and finite terms. The divergent terms were incorporated into the mass and initial charge of the electron, to give what we take as experimental values. Consequently, a gigantic but also formidable mathematical arsenal has been developed to deal with the "infinite" phantom heir to these ambiguities. Sophisticated techniques of renormalization, non-commutative geometry, Hopf algebras, etc. have not been able to provide a definitive solution to this problem.

Although we have advanced enormously on the technical level, physics has remained in an embryonic state on the fundamental level.

A return to wave equations is then justifiable. Firstly, these wave equations are much closer to the inevitable formal structure of quantum mechanics and secondly, the corrections made by field theory are only detectable in the presence of strong fields. In the case of these wave equations, the physical results then only represent the first approximation where the creation and annihilation of particle-antiparticle pairs are neglected but allow their effect to be glimpsed via the tunnel effect.

This thesis is structured as follows: the first chapter is devoted to the basic elements used in this study, such as the Schrödinger equation for non-relativistic particles, the Klein-Gordon equation for relativistic particles of spin-0 (bosons), and the Dirac equation for relativistic particles of spin-1/2 (fermions). The second chapter is dedicated to the theoretical study of scattering theory in classical and quantum mechanics.

The third chapter of this thesis has two parts. The first part will be devoted to unifying the two equations of relativistic quantum mechanics, (Klein-Gordon equation and the second-order Dirac equation or quadratic Dirac equation), into a single equation called the relativistic wave equation of spin-s ($s = 0, 1/2$). In the second part of this chapter, we will construct the scattering matrix formalism for relativistic particles of spin-s in the presence of a localized electromagnetic field.

The last chapter of this thesis is devoted to the application of the $\hat{\mathrm{S}}$-matrix formalism to treat some problems of relativistic quantum mechanics for particles of spin-s, in interaction with certain scalar potentials having some properties of symmetry and range.

Finally, we conclude with a summary of the main results, then, we present a complete bibliography mainly on the subjects covered and those related.

Chapter 1

Klein-Gordon and Dirac equations

1.1 Introduction

Until the end of the 19th century, the physical world was explained by Newtonian mechanics and Maxwell's electromagnetism. However, at the beginning of the 20th century, physicists suddenly found themselves confronted with new phenomena for which the predictions of classical theory are in flagrant disagreement with experience. In order to achieve a coherent interpretation of these experiments, the old quantum physics was abandoned in favor of Schrödinger's wave mechanics (1926) and Heisenberg's matrix mechanics (1927), two formulations of one and the same physics, quantum mechanics [10]. However, quantum mechanics does not satisfy Einstein's principles of special relativity, stated at the beginning of the century. To satisfy covariance, a principle from Einstein's special relativity, physicists developed new theories. Relativistic quantum mechanics thus began with the arrival of the Klein-Gordon equation for relativistic particles of spin-0. Unfortunately, there were still some problems related to it. Dirac, in 1928, introduced the equation that bears his name, which describes in a covariant way the dynamics of a single particle of spin-1/2. It was very successful in explaining the spin of particles and the existence of antiparticles, but it can only describe phenomena where the number of particles does not vary.

Before proceeding to the development of the Klein-Gordon and Dirac equations, it is necessary to first return to the theory of non-relativistic quantum mechanics through the Schrödinger equation.

1.2 Schrödinger equation

The Schrödinger equation is one of the cornerstones of quantum mechanics, revolutionizing our understanding of the microscopic world. Its history and origins are closely linked to the evolution of physics in the early 20th century, marked by surprising discoveries and paradigm shifts.

Thus, by the beginning of the 20th century, it had become clear that light exhibited a wave-particle duality. Louis de Broglie proposed generalizing this duality to all material particles. He also associated each energy-momentum pair $(E, \overrightarrow{p})$ with a vibration characterized by the angular frequency-wavelength pair $\left(\omega, \overrightarrow{k}\right)$ [2, 3, 11], namely:

$$(E, \overrightarrow{p}) = \hbar \left(\omega, \overrightarrow{k}\right), \tag{1.1}$$

where $\hbar = h/2\pi$, and h is Planck's constant.

Inspired by the work of de Broglie, Schrödinger sought to develop a wave theory of matter. His goal was to find an equation that would describe the behavior of the matter waves proposed by de Broglie.

The conceptual scheme used by Schrödinger to derive his equation is based on a formal analogy between optics and mechanics:

Indeed, in physical optics, the propagation equation in a transparent medium of real index n is characterized by an electric field $\overrightarrow{E}(\overrightarrow{r}, t)$ and a magnetic field $\overrightarrow{B}(\overrightarrow{r}, t)$. These fields are deduced from Maxwell's differential equations, which are written in the absence of charges and current [2, 11, 12]:

$$\overrightarrow{\nabla} \wedge \overrightarrow{E} = -\frac{\partial \overrightarrow{B}}{\partial t}, \quad \overrightarrow{\nabla} \wedge \overrightarrow{B} = \varepsilon\mu \frac{\partial \overrightarrow{E}}{\partial t}, \quad \overrightarrow{\nabla}.\overrightarrow{E} = 0, \quad \overrightarrow{\nabla}.\overrightarrow{B} = 0, \tag{1.2}$$

ε and μ being the permittivity and permeability. Using the rotational double formula $\overrightarrow{\nabla} \wedge \left(\overrightarrow{\nabla} \wedge \overrightarrow{a}\right) = \overrightarrow{\nabla}\left(\overrightarrow{\nabla}.\overrightarrow{a}\right) - \Delta \overrightarrow{a}$, we can deduce from (1.2), the general equation that describes the propagation of the wave in free space, in a homogeneous, linear, and isotropic medium [2, 11, 12]:

$$\left\{\Delta - \frac{1}{v_\Phi^2}\frac{\partial^2}{\partial t^2}\right\} \Psi(\overrightarrow{r}, t) = 0 \quad \text{with } \Psi = \overrightarrow{E} \text{ or } \overrightarrow{B}, \tag{1.3}$$

where the operator $\Delta = \overrightarrow{\nabla}^2$ is the Laplacian operator. $v_\Phi = c/n$ designates the phase speed in the medium with optical index $n = \sqrt{\varepsilon\mu}$ and c the speed of light.

If the index n is constant, equation (1.3) admits in particular as a solution $\Psi(\overrightarrow{r}, t) = \Psi(\overrightarrow{r})\, e^{-i\omega t}$. By injecting this solution into equation (1.3), we find that $\Psi(\overrightarrow{r})$ must satisfy the equation

$$\left\{\Delta + k^2\right\} \Psi(\overrightarrow{r}) = 0 \quad \text{with} \quad k^2 = \frac{\omega^2}{v_\Phi^2}. \tag{1.4}$$

An elementary solution of (1.4) is $\Psi(\overrightarrow{r}) = \Psi_0 e^{i\overrightarrow{k}\overrightarrow{r}}$. With this result, the solution to (1.3) takes the form:

$$\Psi(\overrightarrow{r}, t) = \Psi_0 e^{i\left(\overrightarrow{k}.\overrightarrow{r} - \omega t\right)}, \tag{1.5}$$

which represents a vibration of wavelength $\lambda = 2\pi/k$ propagating in the direction of its wave vector $\overrightarrow{k}$ at constant speed. Ψ_0, and k are the amplitude and the wave number in the medium of index n respectively.

On the other hand, for any natural mode of the electromagnetic field in vacuum, the wave vector $\overrightarrow{k}$ and the angular frequency ω define the phase Φ by [2, 11, 12]:

$$\Phi(\overrightarrow{r}, t) = \overrightarrow{k}.\overrightarrow{r} - \omega t, \tag{1.6}$$

where

$$\overrightarrow{k} = \overrightarrow{\nabla}\Phi, \qquad \omega = -\frac{\partial \Phi}{\partial t}. \tag{1.7}$$

As for the Maupertuis Principle, it can be found from the modern form of the action principle, a hypothesis according to which the dynamics of a quantity (position, speed, acceleration, etc.) between two instants can be deduced from a single quantity, noted S, and called action (For convenience, we will consider a system formed by a single particle of mass m, identified by the radius vector $\overrightarrow{r}$ and immersed in a potential $U(\overrightarrow{r})$), defined by the following equality [13, 14]:

$$S(\overrightarrow{r}, t) = \int_0^t L\left(\overrightarrow{r}, \dot{\overrightarrow{r}}, t'\right) dt' = \int_0^t \left(\overrightarrow{p}\dot{\overrightarrow{r}} - H\left(\overrightarrow{p}, \overrightarrow{r}, t'\right)\right) dt', \tag{1.8}$$

where $L\left(\overrightarrow{r},\dot{\overrightarrow{r}},t^{'}\right) = T - U\left(\overrightarrow{r}\right)$ (T is the kinetic energy) is called the Lagrange function, and $H\left(\overrightarrow{p},\overrightarrow{r},t^{'}\right)$ is the hamiltonian, given by:

$$H\left(\overrightarrow{p},\overrightarrow{r},t^{'}\right) = \overrightarrow{p}\dot{\overrightarrow{r}} - L\left(\overrightarrow{r},\dot{\overrightarrow{r}},t^{'}\right), \tag{1.9}$$

and $\overrightarrow{p} = \partial L/\partial\dot{\overrightarrow{r}}$ is the conjugate moment.

In the absence of time-dependent forces, the Hamiltonian H is a constant of motion, we can replace it by the energy E of the system, and directly integrate the equation (1.8) to obtain:

$$S\left(\overrightarrow{r},t\right) = \int_0^t \left(\overrightarrow{p}\dot{\overrightarrow{r}} - E\right) dt^{'} = \int_{M_0}^{M_t} \overrightarrow{p}.d\overrightarrow{r} - Et = S_0 - Et, \tag{1.10}$$

where S_0 is the Maupertuis action, determined by the equation:

$$S_0\left(\overrightarrow{r}\right) = \int_{M_0}^{M_t} \overrightarrow{p}.d\overrightarrow{r} = \int_{M_0}^{M_t} \sqrt{2m\left(E - U\left(\overrightarrow{r}\right)\right)}\overrightarrow{u}_p.d\overrightarrow{r}, \tag{1.11}$$

where $\overrightarrow{u}_p = \overrightarrow{p}/\left|\overrightarrow{p}\right|$. Comparing equation (1.11) with Fermat's least duration equation led Hamilton to assert that the quantity $p = \sqrt{2m(E - U\left(\overrightarrow{r}\right))}$ plays the same role in mechanics as the index n in optics [13, 14, 15]; but Hamilton's optical-mechanical analogy goes even further.

Indeed, if we return to equation (1.10), the total derivative with respect to time of action $S\left(\overrightarrow{r},t\right)$ gives,

$$\frac{dS}{dt} = \frac{\partial S}{\partial r}\frac{d\overrightarrow{r}}{dt} + \frac{\partial S}{\partial t}. \tag{1.12}$$

By the very definition of the action Eq. (1.8), we have:

$$\frac{dS}{dt} = L = \overrightarrow{p}\dot{\overrightarrow{r}} - E \tag{1.13}$$

where it was assumed that L does not explicitly depend on time (conservative system $\partial L/\partial t = 0$).

Comparing (1.12) with (1.13), we find, on the one hand, that the energy E is equal to the opposite of the derivative of S with respect to time; on the other hand, the relations $\overrightarrow{p} = \partial S/\partial \overrightarrow{r}$ can be written with $\overrightarrow{\nabla}$. In total:

$$\overrightarrow{p} = \overrightarrow{\nabla} S = \overrightarrow{\nabla} S_0, \quad \frac{\partial S}{\partial t} = -E. \tag{1.14}$$

The first equation shows that the impulse vector $\overrightarrow{p}$, which defines the tangent to the trajectory at every point, is normal to the surfaces of constant action.

Now, replacing in (1.10) E and $\overrightarrow{p}$ by these expressions (1.1), and taking into account (1.6), we get:

$$S\left(\overrightarrow{r}, t\right) = \hbar \Phi\left(\overrightarrow{r}, t\right). \tag{1.15}$$

Thus, the parallel we have just established shows that the action $S\left(\overrightarrow{r}, t\right)$ plays exactly the same role in analytical mechanics as the phase $\Phi\left(\overrightarrow{r}, t\right)$ in optics.

The condition $S = \left(\overrightarrow{r}, t\right) = Cte$; this clearly defines a surface $\sum$ in $\mathbb{R}^3$ that is parameterized by time, i.e., one that moves (and deforms) as time passes. A given point M on this surface describes a normal line to the surface and moves from M_t to M_{t+dt} between t and $t + dt$; for these two points separated by dl along the normal to $\sum$, the variation of S is formally:

$$dS = \overrightarrow{\nabla} S . d\overrightarrow{r} + \frac{\partial S}{\partial t} dt \quad \Leftrightarrow \quad \frac{dS}{dt} = \mid \overrightarrow{\nabla} S \mid \frac{dl}{dt} + \frac{\partial S}{\partial t}, \tag{1.16}$$

here $dl = \overrightarrow{n} . d\overrightarrow{r}$, and $\overrightarrow{n} = \overrightarrow{\nabla} S / \mid \overrightarrow{\nabla} S \mid$.

By construction, dS is zero (we follow the movement of a surface of constant action), which gives the speed of movement v_Φ of a point marked on such a surface:

$$v_\Phi = \frac{dl}{dt} = -\frac{\partial S/\partial t}{\mid \overrightarrow{\nabla} S \mid} = \frac{E}{\mid \overrightarrow{\nabla} S_0 \mid} = \frac{E}{\sqrt{2m\left(E - U\left(\overrightarrow{r}\right)\right)}}. \tag{1.17}$$

having made this speed appear, Schrödinger makes it play the role of a phase velocity in a certain wave equation for a certain function, noted $\Psi\left(\overrightarrow{r}\right)$, an equation copied from the wave equation of electromagnetism, in which ω must be replaced by $E/\hbar$. By including in equation (1.4) the phase velocity given by relation (1.17), Schrödinger arrives at the time-independent form of his matter wave equation,

$$\left(\Delta + \frac{2m\left(E - U\left(\overrightarrow{r}\right)\right)}{\hbar^2}\right)\Psi\left(\overrightarrow{r}\right) = 0. \tag{1.18}$$

To obtain the equation that governs the evolution over time, the correspondence principle of the Hamiltonian formalism of non-relativistic classical mechanics is used, by replacing the dynamic variables of the system by operators (using the natural units $\hbar = c = 1$) [1]

$$E \leftrightarrow i\frac{\partial}{\partial t}, \qquad \overrightarrow{p} \leftrightarrow -i\overrightarrow{\nabla}, \tag{1.19}$$

we obtain an equation which satisfies these requirements:

$$i\frac{\partial\Psi\left(\overrightarrow{r},t\right)}{\partial t} = H\left(\overrightarrow{r},t\right)\Psi\left(\overrightarrow{r},t\right) = \left(-\frac{\Delta}{2m} + U\left(\overrightarrow{r}\right)\right)\Psi\left(\overrightarrow{r},t\right). \tag{1.20}$$

The Schrödinger equation which describes the evolution over time of a particle of mass m and charge e subjected to an electromagnetic field $A_\mu\left(\overrightarrow{r},t\right) = \left(A_0\left(\overrightarrow{r},t\right), \overrightarrow{A}\left(\overrightarrow{r},t\right)\right)$, is obtained from the Schrödinger equation (1.20) , using the Fock minimal coupling prescription [16, 17], which consists of replacing in the fieldless Hamiltonian $H\left(\overrightarrow{r},t\right)$ (with $U\left(\overrightarrow{r}\right) = 0$),

$$i\frac{\partial}{\partial t} \leftrightarrow i\frac{\partial}{\partial t} - eA_0\left(\overrightarrow{r},t\right), \quad -i\overrightarrow{\nabla} \leftrightarrow -i\overrightarrow{\nabla} - e\overrightarrow{A}\left(\overrightarrow{r},t\right), \tag{1.21}$$

we recover the familiar expression for the Schröedinger equation of a particle in an electromagnetic field.

$$\left\{i\frac{\partial}{\partial t} - eA_0\left(\overrightarrow{r},t\right) + \frac{1}{2m}\left(i\overrightarrow{\nabla} + e\overrightarrow{A}\left(\overrightarrow{r},t\right)\right)^2\right\}\Psi\left(\overrightarrow{r},t\right) = 0. \tag{1.22}$$

It describes the evolution over time of a non-relativistic particle of mass m and charge e subjected to an electromagnetic field $A_\mu\left(\overrightarrow{r},t\right)$, and thus fulfills the same role as the fundamental relation of dynamics in classical mechanics or the equations of Maxwell in electromagnetism.

One way of getting the continuity equation is to take the Schröedinger equation (1.22) multiplied by the complex conjugate $\Psi^\star$ and subtract the complex conjugate equation multiplied by Ψ. One finds

$$\frac{\partial J^0}{\partial t} + \overrightarrow{\nabla} \overrightarrow{J} = 0, \tag{1.23}$$

where

$$J^0 = \Psi\Psi^\star, \quad \overrightarrow{J} = \frac{1}{2im}\left[\left(\Psi^\star \overrightarrow{\nabla}\Psi - \Psi\overrightarrow{\nabla}\Psi^\star\right) - 2ie\overrightarrow{A}\Psi\Psi^\star\right]. \tag{1.24}$$

This equation has all the invariance properties of the Hamiltonian from which it comes. It is also invariant with respect to Galileo's transformations, but it does not have the property of invariance concerning changes in the Lorentz frame of reference required by the principle of relativity (dissymmetry between space and temporal coordinates) and ignores the spins of particles.

To satisfy covariance, a principle arising from Einstein's special relativity, physicists have developed new theories. Relativistic quantum mechanics thus began with the arrival of the Klein-Gordon equation (1926), which describes the dynamics of relativistic particles having a spin-0.

1.3 Klein-Gordon equation

To find the wave equation for relativistic spin-0 particles, we proceed empirically, using the correspondence principle, which consists of replacing classical observables with operators acting on the wave functions. Indeed, according to special relativity, if we take the case without interaction as a starting point, the relativistic equation giving the energy E of a particle of mass m with momentum $\overrightarrow{p}$ is written [6, 7, 8]:

$$E = \sqrt{p^2 + m^2}. \tag{1.25}$$

Afterwards, the same postulates of correspondence as in non-relativistic quantum mechanics are adopted. By replacing the relation (1.19) with a relation between energy and momentum conforming to the theory of relativity, we obtain:

$$i\frac{\partial}{\partial t} = \sqrt{-\overrightarrow{\nabla}^2 + m^2}. \tag{1.26}$$

Taking into account (1.26), the relativistic Schrödinger equation which describes the evolution over time of the wave function $\Psi(\overrightarrow{r},t)$ of a free particle, eigenfunctions of the operator H associated with the total energy E, is written:

$$i\frac{\partial\Psi(\overrightarrow{r},t)}{\partial t}=\left(\sqrt{-\Delta+m^2}\right)\Psi(\overrightarrow{r},t). \tag{1.27}$$

This approach leads to an equation that is not local since it involves arbitrary powers of the Laplacian Δ. Furthermore, space-time symmetry $(\overrightarrow{r},t)$ is not manifest. To circumvent this difficulty, let's start from the relativistic invariant giving the energy of an isolated particle such that:

$$E^2=\overrightarrow{p}^2+m^2. \tag{1.28}$$

If we accept the correspondence principle of quantum mechanics (1.19), which consists of replacing the previous expression with:

$$-\frac{\partial^2}{\partial t^2}=\left(-\Delta+m^2\right), \tag{1.29}$$

and applying this relation to a wave function $\Psi(\overrightarrow{r},t)$, which leads to the Klein-Gordon equation,

$$\left\{\frac{\partial^2}{\partial t^2}-\overrightarrow{\nabla}^2+m^2\right\}\Psi(\overrightarrow{r},t)=0. \tag{1.30}$$

We write equation (1.30) again in a simpler form. For this purpose, we will introduce the four-vector energy impulse p^μ, defined by [6, 7, 8]:

$$p^\mu=i\partial^\mu=(E,\overrightarrow{p})=i\left(\frac{\partial}{\partial t},-\overrightarrow{\nabla}\right), \tag{1.31}$$

next, consider the relativistic invariant (1.28), which is written in the form:

$$p^\mu p_\mu=E^2-\overrightarrow{p}^2=m^2. \tag{1.32}$$

By a direct calculation, and using the definition of the scalar product of two quadrivectors $a^\mu=(a^0,\overrightarrow{a})$ and $b^\mu=\left(b^0,\overrightarrow{b}\right)$, represented by:

$$a^{\mu}b_{\mu} = a^{0}b_{0} - \overrightarrow{a}.\overrightarrow{b}, \tag{1.33}$$

we can write equation (1.30) in the form:

$$\left\{\partial^{\mu}\partial_{\mu} + m^{2}\right\}\Psi\left(\overrightarrow{r}, t\right) = 0, \tag{1.34}$$

usually called the covariant Klein-Gordon equation, since the operator $\partial^{\mu}\partial_{\mu}$ is an invariant and the field $\Psi\left(\overrightarrow{r}, t\right)$ is a scalar.

1.3.1 Klein-Gordon particle in an electromagnetic field

The wave equations of free particles only express those properties that are related to the general requirements of space-time symmetry. However, the physical processes in which particles participate depend on the properties of their interactions.

We would now like to be able to generalize the free Klein-Gordon equation (1.34) that we initially presented above, by introducing the interaction of the Klein-Gordon field with a given external electromagnetic field, composed of a scalar potential $A_{0}\left(\overrightarrow{r}, t\right)$ and a vector potential $\overrightarrow{A}\left(\overrightarrow{r}, t\right)$, which forms a quadrivector that we will designate by $A_{\mu}\left(\overrightarrow{r}, t\right) = \left(A_{0}\left(\overrightarrow{r}, t\right), \overrightarrow{A}\left(\overrightarrow{r}, t\right)\right)$.

To advance in this approach, we first analyze the structure of the Hamiltonian interaction between a classical particle of charge e and the electromagnetic field. Then, we will adopt the same postulates (1.31) and (1.32), as in relativistic quantum mechanics of a free particle to calculate the Hamiltonian of the Klein-Gordon spin-0 particle in an electromagnetic field A_{μ}. The only difference is that we instead use the classical relativistic energy equation for a particle in the presence of an electromagnetic field as a starting point.

As we know from classical electrodynamics, in the presence of electric fields $\overrightarrow{E}\left(\overrightarrow{r}, t\right)$ and magnetic fields $\overrightarrow{B}\left(\overrightarrow{r}, t\right)$, a particle of electric charge e which moves with a speed $\dot{\overrightarrow{r}}$ experiences a force given by the Lorentz formula [12],

$$m\ddot{\overrightarrow{r}} = e\left[\overrightarrow{E}\left(\overrightarrow{r}, t\right) + \dot{\overrightarrow{r}}\left(t\right) \wedge \overrightarrow{B}\left(\overrightarrow{r}, t\right)\right]. \tag{1.35}$$

The potentials $A_0(\overrightarrow{r},t)$ and $\overrightarrow{A}(\overrightarrow{r},t)$ are linked to the electric fields $\overrightarrow{E}$ and magnetic fields $\overrightarrow{B}$ by:

$$\overrightarrow{E} = -\overrightarrow{\nabla}_{\overrightarrow{r}} A_0 - \frac{\partial \overrightarrow{A}}{\partial t}, \quad \overrightarrow{B} = \overrightarrow{\nabla}_{\overrightarrow{r}} \wedge \overrightarrow{A}, \tag{1.36}$$

where $\overrightarrow{\nabla}_{\overrightarrow{r}} = \partial/\partial\overrightarrow{r}$. Substituting the previous expression into equation (1.35), we obtain the following equation

$$m\ddot{\overrightarrow{r}} = e\left[-\overrightarrow{\nabla}_{\overrightarrow{r}} A_0 - \frac{\partial \overrightarrow{A}}{\partial t} + \dot{\overrightarrow{r}} \wedge \left(\overrightarrow{\nabla}_{\overrightarrow{r}} \wedge \overrightarrow{A}\right)\right]. \tag{1.37}$$

To aim for a Lagrangian formulation, we introduce the derivative of the vector potential $\overrightarrow{A}$ with respect to t, we have:

$$\frac{d\overrightarrow{A}}{dt} = \dot{\overrightarrow{r}}.\overrightarrow{\nabla}_{\overrightarrow{r}}\overrightarrow{A} + \frac{\partial \overrightarrow{A}}{\partial t}, \tag{1.38}$$

therefore, we can rewrite (1.37), in the form:

$$\frac{d}{dt}\left(m\dot{\overrightarrow{r}} + e\overrightarrow{A}\right) = e\left[-\overrightarrow{\nabla}_{\overrightarrow{r}} A_0 + \dot{\overrightarrow{r}}.\overrightarrow{\nabla}_{\overrightarrow{r}}\overrightarrow{A} + \dot{\overrightarrow{r}} \wedge \left(\overrightarrow{\nabla}_{\overrightarrow{r}} \wedge \overrightarrow{A}\right)\right]. \tag{1.39}$$

Afterwards, we develop the double vector product,

$$\dot{\overrightarrow{r}} \wedge \left(\overrightarrow{\nabla} \wedge \overrightarrow{A}\right) = \overrightarrow{\nabla}\left(\dot{\overrightarrow{r}}.\overrightarrow{A}\right) - \left(\dot{\overrightarrow{r}}.\overrightarrow{\nabla}\right)\overrightarrow{A}, \tag{1.40}$$

and insert (1.40) into (1.39), we find the following equation

$$\frac{d}{dt}\left(m\dot{\overrightarrow{r}} + e\overrightarrow{A}\right) = \overrightarrow{\nabla}_{\overrightarrow{r}}\left(-eA_0 + e\dot{\overrightarrow{r}}.\overrightarrow{A}\right). \tag{1.41}$$

The potentials A_0 and $\overrightarrow{A}$ are only functions of $\overrightarrow{r}$ and t, and therefore must be independent of $\dot{\overrightarrow{r}}$. Therefore, we can rewrite:

$$\overrightarrow{A} = \overrightarrow{\nabla}_{\dot{\overrightarrow{r}}}\left(\dot{\overrightarrow{r}}.\overrightarrow{A}\right), \quad \dot{\overrightarrow{r}} = \overrightarrow{\nabla}_{\dot{\overrightarrow{r}}}\left(\frac{\dot{\overrightarrow{r}}^2}{2}\right), \tag{1.42}$$

where $\overrightarrow{\nabla}_{\dot{\overrightarrow{r}}} = \partial/\partial\dot{\overrightarrow{r}}$. Then, by inserting this last expression into (1.41), we can write

$$\frac{d}{dt}\left(\vec{\nabla}_{\dot{\vec{r}}}\left(\frac{m\dot{\vec{r}}^{\,2}}{2}+e\,\dot{\vec{r}}.\vec{A}\right)\right)=\vec{\nabla}_{\vec{r}}\left(-eA_0+e\,\dot{\vec{r}}.\vec{A}\right). \qquad (1.43)$$

By adding to the first member of the equation (1.43) a constant with respect to $\dot{\vec{r}}$ therefore arbitrary function $g\left(\vec{r}\right)$, and to the second member by adding a constant relating to $\vec{r}$ therefore arbitrary function $f\left(\dot{\vec{r}}\right)$, we can write

$$\frac{d}{dt}\left(\vec{\nabla}_{\dot{\vec{r}}}\left(\frac{m\dot{\vec{r}}^{\,2}}{2}+e\,\dot{\vec{r}}.\vec{A}+g\left(\vec{r}\right)\right)\right)=\vec{\nabla}_{\vec{r}}\left(-eA_0+e\,\dot{\vec{r}}.\vec{A}+f\left(\dot{\vec{r}}\right)\right). \qquad (1.44)$$

If we take

$$g\left(\vec{r}\right)=-eA_0\left(\vec{r},t\right),\qquad f\left(\dot{\vec{r}}\right)=\frac{m\dot{\vec{r}}^{\,2}}{2}, \qquad (1.45)$$

the two expressions in parentheses of equation (1.44) are identical. With this choice, we can directly verify that the equation (1.44) is written

$$\frac{d}{dt}\left(\vec{\nabla}_{\dot{\vec{r}}}L\left(\vec{r},\dot{\vec{r}},t\right)\right)=\vec{\nabla}_{\vec{r}}L\left(\vec{r},\dot{\vec{r}},t\right), \qquad (1.46)$$

where $L\left(\vec{r},\dot{\vec{r}},t\right)$ is the Lagrangian of a classical particle of mass m and charge e evolving in an electromagnetic field, given by:

$$L\left(\vec{r},\dot{\vec{r}},t\right)=\frac{m\dot{\vec{r}}^{\,2}}{2}-e\left[A_0\left(\vec{r},t\right)-\dot{\vec{r}}.\vec{A}\left(\vec{r},t\right)\right]. \qquad (1.47)$$

The transition between the Lagrangian formulation and the Hamiltonian formulation is executed by a change of variable of the form $\left(\vec{r},\dot{\vec{r}},t\right)\rightarrow\left(\vec{r},\vec{p},t\right)$, where $\vec{p}$ is a new independent variable called conjugate moment of $\vec{r}$, defined by the relation:

$$\vec{p}=\frac{\partial L}{\partial\dot{\vec{r}}}=m\dot{\vec{r}}+e\vec{A}. \qquad (1.48)$$

The passage to these new variables introduces the Hamiltonian $H(\overrightarrow{p}, \overrightarrow{r}, t)$ of the system by Legendre transform with respect to the generalized speed $\dot{\overrightarrow{r}}$ [13],

$$H(\overrightarrow{p}, \overrightarrow{r}, t) = \overrightarrow{p}.\dot{\overrightarrow{r}} - L\left(\overrightarrow{r}, \dot{\overrightarrow{r}}, t\right). \tag{1.49}$$

According to the definition (1.48) of $\overrightarrow{p}$ and equation (1.47), we will express $\dot{\overrightarrow{r}}$ as a function of $\overrightarrow{p}$, and transfer the result to (1.49), we obtain

$$H = \frac{1}{2m}\left(\overrightarrow{p} - e\overrightarrow{A}\right)^2 + eA_0. \tag{1.50}$$

Note that the classical Hamiltonian of a relativistic particle of mass m and charge e, in the presence of an external electromagnetic field $A_\mu = \left(A_0, \overrightarrow{A}\right)$, is obtained by the standard minimal coupling prescription in the same way as that used in non-relativistic quantum mechanics. This requires

$$H \rightarrow (H - eA_0), \qquad \overrightarrow{p} \rightarrow \left(\overrightarrow{p} - e\overrightarrow{A}\right). \tag{1.51}$$

In such a case, the relativistic relation (Einstein's dispersion relation) between energy and momentum (1.28), in the presence of an electromagnetic field is written [6, 7, 8, 9, 10]

$$(E - eA_0)^2 = \left(\overrightarrow{p} - e\overrightarrow{A}\right)^2 + m^2. \tag{1.52}$$

Analogously, the description of electromagnetic interactions of particles in relativistic quantum theory is made possible by the generalization of the correspondence principle used in classical theory and non-relativistic quantum theory. Thus, we start from the classical Hamiltonian (1.52), and admit the minimal coupling principle of Fock [6, 18], which consists of replacing the derivatives ∂_μ by a covariant derivative (covariant with respect to the transformations gauge)

$$\partial_\mu \rightarrow D_\mu = \partial_\mu + ieA_\mu = \left(\frac{\partial}{\partial t} + ieA_0, \overrightarrow{\nabla} - ie\overrightarrow{A}\right), \tag{1.53}$$

and we replace (1.53) in (1.34), we obtain the Klein-Gordon equation which applies to a spinless particle of mass m and charge e moving in an external electromagnetic field $A_\mu(\overrightarrow{r}, t)$,

$$\left(D^\mu D_\mu + m^2\right) \Psi\left(\overrightarrow{r}, t\right) = 0. \tag{1.54}$$

This equation is very similar to the ordinary wave equation, except for an additional term involving mass. It applies to a scalar wave function $\Psi\left(\overrightarrow{r}, t\right)$ describing all particles of integer spin, the bosons. However, it does not apply with particles with half-integer spin (fermions). This relativistic wave equation must converge to the Schrödinger equation in the non-relativistic limit.

Now, it remains to be seen whether this equation has a physical meaning. We know that quantum mechanics interprets the results of a measurement of a state as a probability. Using the same method as used in non-relativistic quantum mechanics (Schrödinger equation), i.e. multiplying Ψ^* by the wave equation and subtracting Ψ multiplied by the conjugate wave equation, we obtain:

$$\partial_\mu \left[\Psi^* \left(\partial^\mu \Psi\right) - \Psi \left(\partial^\mu \Psi^*\right) + 2ieA^\mu \Psi^* \Psi\right] = 0 \tag{1.55}$$

The continuity equation is satisfied by taking J^μ proportional to the bracket of equation (1.55). We fix the constant of proportionality to find the usual definition in the non-relativistic limit:

$$J^\mu = \frac{1}{2im} \left[\Psi^* \partial^\mu \Psi - \Psi \partial^\mu \Psi^* + 2ieA^\mu \Psi^* \Psi\right] = \left(\rho, \overrightarrow{J}\right). \tag{1.56}$$

We introduced the factor $1/2im$ in these definitions to compensate for the additional dimensions introduced by the derivatives of t and $\overrightarrow{\nabla}$.

The Lorentz-invariant scalar product of two scalar wave functions Ψ_1 and Ψ_2 of Klein-Gordon, is defined on the hyperplane $x^0 = const$ as follows [19, 20]

$$(\Psi_1, \Psi_2) = \int \left[\Psi_1^\star \left(i \overleftrightarrow{\partial}_0 - 2eA_0\right) \Psi_2\right] d^3r, \tag{1.57}$$

where $\overleftrightarrow{\partial}_0 = \overrightarrow{\partial}_0 - \overleftarrow{\partial}_0$ and $d^3r = dxdydz$.

The Klein-Gordon equation (1.54) presents two main interpretation difficulties. The first one concerns the appearance of states with negative energy. Indeed, if we look for plane wave solutions $\Psi\left(\overrightarrow{r},t\right)=e^{i\left(\overrightarrow{p}\overrightarrow{r}-Et\right)}$ to the field-free equation, the energy levels which follow from (1.32), are solutions of $E^2=p^2+m^2$ with both signs $E=\pm\sqrt{p^2+m^2}$.

The existence of negative energy levels not lower bound, therefore arbitrarily low, is a major problem, which seems to indicate an instability of the theory.

There is another difficulty in interpreting the Klein-Gordon equation, the density $\rho\left(\overrightarrow{r},t\right)=J^0\left(\overrightarrow{r},t\right)$ defined in (1.56) has no reason to be positive. This is linked to the fact that the Klein-Gordon equation contains a second time derivative. The density must be manufactured from Ψ and $\partial\Psi/\partial t$. One can explicitly test this statement by evaluating J^0 on plane waves, then we find that the probability density J^0 becomes:

$$\rho\left(\overrightarrow{r},t\right)=\frac{E}{m}\Psi^{\star}\left(\overrightarrow{r},t\right)\Psi\left(\overrightarrow{r},t\right). \tag{1.58}$$

Therefore sign (ρ) = sign (E). This means that ρ may be both negative as well as positive and thus can no longer be consistently interpreted as a probability density.

To deal with all these difficulties, Pauli and Weisskopf modified the interpretation of the four-vector J^μ [21]. Following this reinterpretation of the theory, eJ^μ designates the density four-vector; in particular $e\rho$ is the electric charge density. As a result equation (1.55) is a charge conservation equation.

1.4 Dirac equation

In 1928, Dirac succeeded in writing a wave equation for relativistic spin-1/2 particles. This equation, applied to the electron, provided an explanation within the framework of modern quantum theory of the fine structure of the hydrogen atom's spectrum. Furthermore, it allowed Dirac to postulate the existence of positrons, antiparticles associated with electrons, discovered in the study of cosmic radiation as early as 1933 [22].

1.4.1 Construction of the Dirac equation

In an attempt to linearize the Klein-Gordon equation, and to resolve other conceptual problems encountered in the interpretation of this equation (such as that of negative probability density), Dirac hypothesizes that in relativistic quantum mechanics the dynamical state of the system is determined not by a scalar function but by a spinor Ψ forming a vector with n components in a Hilbert space [6, 8, 9]:

$$\Psi = \begin{pmatrix} \Psi_1 \\ . \\ . \\ \Psi_n \end{pmatrix}, \tag{1.59}$$

where Ψ is a function of the classical spatial variables $\overrightarrow{r}$ and t of a Hilbert space ε_0, and of the intrinsic variable or spin variable in a space ε_s. The complete Hilbert space of the particle is thus $\varepsilon_{H_D} = \varepsilon_0 \otimes \varepsilon_s$, where $\otimes$ is the tensor product.

To construct this equation, Dirac follows the historical approach, which is the quickest. He is looking for an equation analogous to Schrödinger's equation (1.20). Applying the correspondence principle (1.26) leads to the following Schrödinger equation:

$$\left(i\frac{\partial}{\partial t} - H_D\right)\Psi\left(\overrightarrow{r}, t\right) = 0, \tag{1.60}$$

where the symbol H_D denotes a linear operator and self adjoint, acting on both spatial and internal variables.

Having established this, we will first consider the free case. The Dirac Hamiltonian H_D must be invariant under spatial translation, therefore independent of $\overrightarrow{r}$. It must be linear in $\overrightarrow{p}$ and m since it is its square which makes $\overrightarrow{p}^2$ and m^2 appear. As $\overrightarrow{p}$ is a vector operator and m a number, the simplest solution leading to a scalar operator consists of putting [6, 8, 9]:

$$H_D\left(\overrightarrow{r}, t\right) = \overrightarrow{\alpha}.\overrightarrow{p} + \beta m, \tag{1.61}$$

where the operator $\overrightarrow{p}$ has the meaning indicated by the correspondence rule (1.19), i.e. $\overrightarrow{p} = -i\overrightarrow{\nabla}$. $\overrightarrow{\alpha} \equiv (\alpha^k,\ k = 1, 2, 3)$ and β are respectively vector and scalar operators acting on internal variables.

To derive from (1.60) a first member resembling the Klein-Gordon equation, it is necessary to manufacture second derivatives in time and space, however without making space-time crossed derivatives appear. Due to these constraints, it is necessary to introduce the operator $(i\frac{\partial}{\partial t}+H_D)$, and make it act on the first member of (1.60), proceeding in this way, it becomes

$$\left(i\frac{\partial}{\partial t}+H_D\right)\left(i\frac{\partial}{\partial t}-H_D\right)\Psi\left(\overrightarrow{r},t\right)=0. \tag{1.62}$$

After some calculation process that is recommended to do for training, the equation above is written:

$$\{E^2-\frac{1}{2}\sum_{k,l=1}^{3}(\left[\alpha^l,\alpha^k\right]_+ +\left[\alpha^l,\alpha^k\right]_-)p^lp^k-m\left(\sum_{k=1}^{3}\left[\alpha^k,\beta\right]_+ p^k\right)$$
$$-\beta^2m^2\}\Psi\left(\overrightarrow{r},t\right)=0, \tag{1.63}$$

where $\left[\alpha^l,\alpha^k\right]_\pm$ is defined as $\left[\alpha^l,\alpha^k\right]_\pm=\alpha^l\alpha^k\pm\alpha^k\alpha^l$, and $\left[\alpha^k,\beta\right]_+=\alpha^k\beta+\beta\alpha^k$. To fix $\overrightarrow{\alpha}$ and β, we require that the solutions of eq. (1.63) obey the Klein-Gordon equation (1.30), i.e.:

$$\left(E^2-\overrightarrow{p}^2-m^2\right)\Psi\left(\overrightarrow{r},t\right)=0, \tag{1.64}$$

which, after expansion, leads to the following algebraic constraints

$$\left[\alpha^k,\alpha^l\right]_+=2\delta^{kl}\mathbb{I}_n,\quad \left[\alpha^k,\beta\right]_+=0, \tag{1.65}$$

and

$$\left(\alpha^k\right)^2=\beta^2=\mathbb{I}_n, \tag{1.66}$$

where $\mathbb{I}_n$ is the identity matrix $n\times n$. Moreover, to guarantee the self-adjoint character of the operator H, these matrices must be hermitic,

$$\alpha^k=\left(\alpha^k\right)^\dagger,\quad \beta=\beta^\dagger. \tag{1.67}$$

Furthermore, from equation (1.65), and from the relation,

$$tr\left(AB\right)=tr\left(BA\right), \tag{1.68}$$

we can show that the matrices α^k and β are of zero trace. Indeed, we have

$$tr\left(\alpha^k\right) = Tr\left(\beta^2\alpha^k\right) = -tr\left(\beta\alpha^k\beta\right) = -tr\left(\alpha^k\right) = 0, \tag{1.69}$$

and in the same way, we find

$$tr\left(\beta\right) = tr\left(\left(\alpha^k\right)^2\beta\right) = -tr\left(\alpha^k\beta\alpha^k\right) = -tr\left(\beta\right) = 0. \tag{1.70}$$

From eq. (1.66) and (1.70), the eigenvalues of these matrices are ± 1. Since their trace is 0, they must have as many times the eigenvalue 1 as -1, so in total, an even number of eigenvalues, therefore:

$$\dim\alpha^k = \dim\beta = 2n, \tag{1.71}$$

where n is an integer other than 0. Relations (1.65), (1.66), (1.67), (1.69), and (1.70) being admitted, it is not difficult to show that there exists a representation where $\overrightarrow{\alpha}$ and β are represented by the following 4×4 Hermitic matrices, written in the form of 2×2 blocks [6]:

$$\overrightarrow{\alpha} = \begin{pmatrix} 0 & \overrightarrow{\sigma} \\ \overrightarrow{\sigma} & 0 \end{pmatrix}, \quad \beta = \begin{pmatrix} \mathbb{I}_2 & 0 \\ 0 & -\mathbb{I}_2 \end{pmatrix}, \tag{1.72}$$

where the $\overrightarrow{\sigma} \equiv (\sigma_x, \sigma_y, \sigma_z)$ are the Pauli matrices. The set of matrices given by (1.72) is called the standard representation, given that there exists an infinity of pairs $(\overrightarrow{\alpha}, \beta)$ verifying (1.65), (1.66), (1.67), (1.69), and (1.70), deducible from (1.72) by any unitary transformation. In any case, in this representation, the Dirac Hamiltonian H_D, for a free particle, has the matrix expression:

$$H_D = \begin{pmatrix} m\mathbb{I}_2 & \overrightarrow{\sigma}.\overrightarrow{p} \\ \overrightarrow{\sigma}.\overrightarrow{p} & -m\mathbb{I}_2 \end{pmatrix} \equiv \overrightarrow{\alpha}.\overrightarrow{p} + \beta m. \tag{1.73}$$

1.4.2 Covariant form of the Dirac equation

Having found a relativistic generalization of the Schrödinger equation of first order in space and time, we still have to show that this equation has the same form in all inertial systems, in accordance with the principle of relativity. Due to the symmetry between t and $\overrightarrow{r}$ for the covariant formulation, we introduce four matrices γ^μ, defined by $\gamma^0 = \beta$ and $\gamma^k = \beta\alpha^k$, where γ^0 is Hermitian [i.e. $(\gamma^0)^\dagger = \gamma^0$] and γ^k is anti-Hermitian [i.e. $\left(\gamma^k\right)^\dagger = -\gamma^k$]. We will also note $\gamma_\mu = g_{\mu\nu}\gamma^\nu$. The properties of the matrices $\overrightarrow{\alpha}$ and β (hermiticity, anticommutation, square $\mathbb{I}_4$) become for the γ^μ [6, 8, 9]:

$$\{\gamma^\mu, \gamma^\nu\} = \gamma^\mu\gamma^\nu + \gamma^\nu\gamma^\mu = 2g^{\mu\nu}, \quad (\gamma^\mu)^\dagger = \gamma^0\gamma^\mu\gamma^0, \tag{1.74}$$

where $g^{\mu\nu}$ denotes the contravariant components of the metric tensor

$$g^{\mu\nu} = diag\,(1, -1, -1, -1)\,. \tag{1.75}$$

By multiplying equation (1.60) on the left by β, we obtain the so-called covariant form of the Dirac equation:

$$(i\gamma^\mu\partial_\mu - m)\,\Psi\,(\overrightarrow{r}, t) = 0. \tag{1.76}$$

1.4.3 Dirac equation in an electromagnetic field

The form of the Dirac equation that we have used so far is only applicable to free particles. We now want to study the interactions of a Dirac particle with an external electromagnetic field characterized by its four-potential $A_\mu = \left(A_0, \overrightarrow{A}\right)$.

In classical mechanics, the Hamiltonian of a particle of charge e, in the presence of an external electromagnetic field, given by its four-potential A_μ is obtained by using the minimal coupling prescription. By replacing in the free Hamiltonian, the energy E by $E - eA_0$, and the spatial momentum $\overrightarrow{p}$ by $\overrightarrow{p} - e\overrightarrow{A}$, then, the four-momentum is substituted by [6, 18]:

$$p_\mu \to p_\mu - eA_\mu. \tag{1.77}$$

Dirac kept this ansatz for quantum mechanics. Since Schrödinger's correspondence rule requires that p_μ becomes the differential operator $i\partial_\mu$, we obtain:

$$D_\mu = \partial_\mu + ieA_\mu. \tag{1.78}$$

Thus, the ordinary derivation ∂_μ is replaced by the covariant derivation D_μ. In the presence of an electromagnetic field, the Dirac equation (1.76) then becomes

$$(i\gamma^\mu D_\mu - m)\,\Psi = 0. \tag{1.79}$$

This wave equation appears sufficient to account for the phenomenon of doubling. Since the matrices γ^μ contain four rows and four columns, it will have four times as many solutions as the non-relativistic wave equation, and twice as many as the previous relativistic wave equation (1.30). Given that half of the solutions must be rejected since they assign a charge $+e$ to the particle of Dirac, we will still have a correct number to account for the splitting phenomenon.

We will define a current density and demonstrate that the current defined with the solutions of the Dirac equation obeys a continuity equation. Starting from the covariant form of the Dirac equation (1.79), the conjugate hermetic of this equation is

$$(i\partial_\mu + eA_\mu)\,\Psi^\dagger\gamma^{\mu\dagger} + m\Psi^\dagger = 0, \tag{1.80}$$

where $\Psi^\dagger = (\Psi^\star)^T$ is the hermetic conjugate of Ψ, written as a row matrix.

Allowing for the relations $\gamma^0(\gamma^\mu)^\dagger\gamma^0 = \gamma^\mu$ and $(\gamma^0)^2 = \mathbb{I}_4$, and after multiplication on the right by γ^0, equation (1.80) then becomes,

$$(i\partial_\mu + eA_\mu)\,\overline{\Psi}\gamma^\mu + m\overline{\Psi} = 0. \tag{1.81}$$

This equation is obviously equivalent to equation (1.79). $\overline{\Psi} = \Psi^\dagger\gamma^0$ is called the adjoint of Ψ and equation (1.81) is called the adjoint equation.

Multiplying Eq. (1.79) on the left by $\overline{\Psi}$ and Eq. (1.81) on the right by Ψ, and adding the results together, leads to a continuity equation of the form

$$\partial_\mu J^\mu = \frac{\partial\rho}{\partial t} + \overrightarrow{\nabla}.\overrightarrow{J} = 0 \quad \text{for} \quad J^\mu = \overline{\Psi}\gamma^\mu\Psi = \left(\rho, \overrightarrow{J}\right), \tag{1.82}$$

where ρ and $\overrightarrow{J}$ are the density and the current for the Dirac equation respectively, namely

$$\rho = J^0 = \Psi^\dagger \Psi, \quad \overrightarrow{J} = \overline{\Psi} \overrightarrow{\gamma} \Psi. \tag{1.83}$$

The scalar product of any two bispinorsΨ_1 and Ψ_2 is defined in a Lorentz-invariant form on the hyperplane $x^0 = const$, as follows [19, 20]

$$(\Psi_1, \Psi_2) = \int \overline{\Psi}_1 \gamma^0 \Psi_2 dr^3 = \int \Psi_1^\dagger \Psi_2 dr^3 = \int \rho dr^3, \tag{1.84}$$

is independent of time t, is therefore constant. This allows us to interpret $|\Psi|^2 = \Psi^\dagger \Psi$ as a probability density in space, and $e\,|\Psi|^2$ as a charge density.

In Dirac's theory, we define a positive density ρ, which was not the case for the Klein-Gordon equation. However, we will see that the difficulty of negative energies, the interpretation proposed by Dirac is schematically the following and confirms the idea that, in any relativistic theory, the number of particles cannot be fixed because of the possibility of creation and annihilation of particles. This scheme allowed Dirac to predict the existence of the positron, antiparticle of the electron (same mass, same spin, opposite charge), discovered a few years later (in 1933) by C. D. Anderson [22].

1.4.4 2nd order Dirac equation

The solutions of the Dirac equation obey, when the electromagnetic field is different from zero, a second-order equation different from the Klein-Gordon equation, but consistent with the correspondence principle.

To form this equation, we start from the covariant form (1.79) and we write that the action of the operator $(i\gamma^\mu D_\mu + m)$ on the first member gives zero:

$$\left(\gamma^\mu \gamma^\nu D_\mu D_\nu + m^2\right) \Psi\left(\overrightarrow{r}, t\right) = 0. \tag{1.85}$$

From the fundamental relations (1.74) between the gamma matrices, we derive:

$$\gamma^\mu \gamma^\nu = g^{\mu\nu} I_4 - i\sigma^{\mu\nu}, \tag{1.86}$$

However, by a simple change in the naming of the mute indices, we have:

$$[\gamma^\mu, \gamma^\nu] D_\mu D_\nu = -[\gamma^\nu, \gamma^\mu] D_\nu D_\mu = \frac{1}{2} [\gamma^\mu, \gamma^\nu] [D_\mu, D_\nu] . \tag{1.87}$$

Now, following the definition of the operator D_μ Eq. (1.78) , we can write

$$[D_\mu, D_\nu] = ie \{[\partial_\mu, A_\nu] + [A_\mu, \partial_\nu]\} = ie (\partial_\mu A_\nu - \partial_\nu A_\mu) = ieF_{\mu\nu}, \tag{1.88}$$

where $\sigma^{\mu\nu} = \frac{i}{2} [\gamma^\mu, \gamma^\nu]$ represents the spin of the particle. $F_{\mu\nu}$ is the electromagnetic tensor defined by the components $F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu$.

Equations (1.86), (1.87) , and (1.88) give:

$$\gamma^\mu \gamma^\nu D_\mu D_\nu = g^{\mu\nu} D_\mu D_\nu + \frac{e}{2} \sigma^{\mu\nu} F_{\mu\nu}. \tag{1.89}$$

Finally, inserting (1.89) into (1.85), we obtain

$$\left\{ \left(D^\mu D_\mu + m^2\right) \mathbb{I}_4 + \frac{e}{2} \sigma^{\mu\nu} F_{\mu\nu} \right\} \Psi (\overrightarrow{r}, t) = 0. \tag{1.90}$$

We can consider this second-order differential equation with respect to time as the fundamental equation of the theory of spin-1/2 particles. As desired, this equation is clearly covariant. If we compare this equation with Eq. (1.54), relating to a particle of spin-0, we see that there is also the term $\frac{e}{2}\sigma^{\mu\nu} F_{\mu\nu}$ which is linked to the interaction of the spin with the external electromagnetic field. This term has no classical analogue and its contribution is negligible when one is in the conditions of validity of the classical approximation. The motion of a Dirac wave packet is then the same as that of a Klein-Gordon wave packet.

We will define a current density and demonstrate that the current defined with the solutions of the previous Dirac equation obeys a continuity equation. Starting from the covariant form of the Dirac equation (1.90), taking the conjugate transpose and multiplying on the right by γ^0, we then have

$$\overline{\Psi} (\overrightarrow{r}, t) \left\{ \left(\underleftarrow{D}^\mu \underleftarrow{D}_\mu + m^2 \right) \mathbb{I}_4 + \frac{e}{2} \sigma^{\mu\nu} F_{\mu\nu} \right\} = 0, \tag{1.91}$$

where $\underleftarrow{D}^\mu = \underleftarrow{\partial}^\mu - ieA^\mu$. Arrows pointing to the left remind that operators are operating on their left.

The following continuity equation can be obtained by multiplying Eq. (1.90) on the right by $\overline{\Psi}$ and Eq. (1.91) on the left by Ψ, and subtracting the two resulting equations:

$$\partial_\mu J^\mu = 0, \tag{1.92}$$

where

$$J^\mu = \frac{1}{2im}\left\{\overline{\Psi}\partial^\mu\Psi - \Psi\partial^\mu\overline{\Psi}\right\} + \frac{e}{m}A^\mu\overline{\Psi}\Psi = \left(\rho, \overrightarrow{J}\right), \tag{1.93}$$

The term $1/(2im)$ is introduced for convenience.

Chapter 2

Scattering theory in classical and quantum mechanics

2.1 Introduction

The world of molecules, atoms, nuclei, and particles is described by the laws of quantum physics which implies that many phenomena occurring at these scales seem unintuitive to our minds formed, by the very nature of our existence, to the macroscopic world and its laws of classical physics. Collision phenomena are no exception to the rule: even the simplest of them manifest themselves in surprising forms for those who only have in mind ideal classical collisions, such as those between billiard balls or celestial bodies.

These phenomena become even more spectacular when we consider more complex collisions, such as inelastic collisions, in which the internal state of the colliding particles is modified during the collision, or reactions, in which it is the very nature of the particles that is altered: in fact, these phenomena would sometimes be purely and simply impossible in classical physics because they would violate the conservation of energy.

This chapter is devoted to the theoretical analysis of scattering experiments. We introduce in the first step the notion of cross-section, which plays a central role in the description of a collision, both from a classical and quantum viewpoint, and more particularly in the description of elastic collisions. Then, we will construct the formalism of the scattering matrix for relativistic particles of spin-s in the presence of a localized electromagnetic field.

2.2 Cross-section

The cross-section is a definition necessary to interpret the results of collision experiments. It is related to the fact that in this type of experiment, we cannot send one particle at a time on the target. The projectile particles are therefore always in a beam. In the same way, the target also contains many particles. We can never know at what moment which incident particle interacts at what location with which target particle. Consequently, the results are of a statistical nature influenced by the details of the beam (the flux) and the target (density and thickness). The cross-section allows us to remove these geometric effects and to measure the dynamics of the interaction between a projectile particle and a target particle.

To describe this reality, let us consider a uniform beam of particles all of the same mass and energy of flux F, i.e., the number of incident particles crossing per unit surface placed perpendicular to the direction of propagation be incident on a scattering center; particles are scattered in all direction. If dn be the number of particles scattered per unit time into the solid angle $d\Omega$ located in the direction θ (deviation) and φ (azimuth) with respect to the bombarding direction as polar axis. Under these conditions, the number of particles dn must be proportional to the incident flux and the solid angle taken [23, 24, 25, 26]. Thus,

$$dn = F\left(\frac{d\sigma}{d\Omega}\right)d\Omega, \tag{2.1}$$

where $d\sigma\left(\theta,\varphi\right)/d\Omega$ is the proportionality coefficient and it is a function of θ and φ. Consideration of eq. (2.1) shows that $d\sigma\left(\theta,\varphi\right)/d\Omega$ has the dimensions of an area. This can be regarded as the cross-section of the incident beam through which all the particles pass that are scattered into the solid angle $d\Omega$ about θ and φ. For this reason, the proportionality constant is known as the differential scattering cross-section.

If eq. (2.1) is integrated over the entire solid angle to give the total flux of particles scattered by the center, the result defines the total scattering cross-section σ.

$$\begin{aligned} n_{scatt} = \int dn = \int\left(\frac{d\sigma}{d\Omega}\right)nd\Omega = n\int\left(\frac{d\sigma}{d\Omega}\right)d\Omega = n\sigma \quad \Rightarrow \\ \sigma = \int\left(\frac{d\sigma}{d\Omega}\right)d\Omega = \int_0^{2\pi}d\varphi\int_0^{\pi}\left(\frac{d\sigma}{d\Omega}\right)\sin\theta d\theta. \end{aligned} \tag{2.2}$$

The cross-section σ measures the field of action of the scattering center. In physical cases (elementary particles) the area where the particle undergoes the most significant part of its deviation is very small compared to the time and distance scales with which we are dealing. The trajectory of the particle therefore seems to be formed by two branches (one for $t \to -\infty$ the other for $t \to +\infty$) for which the motion seems asymptotically free.

2.3 Scattering theory in classical mechanics

In classical mechanics, particles follow trajectories that can be calculated from the equations of motion. In the case of diffusion by a potential of finite range, the trajectory must have two asymptotes that represent the trajectory of the free particle before and after its interaction with the potential. We can therefore define the scattering angle θ as the angle between the two asymptotes of the same trajectory and the impact parameter b as the distance from the center of the potential to one of the asymptotes. Solving the equations of motion allows us to express b as a function of θ.

For the sake of simplicity, first, we consider the diffusion processes, which involve an isolated system consisting of two particles of masses m_1 and m_2, subject only to their mutual interaction, which is described by a potential $V\left(\overrightarrow{r}_1 - \overrightarrow{r}_2\right)$, depending only on their relative positions $\overrightarrow{r}_1 - \overrightarrow{r}_2$; $\overrightarrow{r}_1$ and $\overrightarrow{r}_2$ being the position vectors of the two particles in an inertial frame of origin O [23, 24]. It is further assumed that the dynamics of collisions between these two particles, which initially move at speeds $\overrightarrow{v}_1$ and $\overrightarrow{v}_2$, is governed by an interparticle force. This force is usually a central force $\overrightarrow{F}\left(\overrightarrow{r}\right) = F\left(\overrightarrow{r}\right)\overrightarrow{u}_r$ $\left(\overrightarrow{r} = \overrightarrow{r}_1 - \overrightarrow{r}_2\right)$, deriving from the potential $V\left(\overrightarrow{r}\right)$, but this force has a very short range, so that they move freely most of the time, except when they come very close to each other, they collide.

In the inertial frame, the classical Hamiltonian of the system of two particles is:

$$H = \frac{p_1^2}{2m_1} + \frac{p_2^2}{2m_2} + V\left(\overrightarrow{r}_1 - \overrightarrow{r}_2\right), \tag{2.3}$$

In the center of mass frame, the position and velocity vectors are expressed by the following relationships:

$$\overrightarrow{r}_G = \frac{m_1\overrightarrow{r}_1 + m_2\overrightarrow{r}_2}{m_1 + m_2}, \quad \overrightarrow{v}_G = \frac{m_1\overrightarrow{v}_1 + m_2\overrightarrow{v}_2}{m_1 + m_2}. \tag{2.4}$$

By reporting (2.4) in (2.3), and after certain calculation processes that are recommended to be done for training, we arrive at a

$$H = \frac{1}{2}M\overrightarrow{v}_G^2 + \frac{1}{2}\mu\overrightarrow{v}^2 + V\left(\overrightarrow{r}\right), \tag{2.5}$$

where $M = m_1 + m_2$ is the total mass of the system, and $\mu = m_1m_2/\left(m_1 + m_2\right)$ is the mass of the relative particle of position $\overrightarrow{r}$, initially moving at speed $\overrightarrow{v} = \overrightarrow{v}_1 - \overrightarrow{v}_2$.

Using the relations:

$$M\overrightarrow{v}_G = \overrightarrow{p}_G = \overrightarrow{p}_1 + \overrightarrow{p}_2, \quad \frac{\overrightarrow{p}}{\mu} = \frac{\overrightarrow{p}_1}{m_1} - \frac{\overrightarrow{p}_2}{m_2}, \tag{2.6}$$

where $\overrightarrow{p}_G$ is the total momentum of the system and $\overrightarrow{p}$ the relative momentum of the two particles, the classical Hamiltonian takes the following form:

$$H = \frac{\overrightarrow{p}_G^2}{2M} + \frac{\overrightarrow{p}^2}{2\mu} + V\left(\overrightarrow{r}\right). \tag{2.7}$$

The first term $\overrightarrow{p}_G^2/2M$ of the above equation represents the kinetic energy of the center of mass in the inertial frame. This term is zero in the center of mass frame $\overrightarrow{p}_G = 0$. The second term $\overrightarrow{p}^2/2\mu$ represents the energy of the system of two particles in the center of mass frame.

Motion in a central field conserves the angular momentum of the system relative to the center of the field. For a particle this momentum is

$$\overrightarrow{L} = \overrightarrow{r} \wedge \overrightarrow{p}. \tag{2.8}$$

Since the vectors $\overrightarrow{L}$ and $\overrightarrow{r}$ are perpendicular to each other, the constancy of $\overrightarrow{L}$ means that during the entire motion of the particle its radius vector remains in the same plane, perpendicular to $\overrightarrow{L}$. Thus, the trajectory of the motion of a particle in a central field is contained entirely in a plane.

To obtain a theory that describes scattering at all angles, the equation of motion of the particle must be solved exactly. To this end, we introduce the polar coordinates r, θ, the equations of conservation of energy E, and angular momentum $\overrightarrow{L}$, are then written [23, 24]:

$$E = \frac{1}{2}\mu\left[r^2\dot{\theta}^2 + \dot{r}^2\right] + V\left(\overrightarrow{r}\right) = \frac{\mu\dot{r}^2}{2} + \frac{L^2}{2\mu r^2} + V\left(\overrightarrow{r}\right), \tag{2.9}$$

and

$$L = \left|\overrightarrow{r} \wedge \overrightarrow{p}\right| = \mu r^2\dot{\theta} = \mu v b. \tag{2.10}$$

After some computational process that is recommended to do for training, from these equations (2.9) and (2.10), we obtain a first order differential equation, which is written:

$$\dot{r} = \frac{dr}{dt} = \sqrt{\frac{2}{\mu}\left(E - V\left(\overrightarrow{r}\right)\right) - \frac{L^2}{\mu^2 r^2}}. \tag{2.11}$$

Then, by separating the variables and integrating, we find that

$$t = \int \frac{dr}{\sqrt{\frac{2}{\mu}\left(E - V\left(\overrightarrow{r}\right)\right) - \frac{L^2}{\mu^2 r^2}}} + Cte. \tag{2.12}$$

The equation (2.10) is written in the form

$$d\theta = \frac{L}{\mu r^2}dt. \tag{2.13}$$

From expression (2.11), we deduce dt, insert the result obtained in (2.13), and by performing some simple calculations, we find:

$$d\theta = \pm\frac{\frac{L}{r^2}dr}{\sqrt{2\mu\left(E - V\left(\overrightarrow{r}\right)\right) - \frac{L^2}{r^2}}}. \tag{2.14}$$

Since there are no non-conservative forces, the total energy E is conserved. For a potential $V\left(\overrightarrow{r}\right)$ tends to zero $\left(V\left(\overrightarrow{r}\right) \to 0\right)$ at infinity, the initial energy E is in kinetic form $E = \mu v^2/2$. Substituting this quantity into (2.14), the relationship between the impact parameter b and the scattering angle θ can be written as

$$d\theta = \pm\frac{b}{r^2}\frac{1}{\sqrt{1-\frac{b^2}{r^2}-\frac{2V\left(\overrightarrow{r}\right)}{\mu v^2}}}dr. \tag{2.15}$$

The choice of the sign $\pm$ must be made according to physical arguments. Assuming that r_m is the minimum approach distance corresponding to the angle $\theta\left(r_m\right)$, then we note $\theta > \theta\left(r_m\right)$ the distance r increases with θ and the sign $+$ must be used, for $\theta < \theta\left(r_m\right)$ it is therefore the sign $-$. This minimum approach distance being an extremum, is written

$$\left(\frac{dr}{d\theta}\right)_{r_m} = 0 \quad\Rightarrow\quad 1-\frac{b^2}{r_m^2}-\frac{2V\left(\overrightarrow{r}_m\right)}{\mu v^2} = 0, \tag{2.16}$$

that is to say

$$r_m = \frac{b}{\sqrt{1-\frac{2V\left(\overrightarrow{r}_m\right)}{\mu v^2}}}. \tag{2.17}$$

After slight rearrangements, the integral of (2.15) between $\theta\left(r_m\right)$ and any angle θ, takes the form:

$$\theta-\theta\left(r_m\right) = \pm\int_{r_m}^{r}\frac{b}{\left(\overrightarrow{r}'\right)^2\sqrt{1-\frac{b^2}{\left(\overrightarrow{r}'\right)^2}\frac{2V\left(\overrightarrow{r}'\right)}{\mu v^2}}}dr'. \tag{2.18}$$

Formulas (2.12) and (2.18) give the general solution to the problem posed. The second defines the relationship between r and θ, that is to say the equation of the trajectory. Formula (2.12) implicitly determines the distance r of the moving point from the center as a function of time.

Now consider a beam of identical particles heading towards a scattering center (target) located at O with the same kinetic energy and different impact parameters b. In this case, the main differences from the trajectory of a space probe discussed earlier are that each collision cannot be followed individually and the impact parameters of the microscopic particles are not experimentally accessible.This is because the precise positions of the particles are controllable neither in the beam nor in the target.

To describe this experimental reality, we therefore calculate an average over a large number of collisions, for which we assume that the impact parameters have a uniform probability distribution. Let F be the magnitude of the incident flux, that is, the number of incident particles crossing in unit time a unit surface placed perpendicular to the direction of propagation and stationary relative to the target. After having crossed the target, the deflected particles are recorded by a surface detector dS, placed at a distance r from the target and in a direction of polar angles (θ, φ). This detector is viewed from the target at a solid angle $d\Omega = dS/r^2$. From then on, by following the trajectories, we see that the particles recorded in the aperture counter $d\Omega = \sin\theta d\theta d\varphi$ have been isolated from the initial beam by the angular aperture sector $(\varphi, \varphi + d\varphi)$ of the circular crown of thickness $(b, b + db)$. The area of this sector being $ds = bdbd\varphi$, it sees a number of particles pass through per unit of time [23, 24]

$$dn = Fbdbd\varphi. \tag{2.19}$$

By comparing (2.1) and (2.19), we deduce the expression for the differential scattering cross-section.

$$\left(\frac{d\sigma}{d\Omega}\right) = \frac{b}{\sin\theta}\left|\frac{db}{d\theta}\right|. \tag{2.20}$$

It is therefore sufficient to know the relation $b\left(\theta\right)$, that is to say the geometry of the trajectories, to calculate, in classical mechanics, an effective collision section.

2.4 Scattering theory in quantum mechanics

2.4.1 Introduction

From the perspective of quantum theory, the differences in behavior between classical and quantum objects must necessarily be reflected in the concepts that describe them. There is no proof, a priori, that the concepts of trajectory, and that of impact parameter, which allow us to theoretically treat diffusion processes in classical mechanics, remain adequate for a quantum description. Indeed, in a quantum description and according to the Heisenberg uncertainty principle, the particle cannot have a definite momentum when its position is well defined, because during a movement of a determined speed, the notion of trajectory, and that of impact parameter, loses its meaning. This is why, even from an experimental point of view, at the quantum level, it is necessary to introduce the concept of cross-section, which represents a performed average over this impact parameter [25, 27, 28].

2.4.2 Scattering amplitude and cross-section

Historically, two different yet equivalent ways of doing this have been developed to solve the scattering problems in quantum mechanics. The first approach, dynamic, is more physical: it represents the target particle interaction by a time-dependent perturbation, simulating the passage of a particle coming from infinity and leaving there after collision. This way of doing things is technically cumbersome. The second approach consists in considering exclusively stationary states (static approach), which physically means that at times $t \to \pm\infty$, the particles do not interact. In other words in this limit, the fields evolve only according to the free Hamiltonian H_0. We will choose this approach to derive the scattering equations.

Moving on to the quantum description of the diffusion of a particle of mass m and energy E by a static potential $V(\overrightarrow{r})$, which decreases rapidly ($r^2 V(\overrightarrow{r}) \overset{r\to\infty}{\to} 0$ in all directions). Under these conditions, far from the zone of action of the potential, the incident particle is considered free; it can therefore be represented by the eigenstates of the unperturbed Hamiltonian $H_0 = \overrightarrow{k}^2/2m$ ($\hbar = 1$), the free kets $|\Psi_0\rangle$, solutions of the equation [25, 27, 28]

$$H_0 |\Psi_0\rangle = E |\Psi_0\rangle . \tag{2.21}$$

In the action zone of the potential $V(\overrightarrow{r})$, the eigenstates of $H = H_0 + V(\overrightarrow{r})$ will differ from the free states. However, if we assume that the diffusion process is elastic, the eigenstates of H will have the same energy as those of H_0. The eigenvalue equation that we wish to solve is then:

$$H |\Psi\rangle = (H_0 + V) |\Psi\rangle = E |\Psi\rangle . \tag{2.22}$$

Furthermore, when $V \to 0$, we must have $|\Psi\rangle \to |\Psi_0\rangle$ and equation (2.22) reduces to equation (2.21) with the same proper energy E. The solution to (2.22) is of the form:

$$|\Psi\rangle = |\Psi_0\rangle + \frac{1}{E - H_0} V |\Psi\rangle . \tag{2.23}$$

In representation of positions $|\overrightarrow{r}\rangle$, the wave function is denoted $\Psi(\overrightarrow{r})$, which, by definition, corresponds to $\langle \overrightarrow{r} |\Psi\rangle = \Psi(\overrightarrow{r})$. The scalar product and the closure relation are written as:

$$\langle \overrightarrow{r} \left| \overrightarrow{r}' \right\rangle = \delta\left(\overrightarrow{r} - \overrightarrow{r}'\right), \quad \int d^3r' \left|\overrightarrow{r}'\right\rangle \left\langle \overrightarrow{r}'\right| = 1. \tag{2.24}$$

By making use of the definition of $\Psi(\overrightarrow{r})$, and from the previous expression, equation (2.23) is transformed into an integral equation of scattering [25, 27, 28]:

$$\Psi(\overrightarrow{r}) = \Psi_0(\overrightarrow{r}) + \int d^3r' \langle \overrightarrow{r}| \frac{1}{E - H_0} \left|\overrightarrow{r}'\right\rangle \left\langle \overrightarrow{r}'\right| V |\Psi\rangle , \tag{2.25}$$

where $\Psi_0(\overrightarrow{r})$ is the general solution of the homogeneous equation (2.21), given by:

$$\Psi_0(\overrightarrow{r}) = \langle \overrightarrow{r} |\Psi_0\rangle = e^{i\overrightarrow{k}.\overrightarrow{r}}. \tag{2.26}$$

The resulting equation (2.25) is an integral equation which determining the wave function of the scattering problem.

In equation (2.25), the kernel of the integral equation:

$$G\left(\overrightarrow{r}, \overrightarrow{r}'\right) = \langle \overrightarrow{r}| \frac{1}{E - H_0} \left|\overrightarrow{r}'\right\rangle , \tag{2.27}$$

corresponds to the Green function of the Helmholtz equation [27, 29, 30, 31]:

$$\left(\Delta + k^2\right) G\left(\overrightarrow{r}, \overrightarrow{r}'\right) = \delta^{(3)}\left(\overrightarrow{r} - \overrightarrow{r}'\right). \tag{2.28}$$

To solve this equation, we will use the Fourier transform of the variable ξ, defined by [27, 29, 30, 31]:

$$G\left(\overrightarrow{r}, \overrightarrow{r}'\right) = \left(\frac{1}{2\pi}\right)^3 \int g\left(\overrightarrow{\xi}\right) e^{i\overrightarrow{\xi}.\left(\overrightarrow{r} - \overrightarrow{r}'\right)} d^3\xi, \tag{2.29}$$

where $g\left(\overrightarrow{\xi}\right)$ is the inverse Fourier transform of the function $G\left(\overrightarrow{r} - \overrightarrow{r}'\right)$.

In this spirit, we submit the differential equation for $G\left(\overrightarrow{r}, \overrightarrow{r}'\right)$ to the Fourier transform. To do this, we report the previous expression in (2.28); after some manipulations, we easily verify that the inverse Fourier transform $g\left(\overrightarrow{\xi}\right)$, is given by the following equation:

$$g\left(\overrightarrow{\xi}\right) = \frac{1}{k^2 - \xi^2}. \tag{2.30}$$

By carrying this last expression into (2.29), we arrive at the following integral equation

$$G\left(\overrightarrow{r}, \overrightarrow{r}'\right) = \left(\frac{1}{2\pi}\right)^3 \int \frac{e^{i\overrightarrow{\xi}.\left(\overrightarrow{r}-\overrightarrow{r}'\right)}}{k^2 - \xi^2} d^3\xi. \tag{2.31}$$

The potential $V\left(\overrightarrow{r}\right)$ depends only on the distance r to the origin, in this case, the z axis is an axis of revolution, these are the spherical coordinates ξ, θ and φ, which are best suited to the problem. With these coordinates, by setting $\left|\overrightarrow{r} - \overrightarrow{r}'\right| = \rho$, $y = \cos\theta$ and $\overrightarrow{\xi}.\left(\overrightarrow{r} - \overrightarrow{r}'\right) = \xi\rho y$, and let us insert these expressions in (2.31), after some computational processes, we obtain

$$G\left(\overrightarrow{r}, \overrightarrow{r}'\right) = \left(\frac{1}{2\pi}\right)^3 \int_0^{2\pi} d\varphi \int_0^{\infty} d\xi \frac{\xi^2}{k^2 - \xi^2} \int_{-1}^{1} e^{i\xi\rho y} dy. \tag{2.32}$$

After integration over the variables φ and y, the previous expression is written

$$G\left(\overrightarrow{r}, \overrightarrow{r}'\right) = \frac{1}{4i\pi^2\rho} \int_0^{\infty} d\xi \left[\frac{\xi\left(e^{i\xi\rho} - e^{-i\xi\rho}\right)}{k^2 - \xi^2}\right]. \tag{2.33}$$

After the change $\xi \to -\xi$ in the second integral of the previous expression, we can easily see that equation (2.33) transforms as

$$G\left(\overrightarrow{r}, \overrightarrow{r}'\right) = \frac{1}{4i\pi^2\rho} \int_{-\infty}^{+\infty} \frac{\xi e^{i\xi\rho}}{k^2 - \xi^2} d\xi. \tag{2.34}$$

If we wish to integrate over the variable ξ, we are faced with the problem: what should we do with the simple pôles on the real axis of the integrand at $\xi = \pm k$. We can avoid this difficulty by considering ξ as a complex variable. To illustrate this point, we can consider the term $1/\left(k^2 - \xi^2\right)$ as the limit, when $\varepsilon \to 0$ (ε being a positive real quantity).

Either, by making the change of variable $k \to k + i\varepsilon$, we easily verify that equation (2.34), is written

$$G\left(\overrightarrow{r},\overrightarrow{r}'\right)=-\frac{1}{4i\pi^2\rho}\lim_{\varepsilon\to 0}\int_{-\infty}^{+\infty}\frac{\xi e^{i\xi\rho}}{(\xi-k-i\varepsilon)(\xi+k+i\varepsilon)}d\xi. \tag{2.35}$$

We see that the real pôles k are replaced by the complex pôles $k+i\varepsilon$. We now move on to the calculation of the integral (2.35). To illustrate this, we apply Cauchy's integral formula [29, 32]

$$\oint_C \frac{f(z)}{z-a}dz=\begin{cases}\pm 2\pi i f(a) & \text{if } a \text{ is inside C,}\\ 0 & \text{if } a \text{ is outside C.}\end{cases} \tag{2.36}$$

Here, $f(z)$ is an analytic function inside a closed curve C and on C. We have (+) if the contour is traveled counterclockwise and (−) otherwise. Curve C is the contour composed of the part of the real axis between $-R$ and $+R$, indented by two half-circumferences with centers $(\pm k, 0)$ and radius ε infinitely small, closed by a semi-circle, as shown in figure-2.1.

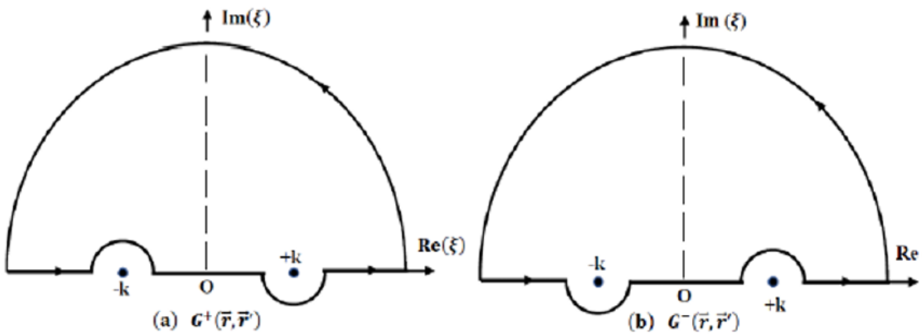

Fig-2.1: Integration contours for Green's functions G^+ and G^-

Our physical intuition tells us that the wave propagating to the right from point $\overrightarrow{r}'$ should not influence the response at point $\overrightarrow{r}$ to the left of $\overrightarrow{r}'$. Thus, for $r>r'$, the contour must go around the pôle $\xi=-k-i\varepsilon$ from above and the pôle $\xi=k+i\varepsilon$ from below, so that only the contour in fig-(2.1.a) contributes. For $r<r'$ the contour is closed downwards and only the contribution of the pôle $\xi=-k-i\varepsilon$ is desired. As shown in fig-(2.1.b).

At this point, we therefore have the following two expressions for the Green function, each expression being associated with a given interval for r.

For $r>r'$, we have:

$$G^{+}\left(\overrightarrow{r},\overrightarrow{r}'\right)=-\frac{1}{4i\pi^{2}\rho}\lim_{\varepsilon\to0}\int_{-\infty}^{+\infty}\frac{f^{+}(\xi)}{(\xi-k-i\varepsilon)}d\xi=$$
$$-\frac{1}{4i\pi^{2}\rho}\lim_{\varepsilon\to0}\oint_{C_a}\frac{f^{+}(\xi)}{(\xi-k-i\varepsilon)}d\xi, \tag{2.37}$$

where $f^{+}(\xi)=\xi e^{i\xi\rho}/(\xi+k+i\varepsilon)$, is an analytic and uniform function inside the simple closed curve C_a and on C_a. Applying Cauchy's integral formula (2.36), we get

$$G^{+}\left(\overrightarrow{r},\overrightarrow{r}'\right)=-\frac{1}{2\pi\rho}\lim_{\varepsilon\to0}f^{+}(k+i\varepsilon)=-\frac{1}{4\pi}\frac{e^{ik\left|\overrightarrow{r}-\overrightarrow{r}'\right|}}{\left|\overrightarrow{r}-\overrightarrow{r}'\right|}. \tag{2.38}$$

Moving to the other region $r<r'$. We now consider the contour of fig-(2.1.b). The function $f^{-}(\xi)=\xi e^{i\xi\rho}/(\xi-k-i\varepsilon)$, is an analytic and uniform function inside the simple closed curve C_b and on C_b. Applying Cauchy's integral formula (2.36), we get

$$G^{-}\left(\overrightarrow{r},\overrightarrow{r}'\right)=-\frac{1}{4i\pi^{2}\rho}\lim_{\varepsilon\to0}\oint_{C_b}\frac{f^{-}(\xi)}{(\xi+k+i\varepsilon)}d\xi=$$
$$-\frac{1}{2\pi\rho}\lim_{\varepsilon\to0}f^{-}(-k-i\varepsilon)=-\frac{1}{4\pi}\frac{e^{-ik\left|\overrightarrow{r}-\overrightarrow{r}'\right|}}{\left|\overrightarrow{r}-\overrightarrow{r}'\right|}. \tag{2.39}$$

Finally, the solutions (2.38) and (2.39) can be grouped together to be written in a single equation including solutions relating to the outgoing (or incoming) waves

$$G^{\pm}\left(\overrightarrow{r},\overrightarrow{r}'\right)=-\frac{1}{4\pi}\frac{e^{\pm ik\left|\overrightarrow{r}-\overrightarrow{r}'\right|}}{\left|\overrightarrow{r}-\overrightarrow{r}'\right|}. \tag{2.40}$$

These two functions have outgoing spherical wave behavior for $G^{+}\left(\overrightarrow{r},\overrightarrow{r}'\right)$ and incoming spherical wave behavior for $G^{-}\left(\overrightarrow{r},\overrightarrow{r}'\right)$ [29, 33].

By carrying this last expression into (2.25), we arrive at

$$\Psi^{\pm}\left(\overrightarrow{r}\right)=e^{i\overrightarrow{k}\overrightarrow{r}}+\int G^{\pm}\left(\overrightarrow{r},\overrightarrow{r}'\right)V\left(\overrightarrow{r}'\right)\Psi^{\pm}\left(\overrightarrow{r}'\right)d^{3}r'. \tag{2.41}$$

The resulting equation (2.41) is the Lippmann-Schwinger equation [27, 29, 34], which is an integral equation determining the wave function of the scattering problem. The first term in this equation can be considered the incident wave, describing the free motion of the particle. The second term describes the scattered wave, which, depending on the choice of the Green's function, can be either outgoing or incoming.

Asymptotically, for large values of r $(r \gg r^{'})$, by a direct calculation, we see immediately that

$$\left|\overrightarrow{r} - \overrightarrow{r}'\right| = r\sqrt{1 + \frac{\left(\overrightarrow{r}'\right)^2 - 2\overrightarrow{r}.\overrightarrow{r}'}{r^2}} \simeq r - r^{'}\cos\theta, \tag{2.42}$$

where θ is the angle between $r^{'}$ and r, r being the direction along which we are calculating the scattered wave $\overrightarrow{k}'$, i.e.,

$$ik\left|\overrightarrow{r} - \overrightarrow{r}'\right| \simeq ikr - ikr^{'}\cos\theta = ikr - i\overrightarrow{k}'.\overrightarrow{r}'. \tag{2.43}$$

By carrying this last expression into (2.40), we arrive at

$$G^{\pm}\left(\overrightarrow{r}, \overrightarrow{r}'\right) = -\frac{e^{\pm ikr}}{4\pi r}e^{\mp i\overrightarrow{k}'.\overrightarrow{r}'}, \tag{2.44}$$

where the vector $\overrightarrow{k}'$ is directed along r and is defined by $\overrightarrow{k}' = k\overrightarrow{r}/r$.

Taking into account the previous expression, for $r >> r^{'}$, asymptotically, the wave function (2.41) can be approximated by the expression

$$\Psi^{\pm}\left(\overrightarrow{r}\right) \simeq e^{i\overrightarrow{k}.\overrightarrow{r}} + \frac{e^{\pm ikr}}{r}\left(-\frac{1}{4\pi}\right)\int e^{\mp i\overrightarrow{k}'.\overrightarrow{r}'}V\left(\overrightarrow{r}'\right)\Psi^{\pm}\left(\overrightarrow{r}'\right)d^3r^{'}. \tag{2.45}$$

Identifying $f^{\pm}(\theta, \varphi)$ as the coefficient of the outgoing wave [25, 27, 28], we find the integral expression for the scattering amplitude

$$f^{\pm}(\theta, \varphi) = -\frac{1}{4\pi}\int e^{\mp i\overrightarrow{k}'.\overrightarrow{r}'}V\left(\overrightarrow{r}'\right)\Psi^{\pm}\left(\overrightarrow{r}'\right)d^3r^{'}. \tag{2.46}$$

The above equation is not a straight-forward formula to calculate $f^{\pm}(\theta, \varphi)$. Because $\Psi\left(\overrightarrow{r}\right)$ which appears in the integral is still not known. However, it provides a very beneficial approximation called the Born approximation to be discussed in the next section [25, 34, 35].

To obtain the differential scattering cross-section $d\sigma/d\Omega$, let us start by relating the flux vector $\overrightarrow{J}$ to the wave functions of equation (2.45). In fact, the plane wave term $e^{i\overrightarrow{k}.\overrightarrow{r}}$ represents the incident wave. In the absence of the vector potential $\overrightarrow{A} = 0$, the flux F_{inc} can be calculated by inserting the plane wave $e^{i\overrightarrow{k}.\overrightarrow{r}}$ into (1.24),

$$F_{inc} = \left| \overrightarrow{J}_{inc} \right| = \frac{k}{m}. \tag{2.47}$$

The flux F_{scatt} of particles passing through an area $d\overrightarrow{S}$ in the direction specified by θ and φ, is related to the second term of equation (2.45) and therefore to the scattering amplitude $f^{\pm}(\theta,\varphi)$. This is given by $F^{\pm}_{scatt} = \left| \overrightarrow{J}^{\pm}_{scatt} . d\overrightarrow{S} \right|$, where $d\overrightarrow{S} = r^2 d\Omega \overrightarrow{u}_r$ and $\overrightarrow{J}^{\pm}_{scatt}$ is the scattered current, whose expression is given by the equation

$$\overrightarrow{J}^{\pm}_{scatt} = \frac{1}{2im}\left(\Psi^{\pm}_{scatt}(\overrightarrow{r})^{\star}\,\overrightarrow{\nabla}\Psi^{\pm}_{scatt}(\overrightarrow{r}) - \Psi^{\pm}_{scatt}(\overrightarrow{r})\,\overrightarrow{\nabla}\Psi^{\pm}_{scatt}(\overrightarrow{r})^{\star}\right), \tag{2.48}$$

where $\Psi^{\pm}_{scatt}(\overrightarrow{r})$ is the scattered wave being expressed in formula (2.45), by

$$\Psi^{\pm}_{scatt}(\overrightarrow{r}) = f^{\pm}(\theta,\varphi)\,\frac{e^{\pm i\overrightarrow{k}\overrightarrow{r}}}{r}. \tag{2.49}$$

To calculate the probability current of the scattered wave, it is convenient to use spherical coordinates. The gradient of a scalar function $\Psi^{\pm}_{scatt}(\overrightarrow{r})$ is given by:

$$\overrightarrow{\nabla}\Psi^{\pm}_{scatt}(\overrightarrow{r}) = \frac{\partial\Psi^{\pm}_{scatt}(\overrightarrow{r})}{\partial r}\overrightarrow{u}_r + \frac{1}{r}\frac{\partial\Psi^{\pm}_{scatt}(\overrightarrow{r})}{\partial\theta}\overrightarrow{u}_\theta + \frac{1}{r\sin\theta}\frac{\partial\Psi^{\pm}_{scatt}(\overrightarrow{r})}{\partial\varphi}\overrightarrow{u}_\varphi. \tag{2.50}$$

Inserting (2.49) into (2.48), and taking into account the previous expression, the components of the scattered current $\overrightarrow{J}_{scatt}$ on the local axes defined by this coordinate system, in the asymptotic region are given by:

$$\left(J^{\pm}_{scatt}\right)_r = \pm\frac{k}{m}\frac{1}{r^2}\left|f^{\pm}\right|^2, \quad \left(J^{\pm}_{scatt}\right)_\theta = \frac{1}{m}\frac{1}{r^3}\,\mathrm{Re}\left[\frac{1}{i}\left(f^{\pm}\right)^{*}\frac{\partial f^{\pm}}{\partial\theta}\right],$$
$$\left(J^{\pm}_{scatt}\right)_\varphi = \frac{1}{m}\frac{1}{r^3\sin\theta}\,\mathrm{Re}\left[\frac{1}{i}\left(f^{\pm}\right)^{*}\frac{\partial f^{\pm}}{\partial\varphi}\right]. \tag{2.51}$$

At large distances the gradient contribution on $f^{\pm}(\theta,\varphi)/r$ is proportional to $1/r^3$, which is negligible for large r. So, only the exponential contributes to the flux. Then $(J_{scatt})_\theta$ and $(J_{scatt})_\varphi$ are negligible compared to $(J_{scatt})_r$, and the flux of particles scattered is practically

$$F^{\pm}_{scatt} = \left|\overrightarrow{J}^{\pm}_{scatt} . d\overrightarrow{S}\right| = \frac{k}{m}\left|f^{\pm}(\theta,\varphi)\right|^2 d\Omega. \tag{2.52}$$

The results of an experiment are usually expressed in terms of a differential cross-section ($d\sigma^{\pm}/d\Omega$) that is defined as the flux of particles scattered in direction (θ, φ) per unit solid angle per unit incident flux. Hence, referring to (2.47) and (2.52), the simple and remarkable relationship between scattering amplitude and differential cross-section:

$$\left(\frac{d\sigma^{\pm}}{d\Omega}\right) = \frac{F^{\pm}_{scatt}}{F_{in}d\Omega} = \left|f^{\pm}(\theta, \varphi)\right|^2 . \tag{2.53}$$

The differential cross-section is therefore simply given by the square of the modulus of the scattering amplitude. We see that this expression is completely analogous to the empirical definition of the scattering cross-section of a classical wave.

2.4.3 Born approximation

The preceding description is very general and applies to any potential $V(\overrightarrow{r})$ which decreases for $r \to \infty$ but arbitrary near the origin. In general, it is very difficult to calculate the solutions of the integral equation of scattering (2.41), and in particular the scattering amplitude $f^{\pm}(\theta, \varphi)$. However, if the interaction can be treated as a small perturbation (weak scattering field), the integral equation (2.41) can be solved by the method of successive approximations. One of the approximate calculation methods is the one developed by Max Born, in which the cross-section is very simply related to the Fourier transform [36, 37].

By solving the Lippmann-Schwinger equation (2.41) by iteration, starting from the incident plane wave $\Psi_0(\overrightarrow{r})$ as the zeroth-order approximation. Indeed, a simple change of notations ($\overrightarrow{r} \to \overrightarrow{r}'$, $\overrightarrow{r}' \to \overrightarrow{r}''$) allows us to write equation (2.41) in the form:

$$\Psi^{\pm}\left(\overrightarrow{r}'\right) = e^{i\overrightarrow{k}.\overrightarrow{r}'} + \int d^3r'' G^{\pm}\left(\overrightarrow{r}', \overrightarrow{r}''\right) V\left(\overrightarrow{r}''\right) \Psi^{\pm}\left(\overrightarrow{r}''\right) . \tag{2.54}$$

Inserting this expression into (2.41) and expanding, we obtain

$$\Psi^{\pm}(\overrightarrow{r}) = e^{i\overrightarrow{k}.\overrightarrow{r}} + \int d^3r' G^{\pm}\left(\overrightarrow{r}, \overrightarrow{r}'\right) V\left(\overrightarrow{r}'\right) e^{i\overrightarrow{k}.\overrightarrow{r}'} + \int d^3r' \times$$
$$\int d^3r'' G^{\pm}\left(\overrightarrow{r}, \overrightarrow{r}'\right) V\left(\overrightarrow{r}'\right) G^{\pm}\left(\overrightarrow{r}', \overrightarrow{r}''\right) V\left(\overrightarrow{r}''\right) \Psi^{\pm}\left(\overrightarrow{r}''\right) \tag{2.55}$$

On the right side of (2.55), the first two terms are known, only the third contains the unknown function $\Psi^{\pm}\left(\overrightarrow{r}''\right)$. We can repeat this process: we change $\overrightarrow{r}$ to $\overrightarrow{r}''$ and $\overrightarrow{r}'$ to $\overrightarrow{r}'''$ in (2.41), resulting in $\Psi^{\pm}\left(\overrightarrow{r}''\right)$, which we insert again in equation (2.55), we lead to

$$\begin{aligned}\Psi^{\pm}\left(\overrightarrow{r}\right) &= e^{i\overrightarrow{k}.\overrightarrow{r}} + \int d^3r' G^{\pm}\left(\overrightarrow{r},\overrightarrow{r}'\right) V\left(\overrightarrow{r}'\right) e^{i\overrightarrow{k}.\overrightarrow{r}'} + \int d^3r' \int d^3r'' G^{\pm}\left(\overrightarrow{r},\overrightarrow{r}'\right) \times \\ & V\left(\overrightarrow{r}'\right) G^{\pm}\left(\overrightarrow{r}',\overrightarrow{r}''\right) V\left(\overrightarrow{r}''\right) e^{i\overrightarrow{k}.\overrightarrow{r}''} + \int d^3r' \int d^3r'' \int d^3r''' G^{\pm}\left(\overrightarrow{r},\overrightarrow{r}'\right) \times \\ & V\left(\overrightarrow{r}'\right) G^{\pm}\left(\overrightarrow{r}',\overrightarrow{r}''\right) V\left(\overrightarrow{r}''\right) G^{\pm}\left(\overrightarrow{r}'',\overrightarrow{r}'''\right) V\left(\overrightarrow{r}'''\right) \Psi^{\pm}\left(\overrightarrow{r}'''\right). \qquad (2.56)\end{aligned}$$

We thus construct step by step what is called the Born development of the scattering stationary wave function, where each nth expansion term is proportional to the potential raised to the nth power. Successive iteration yields

$$\Psi^{\pm}\left(\overrightarrow{r}\right) = \Psi_0\left(\overrightarrow{r}\right) + \Psi_1^{\pm}\left(\overrightarrow{r}\right) + \Psi_2^{\pm}\left(\overrightarrow{r}\right) + \Psi_3^{\pm}\left(\overrightarrow{r}\right) + ..., \qquad (2.57)$$

where

$$\Psi_0^{\pm}\left(\overrightarrow{r}\right) = e^{i\overrightarrow{k}.\overrightarrow{r}}$$

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$$\Psi_n^{\pm}\left(\overrightarrow{r}\right) = e^{i\overrightarrow{k}.\overrightarrow{r}} + \int d^3r' G^{\pm}\left(\overrightarrow{r},\overrightarrow{r}'\right) V\left(\overrightarrow{r}'\right) \Psi_{n-1}^{\pm}\left(\overrightarrow{r}'\right). \qquad (2.58)$$

If we carry this expansion of $\Psi^{\pm}\left(\overrightarrow{r}\right)$ into expression (2.46), we obtain the Born expansion of the scattering amplitude. However, if the scattering potential is small, then the difference between the operators H_0 and $H = H_0 + V$ is small, and hence the difference between their eigenfunctions, $\Psi_0\left(\overrightarrow{r}'\right)$ and $\Psi^{\pm}\left(\overrightarrow{r}'\right)$ should also be small. Therefore, from (2.46), we obtain an approximation of the scattering amplitude by replacing $\Psi^{\pm}\left(\overrightarrow{r}'\right)$ by the plane wave $e^{i\overrightarrow{k}.\overrightarrow{r}'}$. In this approximation we obtain

$$f_B^{\pm}(\theta,\varphi) = -\frac{1}{4\pi}\int e^{i\left(\overrightarrow{k}\mp\overrightarrow{k}'\right)\overrightarrow{r}'} V\left(\overrightarrow{r}'\right) d^3r', \qquad (2.59)$$

which is known as the scattering amplitude in the first Born approximation.

The scattering amplitude (2.59) appears proportional to the matrix element of the scattering potential between the two plane waves, $e^{i\overrightarrow{k}.\overrightarrow{r}'}$ and $e^{\mp i\overrightarrow{k}'.\overrightarrow{r}'}$, representing the free particle before and after the scattering. This is just a Fourier transform of the potential using the momentum transfer $\pm\overrightarrow{q} = \overrightarrow{k} \mp \overrightarrow{k}'$, sometimes called the collision vector, has a magnitude equal to

$$q = |\overrightarrow{q}| = 2k \sin\frac{\theta}{2}, \tag{2.60}$$

where θ is the angle between the vectors $\overrightarrow{k}$ and $\overrightarrow{k}'$, i.e. scattering angle. Recall that the vector $\overrightarrow{k}$ is directed along the incident beam, and the vector $\overrightarrow{k}'$ along the position vector drawn from the scattering center to the point of observation of the scattered particles.

2.5 Asymptotic states in classical and quantum mechanics

In classical mechanics, particles follow trajectories that can be calculated from the equations of motion. In the case of scattering by a finite-range field, the trajectory must have two asymptotes that represent the trajectory of the free particle, before and after its interaction with the potential. We can therefore define the scattering angle θ as the angle between the two asymptotes of the same trajectory and the impact parameter b as the distance from the center of the potential to one of the asymptotes. Solving the equations of motion allows us to express b as a function of θ [23, 24].

At the quantum level, it is then generally not possible to predict with certainty which final state will result from a given collision; we therefore only seek to predict the probabilities for a certain final state. To do this, we will study the evolution of the wave function $\Psi(\overrightarrow{r}, t)$ associated with the incident particle interacting with a localized field. As the classical trajectory tends toward free trajectories, the wave function $\Psi(\overrightarrow{r}, t)$ tends toward free wave functions, $\Psi^{in}(\overrightarrow{r}, t)$ and $\Psi^{out}(\overrightarrow{r}, t)$. The latter are solutions of the free Schrödinger equation, and satisfy the asymptotic conditions [38, 39, 40] $\lim\limits_{t\to-\infty} |\Psi - \Psi^{in}| = \lim\limits_{t\to+\infty} |\Psi - \Psi^{out}| = 0$.

2.5.1 Asymptotic states in classical mechanics

In classical mechanics, the trajectory of the particle can be described by a three-dimensional vector function $\overrightarrow{r}(t)$, which is geometrically a three-dimensional curve. If the particle undergoes the type of motion that has been described above as typical in a scattering experiment, then the trajectory $\overrightarrow{r}(t)$ should have as characteristics the main qualitative features of the curve in figure-2.2.

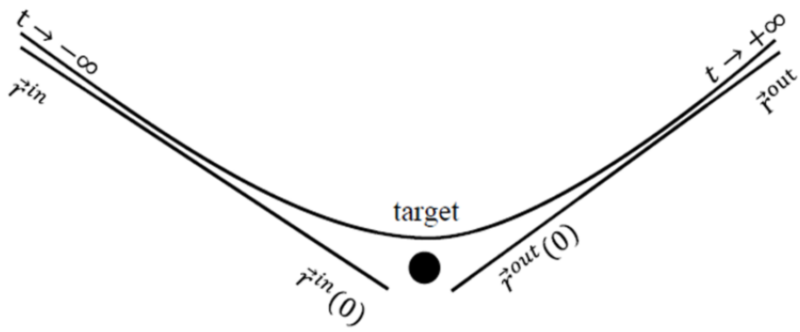

Fig-2.2: Asymptotic states in classical mechanics

Out of the reach of interactions at an initial time in the distant past $t \to -\infty$, the particle's motion should be nearly free, i.e. nearly along a straight line $\overrightarrow{r}^{in}(t)$ at a uniform velocity $\dot{\overrightarrow{r}}^{in}(t)$. Then, for a relatively short period, during which the particle interacts with the scattering center, the motion in general is very complex. Finally, at the end, $t \to +\infty$, of the experiment and for some time before that, the motion of the particle should be again along a straight line $\overrightarrow{r}^{out}(t)$ and at uniform speed $\dot{\overrightarrow{r}}^{out}(t)$.

In classical mechanics a particle is said to be in free motion if its state is of the form

$$\overrightarrow{r}(t) = \overrightarrow{r}_0 + \dot{\overrightarrow{r}}t, \tag{2.61}$$

so that $\ddot{\overrightarrow{r}} = 0$. Hence, at times $t \to -\infty$, we expect that

$$\lim_{t\to-\infty}\left|\overrightarrow{r}(t) - \left(\overrightarrow{r}^{in} + \dot{\overrightarrow{r}}^{in}t\right)\right| = 0, \quad \lim_{t\to-\infty}\left|\dot{\overrightarrow{r}}^{in}(t) - \dot{\overrightarrow{r}}^{in}\right| = 0, \tag{2.62}$$

Similar considerations for $t \to +\infty$, lead to the following corresponding requirements:

$$\lim_{t\to+\infty}\left|\overrightarrow{r}(t)-\left(\overrightarrow{r}^{out}+\dot{\overrightarrow{r}}^{out}t\right)\right|=0,\quad \lim_{t\to+\infty}\left|\dot{\overrightarrow{r}}^{out}(t)-\dot{\overrightarrow{r}}^{out}\right|=0. \tag{2.63}$$

The conditions (2.62) and (2.63) define the asymptotic states of the particle in a precise way. The vectors $\overrightarrow{r}^{in,out}(t)$ and $\dot{\overrightarrow{r}}^{in,out}(t)$ characterize a free state of the particle, which is called the incoming or outgoing asymptotic state.

2.5.2 Asymptotic states in quantum mechanics

Now, we will come to the quantum description. The behavior over time of the wave packet that represents the state of the particle of mass m and charge e in the presence of an external field, is described by a complex wave function $\Psi(\overrightarrow{r},t)$, solution of the Schrödinger equation

$$i\frac{\partial\Psi(\overrightarrow{r},t)}{\partial t}=H\Psi(\overrightarrow{r},t), \tag{2.64}$$

where $H=H_0+V(\overrightarrow{r},t)$ is the Hamiltonian, time-dependent in general, the observable corresponding to the total energy of the system. $V(\overrightarrow{r},t)$ is the Hamiltonian of the interactions, and $H_0=p^2/2m$ is a self-adjoint operator, called the free Hamiltonian.

To use the $\hat{S}$-matrix formalism in scattering processes, it is necessary to assume that the interactions are short-range, so that the initial and final states, in which the particles are well separated from each other, consist of free particle states. For this, we consider the case where the interacting potential $V(\overrightarrow{r},t)$ is to be understood as a perturbation of H_0 whose effects are negligible in the asymptotic regions of space. Intuitively, one expects that the solutions of (2.64) in the asymptotic regions ($|\overrightarrow{r}(t)|\to+\infty$), can be approximated by solutions of the free equation

$$i\frac{\partial\Psi^{in,out}(\overrightarrow{r},t)}{\partial t}=H_0\Psi^{in,out}(\overrightarrow{r},t), \tag{2.65}$$

where $\Psi^{in}(\overrightarrow{r},t)$ is the initial wave function characterizing the motion of the particle at time $t\to-\infty$, and $\Psi^{out}(\overrightarrow{r},t)$ the final wave function describing the particle after the collision at time $t\to+\infty$.

To describe scattering processes and reactions in quantum mechanics, it is convenient to introduce the scattering operator $\hat{\mathbf{S}}$, the matrix elements of which form the scattering matrix. If we know the $\hat{S}$-matrix, we can determine the final state $\Psi^{out}(\overrightarrow{r},t)$ from any initial state $\Psi^{in}(\overrightarrow{r},t)$. Therefore, We can write [38, 39, 40]

$$\Psi^{out}(\overrightarrow{r},t) = \hat{S}\Psi^{in}(\overrightarrow{r},t). \tag{2.66}$$

We introduce eigenfunctions of the operator H_0:

$$H_0\varphi_\alpha^{in} = E_\alpha\varphi_\alpha^{in}, \qquad H_0\varphi_\beta^{out} = E_\beta\varphi_\beta^{out}, \tag{2.67}$$

where E_α and E_β are eigenvalues of H_0. The sets of functions φ_α^{in} and φ_β^{out} form complete orthonormalized systems satisfying the conditions

$$\left(\varphi_\alpha^{in},\varphi_{\alpha'}^{in}\right) = \delta_{\alpha\alpha'}, \qquad \left(\varphi_\beta^{out},\varphi_{\beta'}^{out}\right) = \delta_{\beta\beta'}, \tag{2.68}$$

where (2.68) is the scalar product. We expand the wave functions Ψ^{in} and Ψ^{out} of the initial and final states in terms of the eigenfunctions of the operator H_0

$$\Psi^{in} = \sum_\alpha a_\alpha\varphi_\alpha^{in} \quad \text{and} \quad \Psi^{out} = \sum_\beta b_\beta\varphi_\beta^{out}. \tag{2.69}$$

The problem is to find the coefficients b_β if the set of coefficients a_α is known. For this purpose, inserting (2.69) into (2.66), by a direct calculation, we have

$$\Psi^{out} = \sum_\beta b_\beta\varphi_\beta^{out} = \hat{S}\sum_\alpha a_\alpha\varphi_\alpha^{in} = \sum_\alpha a_\alpha\hat{S}\varphi_\alpha^{in}. \tag{2.70}$$

Afterwards, multiplying the last equation on the left by $\varphi_{\beta'}^{out}$, after some simple computational processes, we obtain

$$\sum_\beta b_\beta\varphi_{\beta'}^{out}.\varphi_\beta^{out} = \sum_\alpha a_\alpha\varphi_{\beta'}^{out}.\hat{S}\varphi_\alpha^{in}. \tag{2.71}$$

By using Eq. (2.68) , the relation (2.71), can be written in the form

$$\sum_\beta b_\beta\varphi_{\beta'}^{out}.\varphi_\beta^{out} = \sum_\beta b_\beta\delta_{\beta\beta'} = b_{\beta'} = \sum_\alpha a_\alpha\hat{S}_{\beta'\alpha}, \tag{2.72}$$

where the coefficient $\hat{S}_{\beta'\alpha}$ is a quantum-mechanical transition amplitude from the state φ_α^{in} to the state $\varphi_{\beta'}^{out}$, given by

$$\hat{S}_{\beta'\alpha} = \left(\varphi_{\beta'}^{out}, \hat{S}\varphi_\alpha^{in}\right). \tag{2.73}$$

Thus, the coefficients b_β to find the scattered state Ψ^{out} after the collision, if initially the system was in the state Ψ^{in}, are the following

$$b_\beta = \sum_\alpha a_\alpha \hat{S}_{\beta\alpha}. \tag{2.74}$$

Equation (2.74) solves the problem: It expresses the coefficients b_β for the scattered wave function in terms of the coefficients a_α for the incident wave function. It is convenient to treat the quantities, $S_{\beta\alpha}$, of Eq. (2.74) a_α the elements of some matrix, $\hat{S}$, which is referred to as the scattering matrix [38, 39, 40].

If the coefficients a_α and b_β are collected into vector columns

$$\hat{b} = \begin{pmatrix} b_1 \\ b_{2.} \\ . \\ . \end{pmatrix}, \quad \hat{a} = \begin{pmatrix} a_1 \\ a_2 \\ . \\ . \end{pmatrix}, \tag{2.75}$$

the corresponding relation simplify to

$$\hat{b} = \hat{S}\hat{a}. \tag{2.76}$$

As we already mentioned, the scattering matrix elements, $\hat{S}_{\beta\alpha}$, are quantum-mechanical amplitudes for a particle in the state Ψ^{in} to be scattered into the state Ψ^{out}. The order of indices is important. We use the convention that the first index for the element $\hat{S}_{\beta\alpha}$ corresponds to a scattered state while the second index corresponds to an incident state.

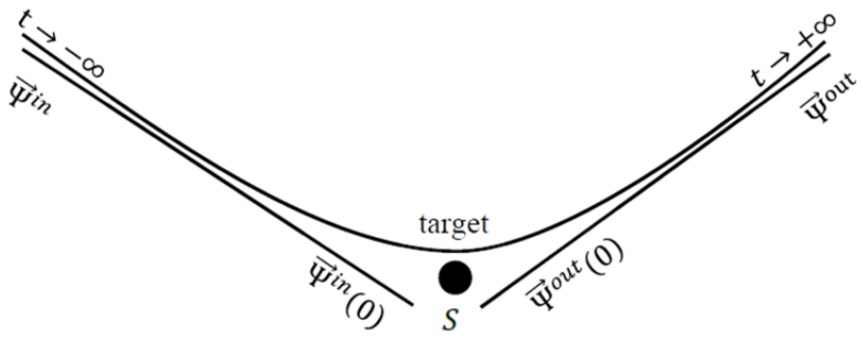

Fig-2.3: Asymptotic states in quantum mechanics

Chapter 3

$\hat{\text{S}}$-matrix formalism in 1D for relativistic particles of spin-s $(s = 0, 1/2)$

3.1 Introduction

The study of one-dimensional scattering problems also has its importance. Indeed, if in physics realistic cases are generally three-dimensional, the one-dimensional case fits into the framework of a model or approximation representing this reality. In what follows, we will adapt the formalism of the diffusion matrix to the one-dimensional case. This matrix finds its physical interpretation by linking it to the transmission and reflection coefficients.

This chapter is devoted to the one-dimensional formalism of the scattering matrix for relativistic particles of spin-s ($s = 0, 1/2$). First, we will try to find a way to gather in a unified writing the two equations of relativistic quantum mechanics, in a single equation that is the so-called wave equation for relativistic particles of spin-s. Then, we will construct the formalism of the scattering matrix $\hat{S}_{-s}$ for particles governed by the relativistic wave equation of spin-s in the presence of a localized electromagnetic field.

3.2 Relativistic wave equation of spin-s $(s = 0, 1/2)$

Remember that the relativistic wave equations which generalize the Schrödinger equation are the Klein-Gordon equation (1.54) , which allows among other things to describe the dynamics of relativistic particles having a spin-0.

$$\left(D^{\mu}D_{\mu} + m^{2}\right)\Psi_{0}\left(x,t\right) = 0, \tag{3.1}$$

and the Dirac equation (1.90) , which is used to describe massive particles of spin-1/2, which obey the Pauli exclusion principle,

$$\left\{\left(D^{\mu}D_{\mu} + m^{2}\right)\mathbb{I}_{4} + \frac{e}{2}\sigma^{\mu\nu}F_{\mu\nu}\right\}\Psi_{1/2}\left(x,t\right) = 0. \tag{3.2}$$

Note that eq. (3.1) differs from (3.2) by the presence of an additional term $\frac{e}{2}\sigma^{\mu\nu}F_{\mu\nu}$, which represents the interaction of the spin with the external electromagnetic field. In the case of zero field, the Dirac equation reduces to the Klein-Gordon equation.

By adopting for any matrix A the following notation:

$$(A)^{2s} = \begin{cases} 1 & \text{for} \quad s = 0, \\ A & \text{for} \quad s = 1/2. \end{cases} \tag{3.3}$$

In this case, equations (3.1) and (3.2) can be expressed by a single relation, called the spin-s relativistic wave equation $(s = 0.1/2)$ [38, 41]

$$\left\{\left[\left(\frac{\partial}{\partial t} + ieA_{0}\right)^{2} - \left(\overrightarrow{\nabla} - ie\overrightarrow{A}\right)^{2} + m^{2}\right]\mathbb{I}_{2^{2s}(2s+1)} + se\left(\sigma F\right)^{2s}\right\}\Psi_{s}\left(x,t\right) = 0. \tag{3.4}$$

Here, $\Psi_{s}\left(x,t\right)$ is a wave function with $2^{2s}\left(2s+1\right)$ components, and I_{d} is the unit matrix of dimension d and $\sigma F = \sigma^{\mu\nu}F_{\mu\nu}$.

For $s = 0$, eq. (3.4) reduces to the Klein-Gordon equation (3.1), and for $s = 1/2$, we thus obtain the Dirac equation (3.2).

We will define a current density and demonstrate that the current defined with the solutions of the relativistic wave equation of spin-s obeys a continuity equation. To do this, starting from equation (3.4), which can be written:

$$\left\{\left[\left(\overrightarrow{\partial}^{\mu} + ieA^{\mu}\right)\left(\overrightarrow{\partial}_{\mu} + ieA_{\mu}\right) + m^2\right]\mathbb{I}_{2^{2s}(2s+1)} + se\left(\sigma F\right)^{2s}\right\}\Psi_s\left(x,t\right) = 0, \tag{3.5}$$

where $\overrightarrow{\partial}^{\mu}$ is the right derivative. Then, taking the hermetic conjugate of the previous equation, multiplying the result on the left by $\left(\gamma^0\right)^{2s}$, and using the fact that

$$\left(\left(\sigma^{\mu\nu}\right)^{2s}\right)^{\dagger} = \left(\sigma^{\mu\nu}\right)^{2s}, \quad \left(\gamma^0\right)^{2s}\left(\sigma^{\mu\nu}\right)^{2s} = \left(\sigma^{\mu\nu}\right)^{2s}\left(\gamma^0\right)^{2s}, \tag{3.6}$$

we then get

$$\overline{\Psi}_s\left(x,t\right)\left\{\left[\left(\overleftarrow{\partial}^{\mu} - ieA^{\mu}\right)\left(\overleftarrow{\partial}_{\mu} - ieA_{\mu}\right) + m^2\right]\mathbb{I}_{2^{2s}(2s+1)} + se\left(\sigma F\right)^{2s}\right\} = 0, \tag{3.7}$$

where $\overline{\Psi}_s = \Psi_s^{\dagger}\left(\gamma^0\right)^{2s}$. Multiplying (3.5) on the left by $\overline{\Psi}_s$ and (3.7) on the right by Ψ_s, then subtracting the equations thus obtained, we get:

$$\frac{\partial J_s^0}{\partial t} + \overrightarrow{\nabla}.\overrightarrow{J}_s = 0, \tag{3.8}$$

the density J_s^0 and the current $\overrightarrow{J}_s$ are given by:

$$J_s^0 = \frac{1}{2im}\left(\overline{\Psi}_s\left(\frac{\partial\Psi_s}{\partial t}\right) - \left(\frac{\partial\overline{\Psi}_s}{\partial t}\right)\Psi_s\right) + \frac{e}{m}A^0\overline{\Psi}_s\Psi_s, \tag{3.9}$$

$$\overrightarrow{J}_s = \frac{i}{2m}\left(\overline{\Psi}_s\left(\overrightarrow{\nabla}\Psi_s\right) - \left(\overrightarrow{\nabla}\overline{\Psi}_s\right)\Psi_s\right) + \frac{e}{m}\overrightarrow{A}\overline{\Psi}_s\Psi_s, \tag{3.10}$$

the term $1/(2im)$ is introduced for convenience.

Similarly, it should be noted that the Lorentz invariant scalar product is defined as [15, 16],

$$\left(\Psi_s, \Psi_s\right) = \int\left\{\overline{\Psi}_s\left[\left(\frac{\partial}{\partial t} + eA^0\right)\Psi_s\right] - \left[\left(\frac{\partial}{\partial t} - eA^0\right)\overline{\Psi}_s\right]\Psi_s\right\}dx. \tag{3.11}$$

3.2.1 Weyl's representation

For the Dirac γ^μ matrices, we select the Weyl representation (also called the chiral representation). In this representation the γ^μ matrices have the following form [6, 42]

$$\gamma^0 = \begin{pmatrix} 0 & \mathbb{I}_2 \\ \mathbb{I}_2 & 0 \end{pmatrix}, \quad \gamma^i = \begin{pmatrix} 0 & -\sigma_i \\ \sigma_i & 0 \end{pmatrix}, \qquad i = 1, 2, 3 \tag{3.12}$$

where $\sigma = (\sigma_1, \sigma_2, \sigma_3)$ are the usual Pauli matrices.

Due to this choice of representation, the matrices $\sigma^{\mu\nu}$ are block diagonal, we find for (i, j, k) cyclic

$$\sigma^{0k} = i \begin{pmatrix} \sigma^k & 0 \\ 0 & -\sigma^k \end{pmatrix}, \quad \sigma^{ij} = \varepsilon_{ijk} \begin{pmatrix} \sigma^k & 0 \\ 0 & \sigma^k \end{pmatrix}, \tag{3.13}$$

where $\varepsilon_{ijk} = \frac{1}{2}(i-j)(j-k)(k-i)$ is the Levi-Civita tensor. If we write

$$\Psi_s(x,t) = \begin{pmatrix} \Psi_s^-(x,t) \\ \Psi_s^+(x,t) \end{pmatrix}. \tag{3.14}$$

Then, inserting the previous expression in eq. (3.4), explicitly developed in the Weyl representation, we get:

$$\begin{pmatrix} H_s^-(x,t) & 0 \\ 0 & H_s^+(x,t) \end{pmatrix} \begin{pmatrix} \Psi_s^-(x,t) \\ \Psi_s^+(x,t) \end{pmatrix} = 0, \tag{3.15}$$

here, $\Psi_s^-(x,t)$ and $\Psi_s^+(x,t)$ are spinors with 2^{2s} components, and the Hamiltonians $H_s^\mp$ are given by:

$$H_s^\mp = \left[\left(\frac{\partial}{\partial t} + ieA_0 \right)^2 - \left(\overrightarrow{\nabla} - ie\overrightarrow{A} \right)^2 + m^2 \right] \mathbb{I}_{2^{2s}} \pm 2ise \left(\overrightarrow{\sigma} \right)^{2s} \left(\overrightarrow{E} \pm i\overrightarrow{B} \right), \tag{3.16}$$

$\overrightarrow{E}$ and $\overrightarrow{B}$ are the electric and magnetic fields.

In the case of spin-1/2, Eq. (3.15) can split into two two-component equations as

$$\begin{pmatrix} H_{1/2}^{-} & 0 \\ 0 & H_{1/2}^{+} \end{pmatrix} \begin{pmatrix} \Psi_{1/2}^{-}(x,t) \\ \Psi_{1/2}^{+}(x,t) \end{pmatrix} = 0, \tag{3.17}$$

where $\Psi_{1/2}^{-}(x,t)$ and $\Psi_{1/2}^{+}(x,t)$ are two-component wave functions which permute under spatial inversion, and

$$H_{1/2}^{\mp} = \left[\left(\frac{\partial}{\partial t} + ieA_0 \right)^2 - \left(\overrightarrow{\nabla} - ie\overrightarrow{A} \right)^2 + m^2 \right] I_2 \pm ie\overrightarrow{\sigma} \left(\overrightarrow{E} \pm i\overrightarrow{B} \right), \tag{3.18}$$

For the spin-0, Eq. (3.15) reduces to

$$\begin{pmatrix} H_{0}^{-} & 0 \\ 0 & H_{0}^{+} \end{pmatrix} \begin{pmatrix} \Psi_{0}^{-}(x,t) \\ \Psi_{0}^{+}(x,t) \end{pmatrix} = 0, \tag{3.19}$$

where $\Psi_0^{-}(\overrightarrow{r},t)$ and $\Psi_0^{+}(\overrightarrow{r},t)$ are one-component wave functions, and,

$$H_0^{-} = H_0^{+} = H_0 = \left(\frac{\partial}{\partial t} + ieA_0 \right)^2 - \left(\overrightarrow{\nabla} - ie\overrightarrow{A} \right)^2 + m^2. \tag{3.20}$$

Note that there is redundancy because $H_0^{-} = H_0^{+}$ and consequently the equations of the system (3.19) are identical.

3.3 Ŝ-matrix formalism in 1D for particles of spin-s

We begin by considering a relativistic particle of mass m, energy E, charge e, and spin-s, evolving in a one-dimensional world. The particle, incident on a scattering center, evolves freely before reaching the region where it will undergo the effects of a localized electromagnetic field $A_\mu(x,t)$. We consider the case where $A_\mu(x,t)$ has the same limit when $x \to \pm\infty$, and following custom we adopt this value ($A_\mu(x,t) \overset{|x|\to+\infty}{\to} 0$). In this case, the evolution equation (3.15) is written as [38, 41]

$$\begin{aligned} \{ & \left[\left(\frac{\partial}{\partial t} + ieA_0(x,t) \right)^2 - \left(\overrightarrow{\nabla} - ie\overrightarrow{A}(x,t) \right)^2 + m^2 \right] \mathbb{I}_{2^{2s}} \\ & + se\left(\sigma F(x,t)\right)^{2s} \} \Psi_s(x,t) = 0, \end{aligned} \tag{3.21}$$

here $\overrightarrow{\nabla} = \overrightarrow{\nabla}_x = (d/dx)\overrightarrow{i}$. At large distance ($|x| \rightarrow \infty$), the field $A_\mu(x,t) \rightarrow 0$. Under these conditions, the Hamiltonian $H_s^{\mp}$ can be approximated by the Hamiltonian of a free particle, $H_s^{\mp,0} = \overrightarrow{p}^2/2m$. Therefore, the equation that governs the evolution of the relativistic particle of spin-s has a special class of solutions, called stationary states, where the time and space variables are separated. More precisely, the stationary solution of the time-dependent equation (3.14) has the following form

$$\Psi_s(x,t) = \Psi_s(x)e^{-iEt} = \begin{pmatrix} \Psi_s^-(x) \\ \Psi_s^+(x) \end{pmatrix} e^{-iEt}. \tag{3.22}$$

Far from the action zone of the scattering center, the field $A_\mu(x,t)$ must be understood as a perturbation of $H_s^{\mp,0}$ whose effects are negligible in the asymptotic regions of space. Asymptotically, the particle is considered free, the stationary solution $\Psi_s(x)$ is a linear combination of plane waves $e^{\pm ikx}$ ($k = \sqrt{E^2 - m^2} > 0$). More precisely, the wave function $\Psi_{s,L}^{\mp}(x)$ (arrival of $-\infty$) and $\Psi_{s,R}^{\mp}(x)$ (arrival of $+\infty$) behave as follows [38, 39, 43]:

$$\Psi_{s,L}^{\mp}(x) = \begin{cases} 1_s^{\mp}e^{ikx} + R_{s,L}^{\mp}e^{-ikx} & x \rightarrow -\infty, \\ T_{s,L}^{\mp}e^{ikx} & x \rightarrow +\infty, \end{cases}$$
$$\Psi_{s,R}^{\mp}(x) = \begin{cases} 1_s^{\mp}e^{-ikx} + R_{s,R}^{\mp}e^{ikx} & x \rightarrow +\infty, \\ T_{s,R}^{\mp}e^{-ikx} & x \rightarrow -\infty. \end{cases} \tag{3.23}$$

Here, $T_{s,L,R}^{\mp}$, $R_{s,L,R}^{\mp}$ and $1_s^{\mp}$ are vectors with 2^{2s} components. $\left(T_{s,L}^{\mp}, R_{s,L}^{\mp}\right)$,and $\left(T_{s,R}^{\mp}, R_{s,R}^{\mp}\right)$ represent the transmission and reflection coefficients left and right respectively, given by:

$$\mathbb{T}_s = \frac{\left(\left|T_{s,L,R}^-\right|^2 + \left|T_{s,L,R}^+\right|^2\right)}{|1_s^-|^2 + |1_s^+|^2}, \quad \mathbb{R}_s = \frac{\left(\left|R_{s,L,R}^-\right|^2 + \left|R_{s,L,R}^+\right|^2\right)}{|1_s^-|^2 + |1_s^+|^2}. \tag{3.24}$$

For the spin-0, $H_0^- = H_0^+$ the equations of the system (3.19) are identical, and consequently, $T_{0,L,R}^- = T_{0,L,R}^+$, $R_{0,L,R}^- = R_{0,L,R}^+$ and $1_0^- = 1_0^+$.

we examine now the general problem. The solution can be written as

$$\Psi_s^{\mp}(x) = \begin{cases} \Psi_s^{\mp}(out,+\infty)e^{ikx} + \Psi_s^{\mp}(in,+\infty)e^{-ikx} & x \longrightarrow +\infty, \\ \Psi_s^{\mp}(in,-\infty)e^{ikx} + \Psi_s^{\mp}(out,-\infty)e^{-ikx} & x \longrightarrow -\infty, \end{cases} \tag{3.25}$$

where $\Psi_s^{\mp}(in, out, \pm\infty)$ are vectors of dimension 2^{2s}. We can say that the vectors $(\Psi_s^{\mp}(in, -\infty), \Psi_s^{\mp}(in, +\infty))$ are the incoming amplitudes (from the left and from the right respectively), and the vectors $(\Psi_s^{\mp}(out, +\infty), \Psi_s^{\mp}(out, -\infty))$ are the outgoing amplitudes (to the right and to the left respectively).

We can see that the spinner $\Psi_s^{\mp}(x)$ can be further written in the form

$$\Psi_s^{\mp}(x) = \Psi_s^{\mp,in}(x) + \Psi_s^{\mp,out}(x), \tag{3.26}$$

where $\Psi_s^{\mp,in}(x)$ and $\Psi_s^{\mp,out}(x)$ are respectively the incident and outgoing parts, given by:

$$\begin{cases} \Psi_s^{\mp,in}(x) = \Psi_s^{\mp}(in, -\infty)\, e^{ikx}\theta(-x) + \Psi_s^{\mp}(in, +\infty)\, e^{-ikx}\theta(x) \\ \Psi_s^{\mp,out}(x) = \Psi_s^{\mp}(out, -\infty)\, e^{-ikx}\theta(-x) + \Psi_s^{\mp}(out, +\infty)\, e^{ikx}\theta(x), \end{cases} \tag{3.27}$$

where $\theta(x)$ is the usual Heaviside function ($\theta(x < 0) = 0$, $\theta(x > 0) = 1$).

A suitable way to describe scattering and reactions is to introduce the scattering operator $\hat{S}_{-\mathbf{s}}$, whose matrix elements form the scattering matrix $\hat{S}_{-s}$. According to (2.66), this operator connects the initial state $\Psi_s^{in}(x)$ with the final state $\Psi_s^{out}(x)$ by means of the relation [38, 39, 41],

$$\Psi_s^{out}(x) = \hat{\mathbf{S}}_{-\mathbf{s}}\Psi_s^{in}(x). \tag{3.28}$$

Or in matrix form, the $\hat{S}$-matrix relates the outgoing wave to the incoming wave by the relation,

$$\begin{pmatrix} \Psi_s^{-}(out, +\infty) \\ \Psi_s^{+}(out, +\infty) \\ \Psi_s^{-}(out, -\infty) \\ \Psi_s^{+}(out, -\infty) \end{pmatrix} = \begin{pmatrix} \hat{s}_{11} & \hat{s}_{12} & \hat{s}_{13} & \hat{s}_{14} \\ \hat{s}_{21} & \hat{s}_{22} & \hat{s}_{23} & \hat{s}_{24} \\ \hat{s}_{31} & \hat{s}_{32} & \hat{s}_{33} & \hat{s}_{34} \\ \hat{s}_{41} & \hat{s}_{42} & \hat{s}_{43} & \hat{s}_{44} \end{pmatrix} \begin{pmatrix} \Psi_s^{-}(in, -\infty) \\ \Psi_s^{+}(in, -\infty) \\ \Psi_s^{-}(in, +\infty) \\ \Psi_s^{+}(in, +\infty) \end{pmatrix}, \tag{3.29}$$

where the elements $\hat{s}_{ij}$ are block-matrices $(2^{2s} \times 2^{2s})$. In the case of spin-0 $H_0^- = H_0^+$, the system (3.29) reduces to

$$\begin{pmatrix} \Psi_0(out, +\infty) \\ \Psi_0(out, -\infty) \end{pmatrix} = \begin{pmatrix} s_{11} & s_{13} \\ s_{31} & s_{33} \end{pmatrix} \begin{pmatrix} \Psi_0(in, -\infty) \\ \Psi_0(in, +\infty) \end{pmatrix}, \tag{3.30}$$

where $\Psi_0\left(in, out, \pm\infty\right)$ and s_{ij} $(i, j = 1, 2)$ are coefficients. In the case of a free particle $A_\mu\left(x, t\right) = 0$, the state vectors $\Psi_s^{\mp}\left(out, \pm\infty\right) \rightarrow \Psi_s^{\mp}\left(in, \mp\infty\right)$. In this case, the $\hat{S}$-matrix then becomes the unit matrix $\mathbb{I}_{2^{(2s+1)}(2s+1)}$.

Combining (3.23) and (3.25), and taking into account (3.29), we have

$$\hat{S}_{-\mathbf{s}} = \begin{pmatrix} \hat{s}_{11} & \hat{s}_{12} & \hat{s}_{13} & \hat{s}_{14} \\ \hat{s}_{21} & \hat{s}_{22} & \hat{s}_{23} & \hat{s}_{24} \\ \hat{s}_{31} & \hat{s}_{32} & \hat{s}_{33} & \hat{s}_{34} \\ \hat{s}_{41} & \hat{s}_{42} & \hat{s}_{43} & \hat{s}_{44} \end{pmatrix} = \begin{pmatrix} \check{T}_{s,L}^{--} & \check{T}_{s,L}^{-+} & \check{R}_{s,R}^{--} & \check{R}_{s,R}^{-+} \\ \check{T}_{s,L}^{+-} & \check{T}_{s,L}^{++} & \check{R}_{s,R}^{+-} & \check{R}_{s,R}^{++} \\ \check{R}_{s,L}^{--} & \check{R}_{s,L}^{-+} & \check{T}_{s,R}^{--} & \check{T}_{s,R}^{-+} \\ \check{R}_{s,L}^{+-} & \check{R}_{s,L}^{++} & \check{T}_{s,R}^{+-} & \check{T}_{s,R}^{++} \end{pmatrix}, \tag{3.31}$$

where $\left(\check{T}_{s,L}^{\mp\mp}, \check{T}_{s,L}^{\mp\pm}, \check{T}_{s,R}^{\mp\mp}, \check{T}_{s,R}^{\mp\pm}\right)$ and $\left(\check{R}_{s,L}^{\mp\mp}, \check{R}_{s,L}^{\mp\pm}, \check{R}_{s,R}^{\mp\mp}, \check{R}_{s,R}^{\mp\pm}\right)$ are blocks of matrices $(2^{2s} \times 2^{2s})$, representing the transmission and reflection coefficients left and right respectively, relative to the wave equation of relativistic particles of spin-s.

3.3.1 Calculation of the $\hat{\mathbf{S}}$-matrix

In quantum mechanics, particles are described by wave functions. Wave functions depend on the space-time coordinates and the variable related to the spin of the particles. Each of the wave functions that describe particles of given spin satisfies a definite equation that is covariant (does not change form) with respect to the Lorentz transformations.

Let us elucidate how the wave function is transformed in discrete Lorentz transformations when equation (3.21) must respect the covariance condition. More precisely, we will study a very important symmetry in particle physics, the $C_sP_sT_s$ symmetry [6, 44, 45], which is the "product" of three fundamental symmetries: C_s is the transformation that associates its antiparticle with any particle, P_s is the one that associates its image in a mirror and T_s is the one that reverses the direction of time.

We begin the study of discrete Lorentz transformations with the operation of reversing the coordinates of space, that is, the parity transformation P_s. When reflecting space $(x, t) \rightarrow (-x, t)$, $\partial/\partial t \rightarrow \partial/\partial t' = \partial/\partial t$, $\overrightarrow{\nabla} \rightarrow \overrightarrow{\nabla}' = -\overrightarrow{\nabla}$, and consequently, the electromagnetic field $A_\mu\left(x, t\right)$, the coupling term (σF) and the wave function (σF) are transformed as follows [6, 44, 45]

$$A_\mu \rightarrow A'_\mu = \left(A_0, -\overrightarrow{A}\right), \qquad \Psi_s(x,t) \rightarrow \Psi_s(-x,t),$$
$$(\sigma F) \rightarrow (\sigma F)' = -\sigma^{0i}F_{0i} + \sigma^{ij}F_{ij}, \quad i,j = 1 \rightarrow 3. \tag{3.32}$$

By inserting these expressions into Eq. (3.21), multiply the result on the left by P_s, and using $P_s^{-1}P_s = \mathbb{I}_{2^{2s}(2s+1)}$, one finds:

$$P_s\{\left(\left(\frac{\partial}{\partial t} + ieA_0\right)^2 - (\overrightarrow{\nabla} - ie\overrightarrow{A})^2 + m^2\right)\mathbb{I}_{2^{2s}(2s+1)} +$$
$$+se\left(-\sigma^{0i}F_{0i} + \sigma^{ij}F_{ij}\right)^{2s}\}P_s^{-1}\Psi^{P_s}(x,t) = 0\,, \tag{3.33}$$

where

$$\Psi_s^{P_s}(x,t) = P_s\Psi_s(-x,t)\,. \tag{3.34}$$

Starting from the fact that due to the invariance with respect to the reflection of space, equations (3.21) and (3.33) must coincide. Comparing these two equations, we find that the operator P_s must satisfy the following conditions:

$$P_s\left(\sigma^{0l}\right)_s^{2s}P_s^{-1} = \left(-\sigma^{0l}\right)^{2s}, \quad P_s\left(\sigma^{ij}\right)^{2s}P_s^{-1} = \left(\sigma^{ij}\right)^{2s}. \tag{3.35}$$

The condition (3.35) is satisfied by the operator $P_s = \eta_{p_s}\left(\gamma^0\right)^{2s}$, where η_{p_s} is an arbitrary complex number. We will subsequently take $\eta_{p_s} = i$. With this phase choice, using the relations (3.25), (3.29), and (3.34), we can easily ensure that $\Psi_s^{P_s}(x,t)$ is obtained from $\Psi_s(x,t)$ by substituting

$$\Psi_s^{\mp}(out,+\infty) \leftrightarrow i\Psi_s^{\pm}(out,-\infty)\,,\;\; \Psi_s^{\mp}(in,+\infty) \leftrightarrow i\Psi_s^{\pm}(in,-\infty)\,. \tag{3.36}$$

In matrix form, by inserting this last expression in (3.29), we obtain the expression

$$(\sigma_1 \otimes P_s)\left(\hat{S}_{-s}\right)(\sigma_1 \otimes P_s)^{-1} = \hat{S}_{-s}. \tag{3.37}$$

The symbol $\otimes$ is the Kronecker product of the matrices. From (3.37), by a simple calculation, we deduce

$$\hat{s}_{11} = \hat{s}_{44}, \quad \hat{s}_{22} = \hat{s}_{33}, \quad \hat{s}_{13} = \hat{s}_{42}, \quad \hat{s}_{31} = \hat{s}_{24}, \quad \hat{s}_{12} = \hat{s}_{43},$$
$$\hat{s}_{21} = \hat{s}_{34}, \quad \hat{s}_{23} = \hat{s}_{32}, \quad \hat{s}_{14} = \hat{s}_{41}. \tag{3.38}$$

Let's now change $(x, t) \to (x, -t)$. This transformation does not change the spatial coordinates, they remain invariable under these conditions: $x \to x^{'} = x$, but changes the sign of the velocities and, consequently, that of the impulses and the kinetic moment $\overrightarrow{L} \to -\overrightarrow{L}$, and $\overrightarrow{s} \to -\overrightarrow{s}$. In this operation the electromagnetic field $A_\mu(x, t)$, the coupling term between the spin of the particle and the electromagnetic field (σF), and the wave function $\Psi_s(x, t)$ are transformed as [6, 44, 45]

$$A_\mu \to A_\mu^{'} = \left(A_0, -\overrightarrow{A}\right), \quad \Psi_s(x, t) \to \Psi_s(x, -t),$$
$$(\sigma F) \to (\sigma F)^{'} = \sigma^{0l} F_{0l} - \sigma^{ij} F_{ij}. \tag{3.39}$$

If we change $t \to -t$, and taking into account (3.39), equation (3.21) transforms into:

$$\{\left(\left(-\frac{\partial}{\partial t} + ieA_0\right)^2 - (\overrightarrow{\nabla} + ie\overrightarrow{A})^2 + m^2\right)\mathbb{I}_{2^{2s}(2s+1)} +$$
$$+ se\left(\sigma^{0k} F_{0k} - \sigma^{ij} F_{ij}\right)^{2s}\}\Psi_s(x, -t) = 0. \tag{3.40}$$

Furthermore, if there is invariance when changing $t \to -t$, a particle and a "reflected" particle in time must be described symmetrically by the same theory, i.e., the wave functions of the particle and the "reflected" particle in time must satisfy the same equation. To obtain Eq. (3.21) again, take the complex conjugate of Eq. (3.40) and multiply the result on the left by the time reversal operator T_s, and taking into account $T_s^{-1} T_s = \mathbb{I}_{2^{2s}(2s+1)}$, we obtain

$$T_s\{\left(\left(\frac{\partial}{\partial t} + ieA_0\right)^2 - (\overrightarrow{\nabla} - ie\overrightarrow{A})^2 + m^2\right)\mathbb{I}_{2^{2s}(2s+1)} +$$
$$se\left(\left(\sigma^{0l}\right)^* F_{0l} - \left(\sigma^{ij}\right)^* F_{ij}\right)^{2s}\} T_s^{-1} \Psi_s^{T_s}(x, t) = 0, \tag{3.41}$$

where

$$\Psi_s^{T_s}(x,t) = T_s \Psi_s^*(x,-t). \tag{3.42}$$

We want the function $\Psi_s^{T_s}(x,t)$ to satisfy the same equation as $\Psi_s(x,t)$. Comparing (3.21) to (3.41), they coincide if the operator T_s that changes $(x,t) \to (x,-t)$ satisfies the relations:

$$T_s \left(\left(\sigma^{0l} \right)^* \right)^{2s} T_s^{-1} = \left(\sigma^{0l} \right)^{2s}, \ T_s \left(\left(\sigma^{ij} \right)^* \right)^{2s} T_s^{-1} = \left(-\sigma^{ij} \right)^{2s}. \tag{3.43}$$

To find the form of the operator T_s, let us use the properties of the matrices $\sigma^{\mu\nu}$:

$$\left(\sigma^{0k} \right)^* = \begin{cases} -\sigma^{0k} \ \text{ if } k \neq 2 \\ \sigma^{02} \quad \text{if} \quad k = 2 \end{cases}, \ \left(\sigma^{ij} \right)^* = \begin{cases} -\sigma^{ij} \text{ if } \ i \neq 2 \text{ and } \ j \neq 2 \\ \sigma^{ij} \ \text{ if } \ \ i = 2 \ \text{ where } \ j = 2 \end{cases}. \tag{3.44}$$

Considering the relations (3.44), then conditions (3.43) are verified by the operator $T_s = \eta_t \left(\gamma^1 \gamma^3 \right)^{2s}$, with the arbitrary constant $\eta_t = i$.

On the other hand, using (3.25), (3.29), and (3.42), one can easily ensure that passing from $\Psi_s(x,t)$ to $\Psi_s^{T_s}(x,t)$ gives

$$\Psi_s^{\mp}(out, +\infty) \leftrightarrow -\sigma_2 \Psi_s^{\mp}(in, +\infty), \quad \Psi_s^{\mp}(out, -\infty) \leftrightarrow -\sigma_2 \Psi_s^{\mp}(in, -\infty). \tag{3.45}$$

Further, by using

$$\begin{aligned} \Psi_s^{T_s,out}(x,t) = \hat{S}_{-s} \Psi_s^{T_s,in}(x,t) = \left(\mathbb{I}_{2^{2s}} \otimes T_s \right) \Psi_s^{*,out}(x,-t), \\ \Psi_s^{T_s,in}(x,t) = \left(\mathbb{I}_{2^{2s}} \otimes T_s \right) \Psi_s^{*,in}(x,-t), \end{aligned} \tag{3.46}$$

and

$$\Psi_s^{*,out}(x,-t) = \hat{S}_{D-s}^* \Psi_s^{*,in}(x,-t) \tag{3.47}$$

In matrix form, with (3.29), (3.45), (3.46) and (3.47), we arrive at the expression

$$\left(S_{-s}\right)\left(\sigma_1 \otimes T_s\right)\left(S^{\star}_{-s}\right)\left(\sigma_1 \otimes T_s\right)^{-1} = \mathbb{I}_{2^{2s+1}(2s+1)}. \tag{3.48}$$

The charge conjugation operation will now be performed. This operation transforms a particle into its antiparticle of identical mass and spin, carrying the same momentum but changing the sign of all other additive quantum numbers: electric charge, baryon number, strangeness, leptonic numbers, etc.

By charge conjugation $e \to -e$, the electromagnetic field $A_\mu(x,t)$ and the coupling term (σF) are transformed as follows [6, 44, 45]

$$A_\mu \to A^{'}_\mu = -A_\mu, \quad (\sigma F) \to (\sigma F)^{'} = -\sigma^{\mu\nu} F_{\mu\nu}. \tag{3.49}$$

To understand how the wave function $\Psi_s(x,t)$ is transformed during the charge conjugation operation, In equation (3.21), we do the substitution $e \to -e$, then, taking the hermitic conjugate, and taking into account (3.49), the result is:

$$\Psi^{\dagger}_s(x,t)\{\left(\left(\frac{\partial}{\partial t} + ieA_0\right)^2 - (\overrightarrow{\nabla} - ie\overrightarrow{A})^2 + m^2\right)\mathbb{I}_{2^{2s}(2s+1)} \\ -se\left(\left(\sigma^{0l}\right)^{\dagger} F_{0l} + \left(\sigma^{ij}\right)^{\dagger} F_{ij}\right)^{2s}\} = 0. \tag{3.50}$$

After multiplying both sides of equation (3.50) on the right by $\left(\gamma^0\right)^{2s}$, and taking into account the relations

$$\left(\sigma^{ij}\right)^{2s}\left(\gamma^0\right)^{2s} = \left(\gamma^0\right)^{2s}\left(\sigma^{ij}\right)^{2s}, \quad \left(\sigma^{0l}\right)^{2s}\left(\gamma^0\right)^{2s} = -\left(\gamma^0\right)^{2s}\left(\sigma^{0l}\right)^{2s} \\ \left(\left(\sigma^{0l}\right)^{2s}\right)^{\dagger} = -\left(\sigma^{0l}\right)^{2s}, \quad \left(\left(\sigma^{ij}\right)^{2s}\right)^{\dagger} = \left(\sigma^{ij}\right)^{2s}, \tag{3.51}$$

equation (3.50) becomes:

$$\overline{\Psi}_s(x,t)\{\left(\left(\frac{\partial}{\partial t} + ieA_0\right)^2 - (\overrightarrow{\nabla} - ie\overrightarrow{A})^2 + m^2\right)\mathbb{I}_{2^{2s}(2s+1)} + \\ -se\left(\left(\sigma^{0l}\right)^{\dagger} F_{0l} + \left(\sigma^{ij}\right)^{\dagger} F_{ij}\right)^{2s}\} = 0, \tag{3.52}$$

where $\overline{\Psi}_s = \Psi_s^{\dagger} (\gamma^0)^{2s}$ and $\Psi^{\dagger} = (\Psi_s^{\star})^T$. This last equation differs from (3.21) by the change of sign in front of $(\sigma F)^{2s}$. To establish the form of the operator C_s, let us take the transpose of both members of equation (3.52), multiply the result on the left by C_s and with $C_s^{-1} C_s = I_{2^{2s}(2s+1)}$, we obtain

$$C_s \{ \left(\left(\frac{\partial}{\partial t} + ieA_0 \right)^2 - (\overrightarrow{\nabla} - ie\overrightarrow{A})^2 + m^2 \right) \mathbb{I}_{2^{2s}(2s+1)}$$
$$-se \left(\left(\sigma^{0l}\right)^T F_{0l} + \left(\sigma^{ij}\right)^T F_{ij} \right)^{2s} \} C_s^{-1} \Psi_s^{C_s} (x,t) = 0, \tag{3.53}$$

Under these conditions, we see that if $\Psi_s (x,t)$ is a solution of (3.21), the function $\Psi_s^{C_s} (x,t)$ such that

$$\Psi_s^{C_s} (x,t) = C_s \overline{\Psi}_s^T (x,t), \tag{3.54}$$

is another one. For equation (3.53) to be reduced to (3.21), the operator C_s must satisfy the following conditions

$$C_s \left(\left(\sigma^{0l}\right)^T \right)^{2s} C_s^{-1} = - \left(\sigma^{0l}\right)^{2s}, \quad C_s \left(\left(\sigma^{ij}\right)^T \right)^{2s} C_s^{-1} = - \left(\sigma^{ij}\right)^{2s}. \tag{3.55}$$

Then the conditions (3.55) are verified by the operator $C_s = \eta_{C_s} (\gamma^2 \gamma^0)^{2s}$ with the arbitrary constant $\eta_{C_s} = i$. Furthermore, with (3.25), (3.29), and (3.54), we can easily ensure that the transition from $\Psi_s (x,t)$ to $\Psi_s^{C_s} (x,t)$ is obtained by changing

$$\Psi_s^{\mp} (out, +\infty) \leftrightarrow \mp i\sigma_2 \left(\Psi_s^{\pm} (in, +\infty)\right)^*,$$
$$\Psi_s^{\mp} (out, -\infty) \leftrightarrow \mp i\sigma_2 \left(\Psi_s^{\pm} (in, -\infty)\right)^*. \tag{3.56}$$

In matrix form, by using

$$\Psi_s^{C_s,in} (x,t) = \left(\mathbb{I}_{2^{2s}} \otimes C_s\right) \overline{\Psi}_s^{T,in} (x,t), \; \Psi_s^{*,out} (x,t) = \hat{S}_{-s}^* \Psi_s^{*,in} (x,t),$$
$$\Psi_s^{C_s,out} (x,t) = \hat{S}_{-s} \Psi_s^{C_s,in} (x,t) = \left(\mathbb{I}_{2^{2s}} \otimes C_s\right) \overline{\Psi}_s^{T,out} (x,t), \tag{3.57}$$

then, by combining the previous expression with (3.25), (3.29) , and (3.57), we get the expression

$$\left(\hat{S}_{-s}\right)(\sigma_1 \otimes C_s)\left(\hat{S}^{\star}_{-s}\right)(\sigma_1 \otimes C_s)^{-1} = \mathbb{I}_{2^{2s+1}(2s+1)}. \tag{3.58}$$

Furthermore, the charge conservation allows to write:

$$\langle \Psi_s^{out} | \Psi_s^{out} \rangle = \langle \Psi_s^{in} | \Psi_s^{in} \rangle \tag{3.59}$$

By making the substitution

$$\overline{\Psi}_s^{out} = \left(\Psi_s^{in}\right)^{\dagger} \hat{S}^{\dagger}_{-s}\left(\mathbb{I}_{2^{2s}} \otimes \left(\gamma^0\right)^{2s}\right), \quad \overline{\Psi}_s^{in} = \left(\Psi_s^{in}\right)^{\dagger}\left(\mathbb{I}_{2^{2s}} \otimes \left(\gamma^0\right)^{2s}\right), \tag{3.60}$$

in (3.59), we easily verify that the matrix $\hat{S}_{-s}$ satisfies:

$$\left(\mathbb{I}_{2^{2s}} \otimes \left(\gamma^0\right)^{2s}\right)\left(\hat{S}^{\dagger}_{-s}\right)\left(\mathbb{I}_{2^{2s}} \otimes \left(\gamma^0\right)^{2s}\right)\left(\hat{S}_{-s}\right) = \mathbb{I}_{2^{(2s+1)}(2s+1)}. \tag{3.61}$$

By combining the relations deduced from the conservation of current, the invariances with respect to the reflection operations of the space P_s (parity), the time reversal T_s, and the charge conjugation C_s, we obtain:

$$\begin{gathered} \hat{s}_{11} = \hat{s}_{44} = \check{T}_s^{+}, \ \hat{s}_{22} = \hat{s}_{33} = \check{T}_s^{-}, \ \hat{s}_{13} = \hat{s}_{42} = \check{R}_s^{+}, \ \hat{s}_{24} = \hat{s}_{31} = \check{R}_s^{-} \\ \hat{s}_{12} = \hat{s}_{21} = \hat{s}_{23} = \hat{s}_{32} = \hat{s}_{14} = \hat{s}_{41} = \hat{s}_{34} = \hat{s}_{43} = 0. \end{gathered} \tag{3.62}$$

By inserting (3.62) into (3.31), we obtain the scattering matrix of a relativistic particle of mass m, energy E, charge e, and spin-s $(s = 0.1/2)$ by a localized electromagnetic field $A_{\mu}(x,t)$.

$$\hat{S}_{-s} = \begin{pmatrix} \check{T}_s^{+} & 0 & \check{R}_s^{+} & 0 \\ 0 & \check{T}_s^{-} & 0 & \check{R}_s^{-} \\ \check{R}_s^{-} & 0 & \check{T}_s^{-} & 0 \\ 0 & \check{R}_s^{+} & 0 & \check{T}_s^{+} \end{pmatrix}, \tag{3.63}$$

where $\check{T}_s^{\pm}$ and $\check{R}_s^{\pm}$ are blocks of matrices $(2^{2s} \times 2^{2s})$, which represent the transmission and reflection coefficients left and right respectively, given by

$$\check{T}_s^{\pm} \begin{pmatrix} t_s & \pm\omega_s \\ \pm\omega_s & t_s \end{pmatrix}, \quad \check{R}_s^{\pm} = \begin{pmatrix} r_s & \pm\rho_s \\ \pm\rho_s & r_s \end{pmatrix}. \tag{3.64}$$

t_s, r_s,ρ_s and ω_s are functions of E, A_μ, and m. For $s = 0$, we have $\rho_0 = \omega_0 = 0$. The matrix $\hat{S}_{-0}$ is symmetric because $\check{T}_0^+ = \check{T}_0^-$ and $\check{R}_0^+ = \check{R}_0^-$. It is pseudo-symmetric for $s = 1/2$ because we have $\sigma_3 \check{T}_{1/2}^+ \sigma_3 = \check{T}_{1/2}^-$ and $\sigma_3 \check{R}_{1/2}^+ \sigma_3 = \check{R}_{1/2}^-$. This last property is specific to the spin of the particles.

On the other hand, by comparing (3.63) with (3.31), we can easily extract

$$\begin{aligned} \check{T}_s^{\pm} = \check{T}_{s,L}^{\mp\mp} = \check{T}_{s,R}^{\pm\pm}, \quad \check{R}_s^{\pm} = \check{R}_{s,L}^{\pm\pm} = \check{R}_{s,R}^{\mp\mp} \\ \check{T}_{s,L}^{\mp\pm} = \check{T}_{s,R}^{\mp\pm} = \check{R}_{s,L}^{\mp\pm} = \check{R}_{s,R}^{\mp\pm} = 0. \end{aligned} \tag{3.65}$$

The previous expression predicts that the probabilities of transmission or reflection for a particle coming from the left are similar to those for a particle coming from the right.

Using the charge conservation condition (3.59), we find

$$\begin{aligned} \left(\check{T}_s^+\right)^\dagger \check{R}_s^- + \left(\check{R}_s^-\right)^\dagger \check{T}_s^+ = \left(\check{T}_s^-\right)^\dagger \check{R}_s^+ + \left(\check{R}_s^+\right)^\dagger \check{T}_s^- = 0\,, \\ \left(\check{T}_s^+\right)^\dagger \check{T}_s^- + \left(\check{R}_s^-\right)^\dagger \check{R}_s^+ = \mathbb{I}_{2^{2s}}\,. \end{aligned} \tag{3.66}$$

3.3.2 $\hat{S}_{-s}$−matrix in the partial waves base

In quantum mechanics, the special mathematical nature of kinetic momentum operator $\overrightarrow{J}_s$ ($\overrightarrow{J}_s = \overrightarrow{L} + \overrightarrow{S}$), has several very special consequences. On one side, the eigenvalues of the observables that are its components and modulus, are quantized. On the other side, only the square of its modulus $\overrightarrow{J}_s^2$ and its component J_{z-s} form, with the Hamiltonian H_s, a complete set of commuting observables. The eigenstates corresponding to these operators form a basis of the space of states. They are called spherical harmonics or partial waves [25, 27].

We now want to express the $\hat{S}_{-s}$−matrix in the partial-waves representation (even and odd waves), in which $\hat{S}_{-s}$ becomes diagonal. To illustrate this point, we apply a unitary transformation on $\hat{S}_{-s}$ so as to obtain a new $\hat{M}_{-s}-$matrix. This can be done by introducing the hermetic operator $\hat{U}_s$, defined by [38, 39, 41]:

$$\varkappa_s^{in}(x) = \hat{U}_s \Psi_s^{in}(x), \quad \varkappa_s^{out}(x) = \hat{U}_s \Psi_s^{out}(x), \tag{3.67}$$

where $\varkappa_s^{in,out}(x) = \left(\varkappa_s^{-,in,out}(x), \varkappa_s^{+,in,out}(x)\right)^T$ are $2^{2s}(2s+1)$ component wave functions. $\hat{U}_s$ is the square matrix $\left(2^{(2s+1)}(2s+1) \times 2^{(2s+1)}(2s+1)\right)$, given by:

$$\hat{U}_s = \frac{1}{\sqrt{2}} \begin{pmatrix} \mathbb{I}_{2^{2s}} & 0 & \mathbb{I}_{2^{2s}} & 0 \\ 0 & \mathbb{I}_{2^{2s}} & 0 & \mathbb{I}_{2^{2s}} \\ i\mathbb{I}_{2^{2s}} & 0 & -i\mathbb{I}_{2^{2s}} & 0 \\ 0 & i\mathbb{I}_{2^{2s}} & 0 & -i\mathbb{I}_{2^{2s}} \end{pmatrix}. \tag{3.68}$$

After some manipulations of expressions (3.25), (3.29), (3.67) and (3.68), we find

$$\varkappa_s^{out}(x) = \hat{U}_s \hat{S}_{-s} \hat{U}_s^{\dagger} \varkappa_s^{in}(x) = \hat{M}_{-s} \varkappa_s^{in}(x). \tag{3.69}$$

where $\hat{M}_{-s}$ is the scattering matrix in the representation of partial waves, given by:

$$\hat{M}_{-s} = \begin{pmatrix} \overline{\check{T}}_s^{+} & 0 & i\overline{\check{R}}_s^{-} & 0 \\ 0 & \overline{\check{T}}_s^{+} & 0 & -i\overline{\check{R}}_s^{-} \\ i\overline{\check{R}}_s^{+} & 0 & \overline{\check{T}}_s^{-} & 0 \\ 0 & -i\overline{\check{R}}_s^{+} & 0 & \overline{\check{T}}_s^{-} \end{pmatrix}, \tag{3.70}$$

and

$$\overline{\check{T}}_s^{\pm} = \begin{pmatrix} t_s \pm r_s & 0 \\ 0 & t_s \pm r_s \end{pmatrix}, \quad \overline{\check{R}}_s^{\pm} = \begin{pmatrix} 0 & \rho_s \pm \omega_s \\ \rho_s \pm \omega_s & 0 \end{pmatrix}. \tag{3.71}$$

Equation (3.69) can be written in matrix form:

$$\begin{pmatrix} \varkappa_s^{-}(out, +\infty) \\ \varkappa_s^{+}(out, +\infty) \\ \varkappa_s^{-}(out, -\infty) \\ \varkappa_s^{+}(out, -\infty) \end{pmatrix} = \hat{M}_{-s} \begin{pmatrix} \varkappa_s^{-}(in, -\infty) \\ \varkappa_s^{+}(in, -\infty) \\ \varkappa_s^{-}(in, +\infty) \\ \varkappa_s^{+}(in, +\infty) \end{pmatrix}. \tag{3.72}$$

Using the current conservation property (3.59), and introducing the phase shifts relative to even waves δ_s^0 and odd waves δ_s^1, we can finally express (3.70) in a more explicit form [38, 39, 41]

$$\hat{M}_{-s} = \mathbb{I}_{2^{2s(2s+1)}} \otimes \begin{pmatrix} e^{2i\delta_s^0} & 0 \\ 0 & e^{2i\delta_s^1} \end{pmatrix}, \tag{3.73}$$

where δ_s^l, $l = 0, 1$, represents respectively the phase shifts of the even and odd wave functions and they are given explicitly by:

$$e^{2i\delta_s^l} = t_s + (-1)^l \sqrt{\omega_s^2 + r_s^2 - \rho_s^2}. \tag{3.74}$$

3.3.3 Phase shift method

The idea of the phase shift method consists in considering the minimal changes in the exact asymptotic development of the free case. The simplest is to add a phase shift. In other words, we assume a priori that the effect of the scattering field is reduced to giving a specific phase shift to each partial wave of the free particle.

To illustrate this point, let's combine the equations (3.27) , (3.29) , and (3.68), and use $\hat{U}_s \hat{U}_s^\dagger = \hat{U}_s^\dagger \hat{U}_s = \mathbb{I}_{2^{(2s+1)}(2s+1)}$, we express the vectors $\Psi_s^\mp(in, \mp\infty)$ and $\Psi_s^\mp(out, \pm\infty)$ as a function of $\varkappa_s^\mp(in, \mp\infty)$ and $\varkappa_s^\mp(out, \pm\infty)$, it becomes:

$$\begin{aligned} \Psi_s^\mp(out, \pm\infty,) &= \frac{1}{\sqrt{2}} \left(\varkappa_s^\mp(out, +\infty) \mp i\varkappa_s^\mp(out, -\infty) \right), \\ \Psi_s^\mp(in, \pm\infty,) &= \frac{1}{\sqrt{2}} \left(\varkappa_s^\mp(in, -\infty) \pm i\varkappa_s^\mp(in, +\infty) \right). \end{aligned} \tag{3.75}$$

And taking the result obtained in (3.27), the incident and transmitted waves are then written:

$$\begin{cases} \Psi_s^{\mp,in}(x) = \frac{1}{\sqrt{2}} \left(\varkappa_s^\mp(in, -\infty) + i\varepsilon\varkappa_s^\mp(in, +\infty) \right) e^{-ik|x|} \\ \Psi_s^{\mp,out}(x) = \frac{1}{\sqrt{2}} \left(\varkappa_s^\mp(out, +\infty) - i\varepsilon\varkappa_s^\mp(out, -\infty) \right) e^{ik|x|}, \end{cases} \tag{3.76}$$

where $\varepsilon = +(-)$ for $x > 0$ $(x < 0)$. Then, carrying the previous expression into equation (3.26), we obtain the asymptotic form ($|x| \to \infty$) of the standing wave function $\Psi_s^{\mp}(x)$, which leads to the asymptotic development (3.25). Is written as:

$$\Psi_s^{\mp}(x) = \frac{1}{\sqrt{2}}\left[\varkappa_s^{\mp}(in, -\infty)\,\psi_s^0(x) + \varkappa_s^{\mp}(in, +\infty)\,\psi_s^1(x)\right], \tag{3.77}$$

with

$$\psi_s^l(x) = (i\varepsilon)^l\, e^{-ik|x|} + (-1)^l\, e^{2i\delta_s^l} e^{ik|x|}). \tag{3.78}$$

This additional phase shift δ_s^l $(l = 0, 1)$ therefore has the following physical interpretation: it is the only visible trace which indicates the presence of a short-range interaction term.

3.3.4 Transmission and reflection coefficients

In scattering problems, we mainly focus on finding the transmission coefficients $\mathbb{T}_s$ and reflection coefficients $\mathbb{R}_s$ defined respectively as the ratios of the fluxes of transmitted and reflected particles to the incident flux. With regard to the probabilistic notions of quantum theory, these fluxes correspond to the fluxes of the associated probability current density vectors.

In order to express the currents, it is necessary to determine the wave function. For a particle coming from the left, the presence of the scattering center gives rise on the left, to two waves $e^{\pm ikx}$ incident and reflected, characterized by their amplitudes. On the right for $x \to +\infty$, there is only one emergent wave, i.e. $\Psi_s^{\mp}(in, +\infty) = 0$. For a particle coming from the right, i.e. there is only one emergent wave for $x \to -\infty$, this imposes $\Psi_s^{\mp}(in, -\infty) = 0$.

As both cases are similar, consider the case of a particle coming from $-\infty$. With this choice, according to (3.75), we have

$$\Psi_s^{\mp}(in, +\infty,) = 0, \qquad \varkappa_s^{\mp}(in, +\infty) = i\varkappa_s^{\mp}(in, -\infty). \tag{3.79}$$

Then, inserting the previous expression in the development (3.77), the wave function of the steady state is written:

$$\Psi_{s,L}^{\mp}(x) = \begin{cases} \sqrt{2}\varkappa_s^{\mp}(in, -\infty)\left[e^{ikx} + f_s^{-} e^{-ikx}\right] & x \to -\infty, \\ \sqrt{2}\varkappa_s^{\mp}(in, -\infty)\left[(1 + f_s^{+}) e^{ikx}\right] & x \to +\infty, \end{cases} \tag{3.80}$$

where $f_s^{\mp}$ are the scattering amplitudes, given by

$$f_s^{\mp} = f_s^0 \mp f_s^1, \quad f_s^l = \frac{1}{2}\left(e^{2i\delta_s^l} - 1\right), \quad l = 0, 1. \tag{3.81}$$

Having obtained the asymptotic form of the wave function $\Psi_{s,L}^{\mp}(x)$ (arrival of $-\infty$), we can then calculate the reflection and transmission coefficients $\mathbb{R}_s$ and $\mathbb{T}_s$, as well as the cross section σ_s^t.

With the choice of $\Psi_s^{\mp}(in, +\infty) = 0$, if we assume that the incident flux is normalized, that is $\Psi_s^{\mp}(in, -\infty) = \sqrt{2}\varkappa_s^{\mp}(in, -\infty) = 1_s^{\mp}$. In this case, comparing (3.23) and (3.80), makes it possible to find

$$T_{s,L}^{\mp} = 1_s^{\mp}\left(1 + f_s^{+}\right), \quad R_{s,L}^{\mp} = 1_s^{\mp} f_s^{-}, \quad T_{s,R}^{\mp} = R_{s,R}^{\mp} = 0. \tag{3.82}$$

The transmission coefficients $\mathbb{T}_s$ and reflection coefficients $\mathbb{R}_s$ can be expressed by inserting (3.82) in (3.24), after some calculation process that is recommended to do for training, and taking into account (3.64) and (3.65), we thus obtain:

$$\mathbb{T}_s = \frac{\left(|1_s^-|^2 + |1_s^+|^2\right)|1 + f_s^+|^2}{|1_s^-|^2 + |1_s^+|^2} = \frac{1}{4}\left|e^{2i\delta_s^0} + e^{2i\delta_s^1}\right|^2 = |t_s|^2, \tag{3.83}$$

and

$$\mathbb{R}_s = \frac{\left(|1_s^-|^2 + |1_s^+|^2\right)|f_s^-|^2}{|1_s^-|^2 + |1_s^+|^2} = \frac{1}{4}\left|e^{2i\delta_s^0} - e^{2i\delta_s^1}\right|^2 = \left|\sqrt{\omega_s^2 + r_s^2 - \rho_s^2}\right|^2, \tag{3.84}$$

and we have, as expected, the relation

$$\mathbb{T}_s + \mathbb{R}_s = 1. \tag{3.85}$$

One interpretation of these coefficients is as follows: if we make a measurement of the position of the particle just after it has finished interacting with the scattering field, the particle will have a probability $\mathbb{R}_s$ of appearing on the left, and a probability $\mathbb{T}_s$ of appearing on the right.

The differential and total scattering cross-sections $\sigma_s^{\mp}$ ($-$ for $x < 0$, $+$ for $x > 0$) and σ_s^t respectively, are given by [38, 46, 47]:

$$\sigma_s^{\mp} = \left|f_s^{\mp}\right|^2, \quad \sigma_s^t = \left|f_s^-\right|^2 + \left|f_s^+\right|^2. \tag{3.86}$$

Chapter 4

Application of the Ŝ-matrix formalism

After having given the elements constituting the formalism of the one-dimensional scattering matrix for relativistic particles of spin-s ($s = 0, 1/2$) interacting with a short-range electromagnetic field $A_\mu \left(A_0\left(x,t\right), \overrightarrow{A}\left(x,t\right)\right)$, we move on to the practical side, namely the application of this formalism to study the scattering of a relativistic particle of spin-s by certain scalar potentials (Woods-Saxon potential, periodic potential) having some properties of symmetry and range.

We begin by considering a relativistic particle of mass m, energy E, charge e, and spin-s ($s = 0, 1/2$) evolving in a one-dimensional world. The incident particle is subject to a localized scattering center, composed of a one-dimensional scalar potential independent of time $A_0\left(x,t\right) = V\left(x\right)$ and a vector potential $\overrightarrow{A}\left(x,t\right) = \overrightarrow{0}$. We consider the case where $V(x)$ has the same limit when $x \to \pm\infty$, and we adopt this value ($\lim\limits_{|x|\to\infty} V(x) \to 0$).

In this case, the Hamiltonian (3.16), namely the electromagnetic potentials A_0 and $\overrightarrow{A}$, related to the electric and magnetic fields by:

$$\overrightarrow{E} = -\overrightarrow{\nabla} A_0 - \frac{\partial \overrightarrow{A}}{\partial t} = -\frac{dV(x)}{dx}\overrightarrow{i}, \ \ \overrightarrow{B} = \overrightarrow{\nabla} \wedge \overrightarrow{A} = \overrightarrow{0}, \tag{4.1}$$

is written:

$$H_s^{\mp} = \left[\left(\frac{\partial}{\partial t} + ieV\left(x\right)\right)^2 - \frac{d^2}{dx^2} + m^2\right]\mathbb{I}_{2^{2s}} \mp 2ise\left(\sigma_1\right)^{2s}\frac{dV(x)}{dx}. \tag{4.2}$$

and by reporting the previous expression in Eq. (3.21), we obtain for the wave function $\Psi_s^{\mp}(x,t)$ the following differential equation:

$$\{\left(\left(\frac{\partial}{\partial t}+ieV(x)\right)^2-\frac{d^2}{dx^2}+m^2\right)\mathbb{I}_{2^{2s}}\mp$$
$$2ise\,(\sigma_1)^{2s}\frac{dV(x)}{dx}\}\Psi_s^{\mp}(x,t)=0. \tag{4.3}$$

The phenomenon studied is stationary, its Hamiltonian operator does not depend explicitly on time ($V(x)$ does not depend on time). In this case, the evolution equation has a class of particular solutions, called stationary states, where the time and space variables are separated. By putting the wave function $\Psi_s^{\mp}(x,t)$ associated with an eigenstate of energy E, in the form of a product of a function of space and another function of time,

$$\Psi_s^{\mp}(x,t)=e^{-iEt}\Psi_s^{\mp}(x)\,. \tag{4.4}$$

If in equation (4.3) we substitute for $\Psi_s^{\mp}(x,t)$ its value (4.4), the variation as a function of time is eliminated, and the time-independent function $\Psi_s^{\mp}(x)$ satisfies the following stationary equation:

$$\left\{D_{KG}^2\mathbb{I}_{2^{2s}}\pm 2ise\,(\sigma_1)^{2s}\frac{dV(x)}{dx}\right\}\Psi_s^{\mp}(x)=0, \tag{4.5}$$

we have noted D_{KG}^2 the operator relative to the Klein-Gordon equation of spin-0 interacting with a scattering field, defined by:

$$D_{KG}^2=\frac{d^2}{dx^2}+(E-eV(x))^2-m^2. \tag{4.6}$$

In order to decouple equation (4.5), let us introduce the function $\Phi_s^{\mp}(x)$, defined by

$$\Psi_s^{\mp}(x)=\left[\frac{\sigma_3+\sigma_1}{2}\right]^{(2s)}\Phi_s^{\mp}(x), \tag{4.7}$$

and reporting this expression in equation (4.5), we obtain for each component of the wave function $\Phi_s^{\mp}(x)$ a Klein-Gordon type equation that also contains a term describing the spin-field coupling

$$\left\{D_{KG}^{2}\mathbb{I}_{2^{2s}} \pm 2ies\left(\sigma_3\right)^{(2s)}\frac{dV\left(x\right)}{dx}\right\}\Phi_s^{\mp}(x)=0. \tag{4.8}$$

The term $\pm 2is\left(\sigma_3\right)^{(2s)}\frac{dV(x)}{dx}$ contains the interaction of the spin with the external electromagnetic field. If we remove it ($s=0$), equation (4.8) reduces to the KLein-Gordon equation of spin-0. By setting ($s=1/2$), we obtain the quadratic Dirac equation of spin-1/2.

Now, we will determine the boundary conditions in the vicinity of unspecified point x_0 where the function $V\left(x\right)$ presents a jump finite amplitude of the form

$$V(x)=\begin{cases} V_1(x) & \text{for} \quad x<x_0, \\ V_2(x) & \text{for} \quad x>x_0. \end{cases} \tag{4.9}$$

In this hypothesis, the singularity induced on the derivative of the function $V(x)$ is naturally more violent in the vicinity of x_0. Indeed, in the vicinity of the discontinuity, we can write [38, 41]

$$\frac{dV(x)}{dx}=\begin{cases} \frac{dV_1(x)}{dx} & \text{if} \quad x<x_0, \\ \left[V_2(x_0^+)-V_1(x_0^-)\right]\delta(x-x_0) & \text{if} \quad x=x_0, \\ \frac{dV_2(x)}{dx} & \text{if} \quad x>x_0. \end{cases} \tag{4.10}$$

The presence of Dirac delta in equation (4.8) implies that the wave function $\Phi_s^{\mp}(x)$ is continuous at the point $x=x_0$,

$$\Phi_s^{\mp}\left(x_0^+\right)=\Phi_s^{\mp}\left(x_0^-\right), \tag{4.11}$$

but its derivative $d\Phi_s^{\mp}\left(x\right)/dx$ is not continuous. This can be seen by integrating Eq. (4.8) from $x_0-\varepsilon$ to $x_0+\varepsilon$ (where ε is positive but arbitrarily small), and we let $\varepsilon\longrightarrow 0$, we obtain

$$\lim_{\varepsilon\to 0}\{\int_{-\varepsilon}^{+\varepsilon}\frac{d^2\Phi_s^{\mp}(x)}{dx^2}dx=-\underbrace{\int_{-\varepsilon}^{+\varepsilon}\left[(E-eV(x))^2-m^2\right]\Phi_s^{\mp}(x)dx}_{0}$$
$$\pm 2ise\left[V_2(x_0^+)-V_1(x_0^-)\right]\left(\sigma_3\right)^{(2s)}\int_{-\varepsilon}^{+\varepsilon}\delta(x-x_0)\Phi_s^{\mp}(x)dx\}\,. \tag{4.12}$$

According to the definition of the δ-Dirac [29, 48], we get

$$\left.\frac{d\Phi_s^{\mp}(x)}{dx}\right|_{x_0^-}^{x_0^+} = \pm 2ise\left[V_2(x_0^+) - V_1(x_0^-)\right](\sigma_3)^{(2s)}\,\Phi_s^{\mp}(x_0). \tag{4.13}$$

4.1 Ŝ-matrix formalism in 1D for particles of spin-s subject to the Woods-Saxon potential

4.1.1 Introduction

In nuclear physics, many theoretical models, detailed in the literature, describe the properties of nuclei very well. One of these most used models is the shell model [49]. This model has made it possible to understand many observables, such as excitation spectra, electromagnetic transitions, magnetic moments, as well as beta transitions. It considers the nucleon moving inside the nucleus under the influence of a mean-field created by all the other nucleons. This mean field consists of a central potential (infinite or finite square well, harmonic oscillator, Woods-Saxon potential, or many other types).

4.1.2 Study in Woods-Saxon potential

We now move on to solving the stationary equation (4.8) in the presence of a potential barrier,

$$V(x) = A_0 = V_0\theta\,(L - |x|) \quad \text{and} \quad \overrightarrow{A} = \overrightarrow{0}, \tag{4.14}$$

where V_0 and L are two positive constants. $\theta\,(x)$ is the Heaviside function. The potential $V(x)$ varies from the value $V(x) \to 0$ for $|x| > L$ to the value $V\,(x) = V_0$ for $|x| < L$.

The potential $V\,(x)$ contains a Heaviside function ; consequently, its derivative introduces a Dirac function $\frac{dV(x)}{dx} = V_0\delta\,(x)$. The problem of solving the equation (4.8) in the presence of a δ-potential represents a serious and complex situation. To get around this problem, we take a regular potential, described by the Woods-Saxon potential $V_\alpha\,(x)$ [50, 51, 52], whose form is as follows (see fig-4.1).

$$V_{\alpha}(x) = \frac{V_0}{1+\exp\left(\frac{|x|-L}{\alpha}\right)} = A_0 \quad \text{and} \quad \overrightarrow{A} = \overrightarrow{0}, \tag{4.15}$$

where V_0, α, and L are positive constants.

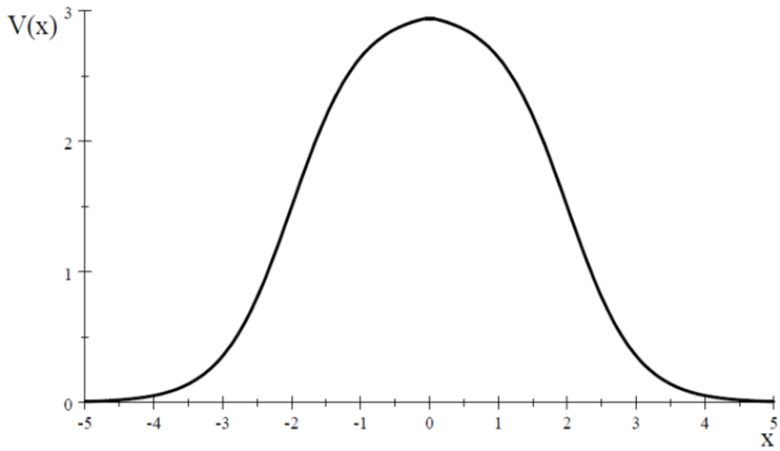

Fig-4.1: Woods-Saxon Potential ($V_0 = 3, L = 2, \alpha = 0.5$)

The wave function, the boundary conditions, and the transmission and reflection coefficients of the potential barrier are deduced by a limit procedure when $\alpha \to 0^+$.

Now move on to solving the steady-state equation (4.8) in the presence of the potential (4.15). In this case, the equation is written as

$$\{\left(\frac{d^2}{dx^2} + \left(E - \frac{eV_0}{1+\exp\left(\frac{|x|-L}{\alpha}\right)}\right)^2 - m^2\right)\mathbb{I}_{2^{2s}} \pm$$
$$2ise\left(\sigma_3\right)^{(2s)}\frac{d}{dx}\left(\frac{V_0}{1+\exp\left(\frac{|x|-L}{\alpha}\right)}\right)\}\Phi_s^{\mp}(x) = 0. \tag{4.16}$$

Since there is an absolute value for the variable x, we distinguish as usual the two regions $x < 0$ and $x > 0$.

We first look for the solutions in the region $x < 0$. The differential Eq. (4.16) has no constant coefficients. The solutions of this equation can be calculated by introducing a new variable $x \to y$ defined by:

$$y = \frac{1}{1 + \exp\left(-\frac{x+L}{\alpha}\right)}. \tag{4.17}$$

So we have for the variation domains $x \in \left]-\infty, 0\right[\rightarrow y \in \left]0, 1\right[$. By a direct calculation, we immediately see that

$$\begin{aligned} \frac{d}{dx} &= \frac{dy}{dx}\frac{d}{dy}, \qquad \frac{d^2}{dx^2} = \left(\frac{dy}{dx}\right)^2 \frac{d^2}{dy^2} + \frac{d^2y}{dx^2}\frac{d}{dy}, \\ \frac{dy}{dx} &= \frac{1}{\alpha} y\left(1-y\right), \qquad \frac{d^2y}{dx^2} = \frac{1}{\alpha^2} y\left(1-y\right)\left(1-2y\right), \end{aligned} \tag{4.18}$$

and by substituting these expressions into (4.16), we obtain for the stationary wave function $\Phi_s^{\mp}(y)$ relative to the new variable (4.17), the following differential equation:

$$\left[D_y^2 \mathbb{I}_{2^{2s}} \pm 2iess\alpha V_0 y\left(1-y\right)\left(\sigma_3\right)^{2s}\right] \Phi_s^{\mp}(y) = 0, \tag{4.19}$$

where D_y^2 is a second order operator, given by:

$$D_y^2 = y^2\left(1-y\right)^2 \frac{d^2}{dy^2} + y\left(1-y\right)\left(1-2y\right)\frac{d}{dy} + \alpha^2\left[\left(E - eV_0 y\right)^2 - m^2\right] \tag{4.20}$$

To solve equation (4.19), we introduce a new function $f_s^{\mp}(y)$ through the relation

$$\Phi_s^{\mp}(y) = y^{\nu}\left(1-y\right)^{\mu} f_s^{\mp}(y), \tag{4.21}$$

where μ and ν are two parameters that we fix later. By a direct calculation, we immediately see that:

$$\frac{d\Phi_s^{\mp}(y)}{dy} = y^{\nu}\left(1-y\right)^{\mu}\left\{\left(\frac{d}{dy} + \frac{\nu}{y} - \frac{\mu}{(1-y)}\right) f_s^{\mp}(y)\right\}, \tag{4.22}$$

and

$$\begin{aligned} \frac{d^2\Phi_s^{\mp}(y)}{dy^2} = y^{\nu}\left(1-y\right)^{\mu} \{ &\frac{d^2}{dy^2} + \left(\frac{2\nu}{y} - \frac{2\mu}{1-y}\right)\frac{d}{dy} + \\ &\left(\frac{-2\mu\nu}{y\left(1-y\right)} + \frac{\mu\left(\mu-1\right)}{\left(1-y\right)^2} + \frac{\nu\left(\nu-1\right)}{y^2}\right)\} f_s^{\mp}(y). \end{aligned} \tag{4.23}$$

Taking into account equations (4.21), (4.22) and (4.23), after some elementary calculations, equation (4.19) transforms into the equation

$$\left\{\left(\widetilde{D}_y^2 + B\left(y\right)\right)\mathbb{I}_{2^{2s}} \pm 2ies\alpha V_0\left(\sigma_3\right)^{2s}\right\} f_s^{\mp}\left(y\right) = 0, \tag{4.24}$$

where

$$\begin{aligned}\widetilde{D}_y^2 = y\left(1-y\right)\frac{d^2}{dy^2} + \left[\left(2\nu+1\right) - 2y\left(\nu+\mu+1\right)\right]\frac{d}{dy} \\ -\left(\mu+\nu+\frac{1}{2}\right)^2 + \frac{1}{4} - \alpha^2 e^2 V_0^2,\end{aligned} \tag{4.25}$$

and

$$B\left(y\right) = \left(\frac{\nu^2}{y} + \frac{\mu^2}{1-y}\right) + \alpha^2\left(\frac{E^2-m^2}{y} + \frac{\left(E-eV_0\right)^2 - m^2}{1-y}\right). \tag{4.26}$$

Equation (4.24) reduces to the standard form of a hypergeometric type equation,

$$\left\{\widetilde{D}_y^2\mathbb{I}_{2^{2s}} \pm 2ies\alpha V_0\left(\sigma_3\right)^{2s}\right\} f_s^{\mp}\left(y\right) = 0, \tag{4.27}$$

if $B\left(y\right) = 0$. Under this condition, the parameters μ and ν have the following values:

$$\mu^2 = \alpha^2\left(m^2 - \left(E-eV_0\right)^2\right) = -\alpha^2 k_1^2, \;\; \nu^2 = \alpha^2\left(m^2 - E^2\right) = -\alpha^2 k^2. \tag{4.28}$$

In this case, the general solution of the differential equation (4.27) is a linear combination of two hypergeometric type functions of the form:

$$f_s^{\mp}\left(y\right) = \begin{pmatrix} C_1^{\mp}{}_2F_1\left(a^{\mp}, b^{\mp}, c, y\right) + C_2^{\mp} y^{-2\nu}{}_2F_1\left(a^{\mp}+1-c, b^{\mp}+1-c, 2-c, y\right) \\ \\ D_1^{\mp}{}_2F_1\left(a^{\pm}, b^{\pm}, c, y\right) + D_2^{\mp} y^{-2\nu}{}_2F_1\left(a^{\pm}+1-c, b^{\pm}+1-c, 2-c, y\right)\end{pmatrix}, \tag{4.29}$$

with

$$\begin{aligned}a^{\mp} = \mu+\nu+\frac{1}{2}+\frac{\vartheta^{\mp}}{2},\; b^{\mp} = \mu+\nu+\frac{1}{2}-\frac{\vartheta^{\mp}}{2}, \\ c = 1+2\nu,\;\; \left(\vartheta^{\mp}\right)^2 = 1 - 4\alpha^2 e^2 V_0^2 \pm 8ise\alpha V_0.\end{aligned} \tag{4.30}$$

Now let's move to the other region $x > 0$. After the change of variable

$$y = \frac{1}{1 + \exp\left(\frac{x-L}{\alpha}\right)}, \tag{4.31}$$

and introduction of a new function $g_s^{\mp}(y)$ according to the formula

$$\Phi_s^{\mp}(x) = y^{\nu}(1-y)^{\mu}\, g_s^{\mp}(y), \tag{4.32}$$

then, by following the previous calculations step by step, we obtain a system of equations that differs from (4.24) only by the sign of the interaction term of the spin with the scattering field

$$\left\{\left[\widetilde{D}_y^2 + B(y)\right]\mathbb{I}_{2^{2s}} \mp 2ies\alpha V_0 (\sigma_3)^{2s}\right\} g_s^{\mp}(y) = 0. \tag{4.33}$$

Taking expression (4.28) as a constraint, the previous equation reduces to a hypergeometric type equation:

$$\left[\widetilde{D}_y^2 \mathbb{I}_{2^{2s}} \mp 2ies\alpha V_0 (\sigma_3)^{2s}\right] g_s^{\mp}(y) = 0, \tag{4.34}$$

which also has the solution

$$g_s^{\mp}(y) = \begin{pmatrix} C_3^{\mp}\, {}_2F_1(a^{\pm}, b^{\pm}, c, y) + C_4^{\mp} y^{-2\nu}\, {}_2F_1(a^{\pm}+1-c, b^{\pm}+1-c, 2-c, y) \\ \\ D_3^{\mp}\, {}_2F_1(a^{\mp}, b^{\mp}, c, y) + D_4^{\mp} y^{-2\nu}\, {}_2F_1(a^{\mp}+1-c, b^{\mp}+1-c, 2-c, y) \end{pmatrix} \tag{4.35}$$

Solutions (4.29) and (4.35) can be grouped together to be written as a single equation including solutions relative to $x < 0$ and $x > 0$:

$$\eta_s^{\mp}(y) = \theta(-x)\, f_s^{\mp}(y) + \theta(x)\, g_s^{\mp}(y) \quad \text{with} \quad y = \frac{1}{1 + e^{\frac{|x|-L}{\alpha}}}. \tag{4.36}$$

Inserting all these relations into (4.7), the stationary solutions at 2^{2s} components $\Psi_s^{-}(x)$ and $\Psi_s^{+}(x)$ of the equation (4.5), in the presence of the Woods-Saxon potential are:

$$\Psi_s^{\mp}(x) = y^{\nu}(1-y)^{\mu}\left[\frac{\sigma_3 + \sigma_1}{2}\right]^{(2s)} \eta_s^{\mp}(y). \tag{4.37}$$

Boundary conditions

Note that the coefficients ($C_j^{\mp}, D_j^{\mp}, j = 1,4$) are not independent of each other: they must be chosen so that expression (4.37) represents the same function in different intervals; this function is the eigenfunction associated with an eigenvalue E.

By the general discussion, the Woods-Saxon potential is contained, that is to say, $V_2(x_0^+) - V_1(x_0^-) = 0$. Taking this condition into account, the wave function as well as its first derivative are continuous at $x = 0$ or $y = \lambda = \left[1 + \exp\left(\frac{-L}{\alpha}\right)\right]^{-1}$, that is:

$$\Psi_s^{\mp}\left(0^-\right) = \Psi_s^{\mp}\left(0^+\right), \qquad \frac{d\Psi_s^{\mp}\left(0^-\right)}{dx} = \frac{d\Psi_s^{\mp}\left(0^+\right)}{dx}, \tag{4.38}$$

which allow the coefficients to be fixed by the following relations:

$$\begin{aligned} C_1^{\mp} &= C_2^{\mp} W_{12}^{\mp} + C_4^{\mp} W_{14}^{\mp}, \quad & C_3^{\mp} &= C_2^{\mp} W_{32}^{\mp} + C_4^{\mp} W_{34}^{\mp}, \\ D_1^{\mp} &= D_2^{\mp} W_{12}^{\pm} + D_4^{\mp} W_{14}^{\pm}, \quad & D_3^{\mp} &= D_2^{\mp} W_{32}^{\pm} + D_4^{\mp} W_{34}^{\pm}, \end{aligned} \tag{4.39}$$

with

$$\begin{aligned} W_{12}^{\mp} = W_{34}^{\pm} &= -\frac{F_1^{\pm}\left(F_2^{\mp}\right)' + F_2^{\mp}\left(F_1^{\pm}\right)'}{F_1^{\pm}\left(F_1^{\mp}\right)' + F_1^{\mp}\left(F_1^{\pm}\right)'}, \\ W_{32}^{\mp} = W_{14}^{\pm} &= \frac{F_2^{\mp}\left(F_1^{\mp}\right)' - F_1^{\mp}\left(F_2^{\mp}\right)'}{F_1^{\pm}\left(F_1^{\mp}\right)' + F_1^{\mp}\left(F_1^{\pm}\right)'} \end{aligned} \tag{4.40}$$

and $F_1^{\mp}$, $F_2^{\mp}$, $\left(F_1^{\mp}\right)'$, and $\left(F_2^{\mp}\right)'$ are defined by:

$$\begin{aligned} \left(F_1^{\mp}\right) &= \left[y^{\nu}\left(1-y\right)^{\mu}\ {}_2F_1\left(a^{\mp}, b^{\mp}, c, y\right)\right]_{y=\lambda}, \\ \left(F_2^{\mp}\right) &= \left[y^{-\nu}\left(1-y\right)^{\mu}\ {}_2F_1\left(a^{\mp}+1-c, b^{\mp}+1-c, 2-c, y\right)\right]_{y=\lambda}, \\ \left(F_1^{\mp}\right)' &= \frac{d}{dx}\left[y^{\nu}\left(1-y\right)^{\mu}\ {}_2F_1\left(a^{\mp}, b^{\mp}, c, y\right)\right]_{y=\lambda}, \\ \left(F_2^{\mp}\right)' &= \frac{d}{dx}\left[y^{-\nu}\left(1-y\right)^{\mu}\ {}_2F_1\left(a^{\mp}+1-c, b^{\mp}+1-c, 2-c, y\right)\right]_{y=\lambda}. \end{aligned} \tag{4.41}$$

Asymptotic states

In a quantum description, the exact calculation of the scattering cross section requires knowledge of the eigenstates of the Hamiltonian. This step is a complex numerical task. To circumvent the complexity of such a description, we always consider the case of observations made "at infinity" ($|x| \to \infty$). Among all the possible forms of the states that satisfy equation (4.16), we will choose solutions for a continuous set of values of the energy E; which correspond to the scattering states $(E - eV_0)^2 - m^2 > 0$. Asymptotically, such solutions are plane waves since the potential is constant when $|x| \to \infty$. By analyzing these solutions correctly, we find that they correspond to the scattering states of asymptotically free particles, scattered by the potential $V(x)$. Admitting, in the case $(E - eV_0)^2 - m^2 \sim E^2 - m^2 = k^2 > 0$, solutions in the form of plane waves $e^{\pm ikx}$ heading towards the right or towards the left [38, 53, 54].

Now find the asymptotic behavior of the stationary wave function (4.37), when $|x| \to \infty$. Under these conditions, we have the following behavior

$$\lim_{|x|\to\infty} y^{\pm\nu} = e^{\pm ik(|x|-L)}, \quad \lim_{|x|\to\infty} (1-y)^{\mu} = 1,$$
$$\lim_{|x|\to\infty} y = 0, \quad k = \sqrt{E^2 - m^2}. \tag{4.42}$$

Having in mind that for $|x| \to \infty$, the argument y of the hypergeometric function is zero. Then, by virtue of the known formula of the hypergeometric function ${}_2F_1(a, b, c, 0) = 1$ [55, 56], and taking into account the relationship (4.42), we obtain the asymptotic expression of the function (4.37)

$$\Psi^{\mp, WS}_{s,asy}(x) = \left[\frac{\sigma_3 + \sigma_1}{2}\right]^{(2s)} \overline{\eta}^{\mp}_s(x), \tag{4.43}$$

where

$$\overline{\eta}^{\mp}_s(x) = \begin{cases} \begin{pmatrix} C_3^{\mp} \\ D_3^{\mp} \end{pmatrix} e^{ik(x-L)} + \begin{pmatrix} C_4^{\mp} \\ D_4^{\mp} \end{pmatrix} e^{-ik(x-L)} & x \to +\infty, \\ \begin{pmatrix} C_2^{\mp} \\ D_2^{\mp} \end{pmatrix} e^{ik(x+L)} + \begin{pmatrix} C_1^{\mp} \\ D_1^{\mp} \end{pmatrix} e^{-ik(x+L)} & x \to -\infty. \end{cases} \tag{4.44}$$

4.1.3 $\hat{\mathbf{S}}^{\mathrm{WS}}$-Matrix formalism

In this section, we construct the scattering matrix formalism relative to the relativistic wave equation describing the interaction of a particle of mass m, energy E, charge e and spin-s ($s = 0, 1/2$) with the Woods-Saxon potential, described by equation (4.15).

To calculate the vectors $\Psi_s^{\mp,WS}(out, \pm\infty)$ and $\Psi_s^{\mp,WS}(in, \pm\infty)$, we insert the expression (4.44) in (4.43). After some elementary calculations, we compare the result obtained with the formula (3.25), and by identifying the coefficients from one member to the other, we obtain the following expressions:

$$\begin{cases} \Psi_s^{\mp,WS}(out, +\infty) = \left[\frac{\sigma_3+\sigma_1}{2}\right]^{(2s)} \begin{pmatrix} C_3^{\mp} \\ D_3^{\mp} \end{pmatrix} e^{-ikL}, \\ \Psi_s^{\mp,WS}(out, -\infty) = \left[\frac{\sigma_3+\sigma_1}{2}\right]^{(2s)} \begin{pmatrix} C_1^{\mp} \\ D_1^{\mp} \end{pmatrix} e^{-ikL}, \\ \Psi_s^{\mp,WS}(in, -\infty) = \left[\frac{\sigma_3+\sigma_1}{2}\right]^{(2s)} \begin{pmatrix} C_2^{\mp} \\ D_2^{\mp} \end{pmatrix} e^{ikL}, \\ \Psi_s^{\mp,WS}(in, +\infty) = \left[\frac{\sigma_3+\sigma_1}{2}\right]^{(2s)} \begin{pmatrix} C_4^{\mp} \\ D_4^{\mp} \end{pmatrix} e^{ikL}. \end{cases} \tag{4.45}$$

The particle is subjected to a localized potential $V(x)$ ($V(x) \overset{|x|\to\infty}{\to} 0$), which is independent of time. In this case, using the methods developed in Chapter-3, we easily find that the final state after scattering $\Psi_s^{out,WS}$ is, according to (3.28), related to the initial state $\Psi_s^{in,WS}$ by the following relation $\Psi_s^{out,WS} = \hat{S}_{-s}^{WS}\Psi_s^{in,WS}$. Or explicitly in matrix form,

$$\begin{pmatrix} \Psi_s^{-,WS}(out, +\infty) \\ \Psi_s^{+,WS}(out, +\infty) \\ \Psi_s^{-,WS}(out, -\infty) \\ \Psi_s^{+,WS}(out, -\infty) \end{pmatrix} = \hat{S}_{-s}^{WS} \begin{pmatrix} \Psi_s^{-,WS}(in, -\infty) \\ \Psi_s^{+,WS}(in, -\infty) \\ \Psi_s^{-,WS}(in, +\infty) \\ \Psi_s^{+,WS}(in, +\infty) \end{pmatrix}. \tag{4.46}$$

To determine the $\hat{S}_{-s}^{WS}-$matrix, we insert (4.39) into (4.45), then we report the result in equation (4.46). After a simple calculation we obtain the following expression:

$$\hat{S}_{-s}^{WS} = \begin{pmatrix} \check{T}_s^{+,WS} & 0 & \check{R}_s^{+,WS} & 0 \\ 0 & \check{T}_s^{-,WS} & 0 & \check{R}_s^{-,WS} \\ \check{R}_s^{-,WS} & 0 & \check{T}_s^{-,WS} & 0 \\ 0 & \check{R}_s^{+,WS} & 0 & \check{T}_s^{+,WS} \end{pmatrix}, \tag{4.47}$$

where

$$\check{T}_s^{\pm,WS} = \begin{pmatrix} t_s^{WS} & \pm\omega_s^{WS} \\ \pm\omega_s^{WS} & t_s^{WS} \end{pmatrix}, \quad \check{R}_s^{\pm,WS} = \begin{pmatrix} r_s^{WS} & \pm\rho_s^{WS} \\ \pm\rho_s^{WS} & r_s^{WS} \end{pmatrix}, \tag{4.48}$$

and

$$\begin{aligned} t_s^{WS} &= \frac{1}{2}\left(W_{14}^{+} + W_{14}^{-}\right)e^{2ikL}, \quad \omega_s^{WS} = \frac{1}{2}\left(W_{14}^{+} - W_{14}^{-}\right)e^{2ikL}, \\ r_s^{WS} &= \frac{1}{2}\left(W_{12}^{+} + W_{12}^{-}\right)e^{2ikL}, \quad \rho_s^{WS} = \frac{1}{2}\left(W_{12}^{+} - W_{12}^{-}\right)e^{2ikL}. \end{aligned} \tag{4.49}$$

Representation in the partial wave base

Let us now express the scattering matrix in the partial waves basis. To illustrate this point, we apply the unitary transformation (3.68) which transforms $\Psi_s^{out,WS}$ and $\Psi_s^{in,WS}$ in $\varkappa_s^{out,WS}$ and $\varkappa_s^{in,WS}$, given by:

$$\varkappa_s^{out,WS}(x) = \hat{U}_s\Psi_s^{out,WS}(x), \quad \varkappa_s^{in,WS}(x) = \hat{U}_s\Psi_s^{in,WS}(x). \tag{4.50}$$

After some manipulations, deduce $\Psi_s^{out,WS}(x)$ and $\Psi_s^{in,WS}(x)$ respectively as a function of $\varkappa_s^{out,WS}(x)$ and $\varkappa_s^{in,WS}(x)$, and use the property of unitary matrices $\hat{U}_s\hat{U}_s^{\dagger} = \mathbb{I}_{2^{2s+1}(2s+1)}$, we obtain after a simple calculation

$$\varkappa_s^{out,WS}(x) = \left(\hat{U}_s\hat{S}_{-s}^{WS}\hat{U}_s^{\dagger}\right)\varkappa_s^{in,WS}(x) = \hat{M}_{-s}^{WS}\varkappa_s^{in,WS}(x), \tag{4.51}$$

where $\hat{M}_{-s}^{WS}$ is scattering matrix in the partial wave representation, given by:

$$\hat{M}_{-s}^{WS} = \hat{U}_s \hat{S}_{-s}^{WS} \hat{U}_s^{\dagger} = \begin{pmatrix} \overline{\breve{T}}_s^{+,WS} & 0 & i\overline{\breve{R}}_s^{-,WS} & 0 \\ 0 & \overline{\breve{T}}_s^{+,WS} & 0 & -i\overline{\breve{R}}_s^{-,WS} \\ i\overline{\breve{R}}_s^{+,WS} & 0 & \overline{\breve{T}}_s^{-,WS} & 0 \\ 0 & -i\overline{\breve{R}}_s^{+,WS} & 0 & \overline{\breve{T}}_s^{-,WS} \end{pmatrix}, \tag{4.52}$$

where

$$\overline{\breve{T}}_s^{\pm,WS} = \begin{pmatrix} t_s^{WS} \pm r_s^{WS} & 0 \\ 0 & t_s^{WS} \pm r_s^{WS} \end{pmatrix}, \tag{4.53}$$

and

$$\overline{\breve{R}}_s^{\pm,WS} = \begin{pmatrix} 0 & \rho_s^{WS} \pm \omega_s^{WS} \\ \rho_s^{WS} \pm \omega_s^{WS} & 0 \end{pmatrix}. \tag{4.54}$$

It is easy to show that when we go to the even-odd basis, $\hat{M}_{-s}^{WS}$ can be diagonalized in each case $s = 0, 1/2$. To illustrate this, as usual, we write the eigenvalue equation

$$\det\left(\hat{M}_{-s}^{WS} - \beta \mathbb{I}_{2^{(2s+1)}(2s+1)}\right) = 0. \tag{4.55}$$

By a simple calculation, we find the associated eigenvalues which we format as follows:

$$\beta^{\pm} = t_s^{WS} \pm \sqrt{(\omega_s^{WS})^2 + (r_s^{WS})^2 - (\rho_s^{WS})^2}, \tag{4.56}$$

and the diagonal matrix $\hat{M}_{-s}^{WS}$ which represents $\hat{S}_{-s}^{WS}$ as follows:

$$\hat{M}_{-s}^{WS} = \mathbb{I}_{2^{2s(2s+1)}} \otimes \begin{pmatrix} e^{2i\delta_s^{0,WS}} & 0 \\ 0 & e^{2i\delta_s^{1,WS}} \end{pmatrix}, \tag{4.57}$$

where

$$e^{2i\delta_s^{l,WS}} = t_s^{WS} + (-1)^l \sqrt{(\omega_s^{WS})^2 + (r_s^{WS})^2 - (\rho_s^{WS})^2}, \tag{4.58}$$

this additional phase shift $\delta_s^{l,WS}$ $(l = 0, 1)$ therefore has the following physical interpretation: it is the only trace visible at a long distance in the wave function in the presence of a short-range interaction term. This phase shift is a function of the energy E, the mass m, as well as the parameters V_0 and α.

Transmission and reflection coefficients

To calculate the transmission and reflection coefficients $\mathbb{T}_s^{WS}$ and $\mathbb{R}_s^{WS}$, consider the usual physical situation where the particle coming from the left, the presence of the potential gives rise, on the left, to two waves, incident and reflected, characterized by their amplitudes. On the right there is only one emergent wave, In this case the incoming amplitude from the right $\Psi_s^{\mp,WS}(in,+\infty)=0$. With this choice, according to (3.75), we have $\varkappa_s^{\mp,WS}(in,+\infty)=i\varkappa_s^{\mp,WS}(in,-\infty)$. Under these conditions, equation (3.77) for a relativistic particle of spin-s placed in the Woods-Saxon potential becomes:

$$\Psi_{s,L}^{\mp,WS}(x)=\begin{cases}\sqrt{2}\varkappa_s^{\mp,WS}(in,-\infty)\left[e^{ikx}+f_s^{-,WS}e^{-ikx}\right] & x\to-\infty,\\ \sqrt{2}\varkappa_s^{\mp,WS}(in,-\infty)\left[\left(1+f_s^{+,WS}\right)e^{ikx}\right] & x\to+\infty,\end{cases}\tag{4.59}$$

where $f_s^{\mp,WS}$ are the scattering amplitudes, given by

$$f_s^{\mp,WS}=f_s^{0,WS}\mp f_s^{1,WS},\quad \text{where}\quad f_s^{l,WS}=\frac{1}{2}\left(e^{2i\delta_s^{l,WS}}-1\right),\quad l=0,1.\tag{4.60}$$

Having obtained the asymptotic form of the wave function $\Psi_{s,L}^{\mp,WS}(x)$ (arrival of $-\infty$), we can then calculate the transmission and reflection coefficients $\mathbb{T}_s$ and $\mathbb{R}_s$, as well as the cross-section σ_s^t.

Knowing that the interpretation of the wave function remains the same if it is multiplied by a constant vector, we can pose $\sqrt{2}\varkappa_s^{\mp,WS}(in,-\infty)=1_s^{\mp}$. In this case, comparing (3.23) and (4.59), we then easily verify

$$T_{s,L}^{\mp,WS}=1_s^{\mp}\left(1+f_s^{+,WS}\right),\quad R_{s,L}^{\mp,WS}=1_s^{\mp}f_s^{-,WS},\quad T_{s,R}^{\mp,WS}=R_{s,R}^{\mp,WS}=0.\tag{4.61}$$

Then, by inserting the previous expression into equation (3.24), after some calculation process that it is recommended to do for training, and taking into account (4.60), and (4.61), we thus obtain:

$$\mathbb{T}_s^{WS} =\mid 1+f_s^{+,WS}\mid^2 = \frac{1}{4}\left|e^{2i\delta_s^{0,WS}}+e^{2i\delta_s^{1,WS}}\right|^2,$$
$$\mathbb{R}_s^{WS} =\mid f_s^{-,WS}\mid^2 = \frac{1}{4}\mid e^{2i\delta_s^{0,WS}}-e^{2i\delta_s^{1,WS}}\mid^2, \quad (4.62)$$

and

$$\sigma_s^{t,WS} = \left|f_s^{+,WS}\right|^2+\left|f_s^{-,WS}\right|^2 = 2\left(\sin^2\delta_s^{0,WS}+\sin^2\delta_s^{1,WS}\right). \quad (4.63)$$

and we have, as expected, the relation

$$\mathbb{T}_s^{WS}+\mathbb{R}_s^{WS} = 1. \quad (4.64)$$

4.1.4 Ŝ-matrix formalism in 1D for particles of spin-s subject to the rectangular barrier potential

Now consider the limiting case when the smooth potential tends towards the rectangular barrier. The latter is found as a limiting case of the Woods-Saxon potential for $\alpha \rightarrow 0^+$,

$$V^b(x) = \lim_{\alpha\rightarrow 0^+}\frac{V_0}{1+e^{\frac{|x|-L}{\alpha}}} = V_0\theta\left(L-\mid x\mid\right). \quad (4.65)$$

For $|x| > L$, we have

$$\lim_{\alpha\rightarrow 0^+}(1-\lambda)^{-2\mu} = e^{-2ik_1L},\ \lim_{\alpha\rightarrow 0^+}\frac{1}{\alpha}(1-\lambda) = 0,$$
$$\lim_{\alpha\rightarrow 0^+}\lambda = 1,\ \lim_{\alpha\rightarrow 0^+}y^{\nu} = e^{ik(|x|-L)},\ \lim_{\alpha\rightarrow 0^+}y = 0,$$
$$\lim_{\alpha\rightarrow 0^+}y^{-2\nu} = e^{-2ik(|x|-L)},\ \lim_{\alpha\rightarrow 0^+}(1-y)^{\mu} = 1, \quad (4.66)$$

where $\mu = -i\alpha k_1$, $\nu = -i\alpha k$. By using (4.66) and the relations to the hypergeometric functions, as well as the properties of the functions Γ [55, 56]

$$
\begin{aligned}
{}_2F_1\left(a,b,c,0\right)=1,\quad & \frac{d}{dz}\left[{}_2F_1\left(a,b,c,z\right)\right] \\
&=\frac{ab}{c}\,{}_2F_1\left(a+1,b+1,c+1,z\right), \\
z\Gamma\left(z\right)=\Gamma\left(z+1\right),\quad & \lim_{z\to 0^+}\Gamma\left(z\right)=\frac{1}{z},
\end{aligned} \tag{4.67}
$$

we easily check that

$$
\begin{aligned}
\lim_{\alpha\to 0^+} W_{32}^{\mp}=\lim_{\alpha\to 0^+} W_{32}^{\pm}=\lim_{\alpha\to 0^+} W_{14}^{\mp}=\lim_{\alpha\to 0^+} W_{14}^{\pm}=\varrho_s, \\
\lim_{\alpha\to 0^+} W_{12}^{\mp}=\lim_{\alpha\to 0^+} W_{34}^{\pm}=\varsigma_s^{\mp},
\end{aligned} \tag{4.68}
$$

with

$$
\begin{aligned}
\varrho_s &= \frac{(2k_1k)}{(2k_1k)\cos\left(2k_1L\right)-i\left(k_1^2+k^2-4s^2e^2V_0^2\right)\sin\left(2k_1L\right)}, \\
\varsigma_s^{\mp} &= \frac{i\left(k_1^2-\left(k\mp 2seV_0\right)^2\right)sin\left(2k_1L\right)}{(2k_1k)\cos\left(2k_1L\right)-i\left(k_1^2+k^2-4s^2e^2V_0^2\right)\sin\left(2k_1L\right)}.
\end{aligned} \tag{4.69}
$$

Insert all these expressions into equation (4.37), we obtain

$$
\Psi_s^{\mp,b}(x)=\lim_{\alpha\to 0^+}\Psi_s^{\mp,WS}(x)=\left[\frac{\sigma_3+\sigma_1}{2}\right]^{(2s)}\eta_s^{\mp,b}\left(x\right). \tag{4.70}
$$

where

$$
\begin{aligned}
\eta_s^{\mp,b}\left(x\right)=&\left\{\begin{pmatrix} C_2^{\mp}\varsigma_s^{\mp}+C_4^{\mp}\varrho_s \\ D_2^{\mp}\varsigma_s^{\pm}+D_4^{\mp}\varrho_s\end{pmatrix}e^{-ik(x+L)}+\begin{pmatrix} C_2^{\mp} \\ D_2^{\mp}\end{pmatrix}e^{ik(x+L)}\right\}\theta\left(-x-L\right) \\
&+\left\{\begin{pmatrix} C_2^{\mp}\varrho_s+C_4^{\mp}\varsigma_s^{\pm} \\ D_2^{\mp}\varrho_s+D_4^{\mp}\varsigma_s^{\mp}\end{pmatrix}e^{ik(x-L)}+\begin{pmatrix} C_4^{\mp} \\ D_4^{\mp}\end{pmatrix}e^{-ik(x-L)}\right\}\theta\left(x-L\right)
\end{aligned}. \tag{4.71}
$$

For $\mid x\mid< L$, using

$$\lim_{\alpha\to 0^+}(1-y)^{-2\mu}=e^{2ik_1(|x|-L)},\quad \lim_{\alpha\to 0^+}(1-y)^{\mu}=e^{-ik_1(|x|-L)}$$
$$\lim_{\alpha\to 0^+}y^{\nu}=\lim_{\alpha\to 0^+}y^{-2\nu}=1,\quad \lim_{\alpha\to 0^+}y=1, \tag{4.72}$$

and the formula relating the hypergeometric functions of arguments z and $1-z$ [55, 56], we find

$$\lim_{\alpha\to 0^+}{}_2F_1\left(a^{\mp}+1-c,b^{\mp}+1-c,2-c,y\right)=\overline{B}^{\mp}+\overline{A}^{\pm}e^{2ik_1(|x|-L)},$$
$$\lim_{\alpha\to 0^+}{}_2F_1\left(a^{\mp},b^{\mp},c,y\right)=\overline{A}^{\mp}+\overline{B}^{\pm}e^{2ik_1(|x|-L)}, \tag{4.73}$$

where

$$\overline{A}^{\mp}=\frac{k_1-k\mp 2seV_0}{2k_1},\quad \overline{B}^{\pm}=\frac{k_1+k\pm 2seV_0}{2k_1}. \tag{4.74}$$

These relations reported in (4.37), give the following result:

$$\Psi_s^{\mp,b}(x)=\lim_{\alpha\to 0^+}\Psi_s^{\mp,WS}(x)=\left[\frac{\sigma_3+\sigma_1}{2}\right]^{(2s)}\overline{\eta}_s^{\mp}(x)\,\theta\left(L-|x|\right) \tag{4.75}$$

where

$$\overline{\eta}_s^{\mp}(x)=f_s^{\mp,b}(y)\,\theta(-x)+g_s^{\mp,b}(y)\,\theta(x) \tag{4.76}$$

with

$$f_s^{\mp,b}(y)=\begin{pmatrix}\left(C_2^{\mp}\varsigma_s^{\mp}+C_4^{\mp}\varrho_s\right)\overline{A}^{\mp}+C_2^{\mp}\overline{B}^{\mp}\\ \\ \left(D_2^{\mp}\varsigma_s^{\pm}+D_4^{\mp}\varrho_s\right)\overline{A}^{\pm}+D_2^{\mp}\overline{B}^{\pm}\end{pmatrix}e^{ik_1(x+L)}+$$
$$\begin{pmatrix}\left(C_2^{\mp}\varsigma_s^{\mp}+C_4^{\mp}\varrho_s\right)\overline{B}^{\pm}+C_2^{\mp}\overline{A}^{\pm}\\ \\ \left(D_2^{\mp}\varsigma_s^{\pm}+D_4^{\mp}\varrho_s\right)\overline{B}^{\mp}+D_2^{\mp}\overline{A}^{\mp}\end{pmatrix}e^{-ik_1(x+L)} \tag{4.77}$$

and

$$g_s^{\mp,b}(y) = \begin{pmatrix} \left(C_2^{\mp}\varrho_s + C_4^{\mp}\varsigma_s^{\pm}\right)\overline{A}^{\pm} + C_4^{\mp}\overline{B}^{\pm} \\ \\ \left(D_2^{\mp}\varrho_s + D_4^{\mp}\varsigma_s^{\mp}\right)\overline{A}^{\mp} + D_4^{\mp}\overline{B}^{\mp} \end{pmatrix} e^{-ik_1(x-L)} + \begin{pmatrix} \left(C_2^{\mp}\varrho_s + C_4^{\mp}\varsigma_s^{\pm}\right)\overline{B}^{\mp} + C_4^{\mp}\overline{A}^{\mp} \\ \\ \left(D_2^{\mp}\varrho_s + D_4^{\mp}\varsigma_s^{\mp}\right)\overline{B}^{\pm} + D_4^{\mp}\overline{A}^{\pm} \end{pmatrix} e^{ik_1(x-L)}. \tag{4.78}$$

We can also give the scattering matrices $\hat{S}_{-s}^{b}$ and $\hat{M}_{-s}^{b}$, the phase shifts $\delta_s^{l,b}$ $(l = 0, 1)$, the transmission and reflection coefficients $\mathbb{T}_s^b$ and $\mathbb{R}_s^b$, as well as the total scattering cross-section $\sigma_s^{t,b}$ by a limit case $\alpha \to 0^+$.

$$\hat{S}_{-s}^{b} = \lim_{\alpha\to 0^+} \hat{S}_{-s}^{WS} = \begin{pmatrix} \check{T}_s^{+,b} & 0 & \check{R}_s^{+,b} & 0 \\ 0 & \check{T}_s^{-,b} & 0 & \check{R}_s^{-,b} \\ \check{R}_s^{-,b} & 0 & \check{T}_s^{-,b} & 0 \\ 0 & \check{R}_s^{+,b} & 0 & \check{T}_s^{+,b} \end{pmatrix}, \tag{4.79}$$

with

$$\check{T}_s^{\pm,b} = \begin{pmatrix} t_s^b & \pm\omega_s^b \\ \pm\omega_s^b & t_s^b \end{pmatrix}, \quad \check{R}_s^{\pm,b} = \begin{pmatrix} r_s^b & \pm\rho_s^b \\ \pm\rho_s^b & r_s^b \end{pmatrix}, \tag{4.80}$$

and

$$r_s^b = \lim_{\alpha\to 0^+} r_s^{WS} = \frac{1}{2}\left(\varsigma_s^+ + \varsigma_s^-\right)e^{2ikL}, \quad \rho_s^b = \lim_{\alpha\to 0^+} \rho_s^{WS} = \frac{1}{2}\left(\varsigma_s^+ - \varsigma_s^-\right)e^{2ikL}$$
$$t_s^b = \lim_{\alpha\to 0^+} t_s^{WS} = \varrho_s e^{2ikL}, \quad \omega_s^b = \lim_{\alpha\to 0^+} \omega_s^{WS} = 0. \tag{4.81}$$

$$\hat{M}_{-s}^{b} = \lim_{\alpha\to 0^+} \hat{M}_{-s}^{WS} = \mathbb{I}_{2^{2s(2s+1)}} \otimes \begin{pmatrix} e^{2i\delta_s^{0,b}} & 0 \\ 0 & e^{2i\delta_s^{1,b}} \end{pmatrix}, \tag{4.82}$$

where

$$e^{2i\delta_s^{l,b}} = \left(\varrho_s + (-1)^l\sqrt{\varsigma_s^+\varsigma_s^-}\right)e^{2ikL}. \tag{4.83}$$

For the coefficients $\mathbb{T}_s^b$ and $\mathbb{R}_s^b$, we have

$$\mathbb{T}_s^b = \lim_{\alpha\to 0^+} \mathbb{T}_s^{WS} = |\varrho_s|^2 = \frac{4k_1^2k^2}{4k_1^2k^2 + \left[k_1^2 - (k+2seV_0)^2\right]\left[k_1^2 - (k-2seV_0)^2\right]\sin^2(2k_1L)}, \tag{4.84}$$

$$\mathbb{R}_s^b = \lim_{\alpha\to 0^+} \mathbb{R}_s^{WS} = \varsigma_s^-\left(\varsigma_s^+\right)^\star = \frac{\left[k_1^2 - (k+2seV_0)^2\right]\left[k_1^2 - (k-2seV_0)^2\right]\sin^2(2k_1L)}{4k_1^2k^2 + \left[k_1^2 - (k+2seV_0)^2\right]\left[k_1^2 - (k-2seV_0)^2\right]\sin^2(2k_1L)}. \tag{4.85}$$

And for the total scattering cross-section for the barrier, we have

$$\sigma_s^{t,b} = \lim_{\alpha\to 0^+} \sigma_s^{t,WS} = \left|f_s^{+,b}\right|^2 + \left|f_s^{-,b}\right|^2 = 2\left(\sin^2\delta_s^{0,b} + \sin^2\delta_s^{1,b}\right). \tag{4.86}$$

Figures (4.2.a) and (4.2.b) respectively represent $(\mathbb{T}_0, \mathbb{R}_0)$ and $(\mathbb{T}_{1/2}, \mathbb{R}_{1/2})$ as a function of the energy E of the particle.

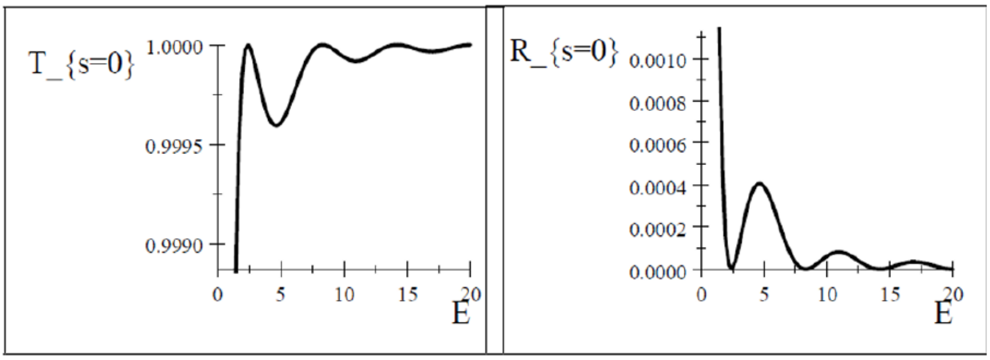

Fig-4.2.a: $\mathbb{T}_{s=0}$ and $\mathbb{R}_{s=0}$ for $V = m = 0.1, \alpha = 6$

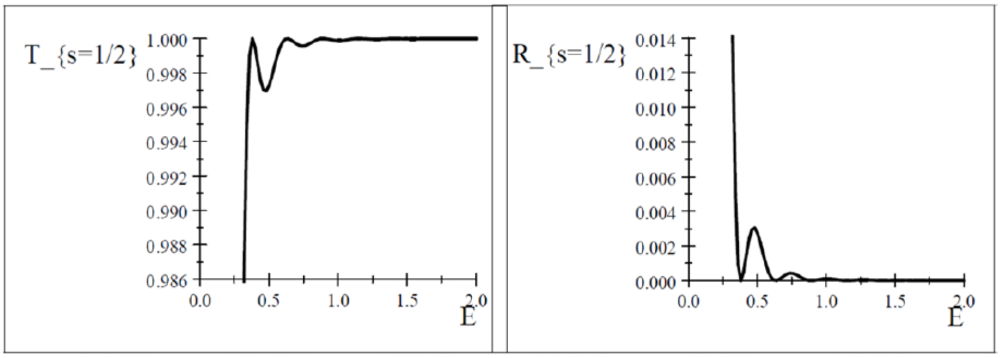

Fig-4.2.b: $\mathbb{T}_{s=1/2}$ and $\mathbb{R}_{s=1/2}$ for $V = m = 0.1, \alpha = 6$

4.2 Ŝ-matrix formalism in 1D for particles of spin-s with periodic potential

4.2.1 Introduction

According to the relative arrangement of the atoms, molecules and ions that constitute them, solid substances are divided into two groups: crystalline substances and amorphous substances. The difference between these two groups lies in the order in which the constituent particles are arranged in space. Amorphous substances show a short-range order, i.e. a definite law of the relative arrangement of neighboring atoms which does not, however, extend to large parts of the body and does not repeat itself periodically in space. Crystalline substances are characterized by a long-range order in the arrangement of atoms, i.e. they have a periodic structure ordered in space, which is preserved over time if the external conditions remain unchanged, and is known as a crystal lattice. Indeed, this arrangement is characterized by the periodic and ordered repetition of an identical pattern made up of ions, atoms, or molecules, which presents interesting symmetry properties in space.

In quantum mechanics, the particle in a one-dimensional lattice is a problem arising in the periodic crystal lattice model. The typical example of this problem is the behavior of electrons in a periodic crystal lattice (metal, semiconductor or insulator) which experience a periodic regular potential caused by the ions forming the crystal structure, and therefore arranged in a regular way. Although the actual form of this potential is quite complex, the new features that appear in this problem can be extracted by considering a simpler model of the potential due to Kronig and Penney. In the Kronig-Penney model [57, 58], we consider the one-dimensional motion of a particle in a periodic potential.

4.2.2 Study in the periodic potential

Let us now consider the scattering of a relativistic particle of mass m, energy E, charge e, and spin-s by a locally periodic potential: that is, it is periodic over a finite interval and zero elsewhere. This potential comprises N identical cells, each cell having a length L ($L = 2a + 2b$), called the period of the potential, and consists of a rectangular potential barrier of width $2a$ and height V_0, separated by a quantum well of size $2b$ (fig-4.3).

For simplicity, we assume that the unit cell is defined on the interval $(-a, a)$, and zero elsewhere. The cells are separated by a distance $r = 2b \geq 2a$. In this ordered system, the scattering potential in which the particle moves is given by

$$V(x) = \begin{cases} V_0 & \text{if} \quad -a < x < a, \\ 0 & \text{if} \quad |x| > a. \end{cases} \tag{4.87}$$

Here, V_0, a and b are positive constants.

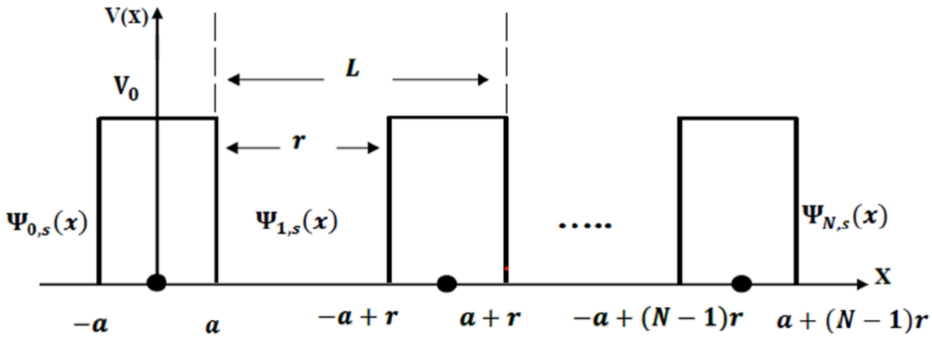

Fig-4.3: A periodic potential $V(x)$ in one dimension

The particle is subjected to a potential $V(x)$ which does not depend on time. In this case, the evolution equation can be simplified by writing the wave function associated with an eigenstate of energy E in the form $\Psi_s^{\mp}(x,t) = e^{-iEt}\Psi_s^{\mp}(x)$. Then, by carrying this expression into (4.3), and making the variable change

$$\Psi_s^{\mp,\mathrm{Pr}}(x) = \left[\frac{\sigma_3 + \sigma_1}{2}\right]^{(2s)} \Phi_s^{\mp,\mathrm{Pr}}(x), \tag{4.88}$$

we obtain for the spinors $\Phi_s^{-}(x)$ and $\Phi_s^{+}(x)$ with 2^{2s} components, the following equation:

$$\left\{ D_{KG}^2 \mathbb{I}_{2^{2s}} \pm 2is\left(\sigma_3\right)^{(2s)} \frac{dV\left(x\right)}{dx} \right\} \Phi_s^{\mp,\mathrm{Pr}}(x) = 0, \tag{4.89}$$

where D_{KG}^2 is the operator relative to the Klein-Gordon equation of spin-0, defined by Eq. (4.6).

The same equation (4.10) can also be written in $x+L$:

$$\left\{ \tilde{D}_{KG}^2 \mathbb{I}_{2^{2s}} \pm 2ise\left(\sigma_3\right)^{2s} \frac{dV(x+L)}{dx} \right\} \Phi_s^{\mp,\mathrm{Pr}}(x+L) = 0, \tag{4.90}$$

where

$$\tilde{D}_{KG}^2 = \frac{d^2}{dx^2} + (E - eV(x+L))^2 - m^2. \tag{4.91}$$

However, by applying the periodicity to $V\left(x\right) = V\left(x+L\right)$, and by reporting this expression in (4.90), and since the derivatives in equation (4.89) are the same for the new variable $(x+L)$, we obtain for the stationary wave function $\Phi_s^{\mp,\mathrm{Pr}}(x+L)$ a differential equation of type,

$$\left\{ D_{KG}^2 \mathbb{I}_{2^{2s}} \pm 2ise\left(\sigma_3\right)^{2s} \frac{dV(x)}{dx} \right\} \Phi_s^{\mp,\mathrm{Pr}}(x+L) = 0. \tag{4.92}$$

In other words $\Phi_s^{\mp,\mathrm{Pr}}(x+L)$ is also a solution in x of the same eigenvalue problem; the only way to achieve this is that the two functions $\Phi_s^{\mp,\mathrm{Pr}}(x)$ and $\Phi_s^{\mp,\mathrm{Pr}}(x+L)$ can therefore only differ by a multiplicative constant ς, i.e.

$$\Phi_s^{\mp,\mathrm{Pr}}(x+L) = \varsigma \Phi_s^{\mp,\mathrm{Pr}}(x) \tag{4.93}$$

Applying this relation again to $\Phi_s^{\mp,\mathrm{Pr}}(x+2L)$, we obtain

$$\Phi_s^{\mp,\mathrm{Pr}}(x+2L) = \varsigma\Phi_s^{\mp,\mathrm{Pr}}(x+L) = \varsigma^2\Phi_s^{\mp,\mathrm{Pr}}(x), \tag{4.94}$$

and, little by little, we see that we have

$$\Phi_s^{\mp,\mathrm{Pr}}(x+nL) = \varsigma^n\Phi_s^{\mp,\mathrm{Pr}}(x). \tag{4.95}$$

By successive shifts to the left, we obtain the same

$$\Phi_s^{\mp,\mathrm{Pr}}(x-nL) = \varsigma^{-n}\Phi_s^{\mp,\mathrm{Pr}}(x). \tag{4.96}$$

Under these conditions we see from (4.95) that if $|\varsigma| > 1$, the wave function $\Phi_s^{\mp,\mathrm{Pr}}(x)$ tends to infinity when $x \to +\infty$. We see similarly from (4.96) that if $|\varsigma| < 1$, the wave function $\Phi_s^{\mp,\mathrm{Pr}}(x)$ tends to infinity when $x \to -\infty$. For $\Phi_s^{\mp,\mathrm{Pr}}(x)$ to remain finite for $x \to \pm\infty$, it is therefore necessary that $|\varsigma| = 1$, i.e. that ς is a phase factor of the type

$$\varsigma = e^{i\theta} \qquad \text{and} \qquad \Phi_s^{\mp,\mathrm{Pr}}(x \pm nL) = \varsigma^{\pm n}\Phi_s^{\mp,\mathrm{Pr}}(x). \tag{4.97}$$

Thus, for any wave function, solution of the relativistic equation (4.89), there exists a number ς such that the translation by the mesh parameter L is equivalent to a multiplication by the phase factor $e^{i\theta}$: this is what is called Bloch's theorem [58].

We move on to solving the stationary equation (4.89) in the presence of a periodic potential $V(x)$, described by equation (4.87).

Equation (4.89) is a second-order differential equation, whose general solution is expressed as a combination of two independent particular solutions; which obviously depend on the particular form of the function $V(x)$. A simple examination of this equation leads to distinguishing two possible cases depending on whether $(E - eV(x))^2 - m^2 > 0$ (scattering states) or $(E - eV(x))^2 - m^2 < 0$ (bound states). We will look first at the scattering states.

scattering states

First, we examine the case $(E - eV(x))^2 - m^2 > 0$. The variation of the potential energy $eV(x)$ which is equal to eV_0 ($V_0 > 0$), in the region $|x| < a$ and zero outside this interval.

Under these conditions, between the cells when $(n-1)\,r+a < x < nr-a$, where $0 < n < N$, $V(x) = 0$. The equation (4.89) for stationary states, takes the form:

$$\left[\left(\frac{d^2}{dx^2} + E^2 - m^2\right)\mathbb{I}_{2^{2s}}\right]\Phi_s^{\mp,well}(x) = 0. \tag{4.98}$$

In the nth well, the solution of this second order differential equation is obviously:

$$\Phi_{s,n}^{\mp,well}(x) = \begin{pmatrix} A_n^{\mp} \\ B_n^{\mp} \end{pmatrix} e^{ik(x-nr)} + \begin{pmatrix} C_n^{\mp} \\ D_n^{\mp} \end{pmatrix} e^{-ik(x-nr)}, \tag{4.99}$$

where $k = \sqrt{E^2 - m^2} > 0$ and $(A_n^{\mp}, B_n^{\mp}, C_n^{\mp}, D_n^{\mp})$, are constants.

In the region when $nr - a < x < nr + a$, the potential for each unit cell $V\,(x) = V_0$. Under these conditions, the equation (4.89) for stationary states, takes the form:

$$\left[\left(\frac{d^2}{dx^2} + (E - eV_0)^2 - m^2\right)\mathbb{I}_{2^{2s}}\right]\Phi_s^{\mp,b}(x) = 0. \tag{4.100}$$

In the nth unit cell, the general solution of this second-order differential equation is a superposition of plane waves $e^{\pm ik_1x}$, which we write as

$$\Phi_{s,n}^{\mp,b}(x) = \begin{pmatrix} a_n^{\mp} \\ b_n^{\mp} \end{pmatrix} e^{ik_1(x-nr)} + \begin{pmatrix} c_n^{\mp} \\ d_n^{\mp} \end{pmatrix} e^{-ik_1(x-nr)}, \tag{4.101}$$

where $k_1 = \sqrt{(E - eV_0)^2 - m^2} > 0$ and $(a_n^{\mp}, b_n^{\mp}, c_n^{\mp}, d_n^{\mp})$, are constants.

Finally, in the $(n+1)$th well, $nr + a < x < (n+1)\,r - a$, the potential $V(x)$ is again identically zero ($V(x) = 0$). The eigenvalue equation takes a form absolutely analogous to (4.98). Its general solution in the $(n+1)$-th valley can be written by replacing n in the equation (4.99) by $n+1$ as

$$\Phi_{s,n+1}^{\mp,well}(x) = \begin{pmatrix} A_{n+1}^{\mp} \\ B_{n+1}^{\mp} \end{pmatrix} e^{ik(x-(n+1)r)} + \begin{pmatrix} C_{n+1}^{\mp} \\ D_{n+1}^{\mp} \end{pmatrix} e^{-ik(x-(n+1)r)}, \tag{4.102}$$

where $(A_{n+1}^{\mp}, B_{n+1}^{\mp}, C_{n+1}^{\mp}, D_{n+1}^{\mp})$, are again constants.

At this point, we therefore have the following three expressions for the generic eigenfunction $\Phi_s^{\mp,\mathrm{Pr}}(x)$, each expression being associated with a given interval for x:

$$\Phi_s^{\mp,\mathrm{Pr}}(x) = \begin{cases} \Phi_{s,n}^{\mp,well}(x) & \text{if} \quad (n-1)\,r + a < x < nr - a, \\ \Phi_{s,n}^{\mp,barrier}(x) & \text{if} \quad nr - a < x < nr + a, \\ \Phi_{s,n+1}^{\mp,well}(x) & \text{if} \quad nr + a < x < (n+1)\,r - a. \end{cases} \tag{4.103}$$

To the time-independent solutions of eq. (4.5), correspond time-dependent solutions of Eq. (4.3), which are traveling waves propagating in the positive x or negative x directions. Inserting (4.103) into (4.88), and taking into account of eq. (4.4), the solution $\Psi\,(x,t)$ with $2^{2s}\,(2s+1)$ components of equation (4.3) in the presence of a scalar potential (periodic potential) is given by:

$$\Psi^{\mathrm{Pr}}\,(x,t) = \begin{pmatrix} \Psi^{-,\mathrm{Pr}}\,(x) \\ \Psi^{+,\mathrm{Pr}}\,(x) \end{pmatrix} e^{-iEt}, \quad \Psi_s^{\mp,\mathrm{Pr}}(x) = \left[\frac{\sigma_3+\sigma_1}{2}\right]^{(2s)} \Phi_s^{\mp,\mathrm{Pr}}(x). \tag{4.104}$$

The coefficients $(A_i^{\mp}, B_i^{\mp}, C_i^{\mp}, D_i^{\mp}, i = n, n+1)$ and $(a_j^{\mp}, b_j^{\mp}, c_j^{\mp}, d_j^{\mp}, j = n)$ are not independent of each other. They are determined by the boundary conditions (4.11) and (4.13) at the points $x - nr = \pm a$.

By the play of the conditions of continuity of the wave function $\Phi_s^{\mp,\mathrm{Pr}}\,(x)$ and its derivative at $x - nr = -a$, and taking into account that $V_1(-a^-) = 0$ and $V_2(-a^+) = V_0$, we obtain:

$$\Phi_s^{\mp,\mathrm{Pr}}\left(-a^-\right) = \Phi_s^{\mp,\mathrm{Pr}}\left(-a^+\right), \tag{4.105}$$

and

$$\frac{d\Phi_s^{\mp,\mathrm{Pr}}(x)}{dx}\,|_{-a^+} = \frac{d\Phi_s^{\mp,\mathrm{Pr}}(x)}{dx}\,|_{-a^-} \pm 2iseV_0\,(\sigma_3)^{2s}\,\Phi_s^{\mp,\mathrm{Pr}}(-a). \tag{4.106}$$

$(A_i^{\mp}, B_i^{\mp}, C_i^{\mp}, D_i^{\mp}, i = n, n+1)$ and $(a_j^{\mp}, b_j^{\mp}, c_j^{\mp}, d_j^{\mp}, j = n)$. The two previous equations provide a linear system for the unknowns coefficients $(a_n^{\mp}, b_n^{\mp}, c_n^{\mp}, d_n^{\mp})$ that we can expressed them as a function of the coefficients $(A_n^{\mp}, B_n^{\mp}, C_n^{\mp}, D_n^{\mp})$. After some calculation process that is recommended to do for training, we find:

$$\begin{pmatrix} a_n^{\mp} \\ b_n^{\mp} \\ c_n^{\mp} \\ d_n^{\mp} \end{pmatrix} = \frac{1}{2k_1} \begin{pmatrix} \hat{D}_s^{\pm} & 0 & \hat{G}_s^{\pm} & 0 \\ 0 & \hat{D}_s^{\mp} & 0 & \hat{G}_s^{\mp} \\ \hat{Q}_s^{\mp} & 0 & \hat{U}_s^{\mp} & 0 \\ 0 & \hat{Q}_s^{\pm} & 0 & \hat{U}_s^{\pm} \end{pmatrix} \begin{pmatrix} A_n^{\mp} \\ B_n^{\mp} \\ C_n^{\mp} \\ D_n^{\mp} \end{pmatrix}, \tag{4.107}$$

where

$$\hat{D}_s^{\mp} = \alpha_s^{\mp} e^{i(k_1-k)a}, \quad \hat{U}_s^{\mp} = \alpha_s^{\mp} e^{-i[k_1-k]a} = \left(\hat{D}_s^{\mp}\right)^{\star},$$
$$\hat{G}_s^{\mp} = \beta_s^{\mp} e^{i[k_1+k]a}, \quad \hat{Q}_s^{\mp} = \beta_s^{\mp} e^{-i[k_1+k]a} = \left(\hat{G}_s^{\mp}\right)^{\star}, \tag{4.108}$$

and

$$\alpha_s^{\mp} = (k_1 + k \mp 2seV_0), \quad \beta_s^{\mp} = (k_1 - k \mp 2seV_0). \tag{4.109}$$

Let us now write explicitly the conditions of continuity of the wave function $\Phi_s^{\mp,\mathrm{Pr}}(x)$ and its derivative at the point $x - nr = a$. By an argument similar to that which leads to equations (4.105) and (4.106), and taking $V_1(a) = V_0$ and $V_2(a) = 0$, we obtain:

$$\Phi_s^{\mp,\mathrm{Pr}}\left(a^-\right) = \Phi_s^{\mp,\mathrm{Pr}}\left(a^+\right), \tag{4.110}$$

and

$$\frac{d\Phi_s^{\mp,\mathrm{Pr}}(x)}{dx}\,|_{a^+} = \frac{d\Phi_s^{\mp,\mathrm{Pr}}(x)}{dx}\,|_{a^-} \mp 2iseV_0\left(\sigma_3\right)^{2s}\Phi_s^{\mp,\mathrm{Pr}}(a). \tag{4.111}$$

The two previous equations provide a linear system for $(A_{n+1}^{\mp}, B_{n+1}^{\mp}, C_{n+1}^{\mp}, D_{n+1}^{\mp})$ that we can express them in terms of $(a_n^{\mp}, b_n^{\mp}, c_n^{\mp}, d_n^{\mp})$. After some manipulations, we obtain:

$$\begin{pmatrix} A_{n+1}^{\mp} \\ B_{n+1}^{\mp} \\ C_{n+1}^{\mp} \\ D_{n+1}^{\mp} \end{pmatrix} = \frac{1}{2k} \begin{pmatrix} \hat{D}_s^{\mp} e^{ikr} & 0 & -\hat{Q}_s^{\pm} e^{ikr} & 0 \\ 0 & \hat{D}_s^{\pm} e^{ikr} & 0 & -\hat{Q}_s^{\mp} e^{ikr} \\ -\hat{G}_s^{\mp} e^{-ikr} & 0 & \hat{U}_s^{\pm} e^{-ikr} & 0 \\ 0 & -\hat{G}_s^{\pm} e^{-ikr} & 0 & \hat{U}_s^{\mp} e^{-ikr} \end{pmatrix} \begin{pmatrix} a_n^{\mp} \\ b_n^{\mp} \\ c_n^{\mp} \\ d_n^{\mp} \end{pmatrix}. \tag{4.112}$$

Eliminating $(a_n^{\mp}, b_n^{\mp}, c_n^{\mp}, d_n^{\mp})$ from Eqs. (4.107) and (4.112), we get a relation connecting the solutions in the n-th and $(n+1)$-th valley

$$\begin{pmatrix} A_{n+1}^{\mp} \\ B_{n+1}^{\mp} \\ C_{n+1}^{\mp} \\ D_{n+1}^{\mp} \end{pmatrix} = \hat{M}_s \begin{pmatrix} A_n^{\mp} \\ B_n^{\mp} \\ C_n^{\mp} \\ D_n^{\mp} \end{pmatrix}, \tag{4.113}$$

where $\hat{M}_s$ is the individual transfer matrix for each cell of dimension $(2^{2s+1}(2s+1) \times 2^{2s+1}(2s+1))$, given by:

$$\hat{M}_s = \left(\begin{pmatrix} e^{ikr} & 0 \\ 0 & e^{-ikr} \end{pmatrix} \otimes \mathbb{I}_{2^{2s}(2s+1)} \right) P_s, \tag{4.114}$$

and P_s is a square matrix that does not depend on n, given by:

$$P_s = \begin{pmatrix} \rho_s^{\mp} & 0 & \sigma_s^{\mp} & 0 \\ 0 & \rho_s^{\mp} & 0 & \sigma_s^{\pm} \\ (\sigma_s^{\pm})^* & 0 & (\rho_s^{\mp})^* & 0 \\ 0 & (\sigma_s^{\mp})^* & 0 & (\rho_s^{\mp})^* \end{pmatrix}, \tag{4.115}$$

with

$$\begin{aligned} \rho_s^{\mp} &= \frac{1}{4kk_1} \left[\alpha_s^{\mp} \alpha_s^{\pm} e^{2ik_1 a} - \beta_s^{\mp} \beta_s^{\pm} e^{-2ik_1 a} \right] e^{-2ika}, \\ \sigma_s^{\mp} &= \left(\frac{\alpha_s^{\mp} \beta_s^{\pm}}{4kk_1} \right) \left[e^{2ik_1 a} - e^{-2ik_1 a} \right]. \end{aligned} \tag{4.116}$$

Using Eq. (4.113) recursively, we can express the column vector $(A_n^{\mp}, B_n^{\mp}, C_n^{\mp}, D_n^{\mp})^T$, which determines the solution of Eq. (4.89) in the n-th valley, in terms of the solution in the zeroth valley:

$$\begin{pmatrix} A_n^{\mp} \\ B_n^{\mp} \\ C_n^{\mp} \\ D_n^{\mp} \end{pmatrix} = \hat{M}_s \begin{pmatrix} A_{n-1}^{\mp} \\ B_{n-1}^{\mp} \\ C_{n-1}^{\mp} \\ D_{n-1}^{\mp} \end{pmatrix} = \hat{M}_s^2 \begin{pmatrix} A_{n-2}^{\mp} \\ B_{n-2}^{\mp} \\ C_{n-2}^{\mp} \\ D_{n-2}^{\mp} \end{pmatrix} = ... = \hat{M}_s^n \begin{pmatrix} A_0^{\mp} \\ B_0^{\mp} \\ C_0^{\mp} \\ D_0^{\mp} \end{pmatrix}, \tag{4.117}$$

where $0 < n < N$, and

$$\hat{M}_s^n = \left(\begin{pmatrix} e^{inkr} & 0 \\ 0 & e^{-inkr} \end{pmatrix} \otimes \mathbb{I}_{2^{2s}(2s+1)} \right) P_s^n. \tag{4.118}$$

From Eq. (4.117) we have

$$\begin{pmatrix} A_N^{\mp} \\ B_N^{\mp} \\ C_N^{\mp} \\ D_N^{\mp} \end{pmatrix} = \hat{M}_s^N \begin{pmatrix} A_0^{\mp} \\ B_0^{\mp} \\ C_0^{\mp} \\ D_0^{\mp} \end{pmatrix}. \tag{4.119}$$

This equation expresses the wave function to the right of the periodic potential ($x > (N-1)\,r + a$) in terms of the wave function to the left of the periodic potential ($x < -a$).

4.2.3 $\hat{\mathbf{S}}^{\mathrm{Pr}}$-Matrix formalism

Construct now the formalism of the scattering matrix for a relativistic particle of mass m, energy E, charge e, and spin-s subject to a localized periodic potential, described by equation (4.87). To analyze this problem, we always consider the case of observations made outside the action zone of the potential, i.e. to the left ($x < -a$), and to the right ($x > (N-1)r+a$). Under these conditions, the stationary solution of equation (4.3) is written:

$$\Psi_s^{\mp,\mathrm{Pr}}(x) = \begin{cases} \left[\frac{\sigma_3+\sigma_1}{2}\right]^{(2s)} \Phi_{s,0}^{\mp,\mathrm{Pr}}(x) & \text{if} \quad x < -a, \\ \left[\frac{\sigma_3+\sigma_1}{2}\right]^{(2s)} \Phi_{s,N}^{\mp,\mathrm{Pr}}(x) & \text{if} \quad x > (N-1)r + a, \end{cases} \tag{4.120}$$

where

$$\Phi_{s,0}^{\mp,\mathrm{Pr}}(x) = \begin{pmatrix} A_0^{\mp} \\ B_0^{\mp} \end{pmatrix} e^{ikx} + \begin{pmatrix} C_0^{\mp} \\ D_0^{\mp} \end{pmatrix} e^{-ikx}, \tag{4.121}$$

and

$$\Phi_{s,N}^{\mp,\mathrm{Pr}}(x) = \begin{pmatrix} A_N^{\mp} \\ B_N^{\mp} \end{pmatrix} e^{ik(x-Nr)} + \begin{pmatrix} C_N^{\mp} \\ D_N^{\mp} \end{pmatrix} e^{-ik(x-Nr)} \tag{4.122}$$

To calculate vectors $\Psi_s^{\mp,\mathrm{Pr}}(out,\pm\infty)$ and $\Psi_s^{\mp,\mathrm{Pr}}(in,\pm\infty)$, insert expressions (4.121) and (4.122) into equation (4.120), compare the result obtained with formula (3.25), and by identifying the coefficients from one member to the other, we finally find

$$\begin{cases} \Psi_s^{\mp,\mathrm{Pr}}(out,+\infty) = \left[\frac{\sigma_3+\sigma_1}{2}\right]^{(2s)} \begin{pmatrix} A_N^{\mp} \\ B_N^{\mp} \end{pmatrix} e^{-iNkr}, \\ \Psi_s^{\mp,\mathrm{Pr}}(out,-\infty) = \left[\frac{\sigma_3+\sigma_1}{2}\right]^{(2s)} \begin{pmatrix} C_0^{\mp} \\ D_0^{\mp} \end{pmatrix}, \\ \Psi_s^{\mp,\mathrm{Pr}}(in,-\infty) = \left[\frac{\sigma_3+\sigma_1}{2}\right]^{(2s)} \begin{pmatrix} A_0^{\mp} \\ B_0^{\mp} \end{pmatrix}, \\ \Psi_s^{\mp,\mathrm{Pr}}(in,+\infty) = \left[\frac{\sigma_3+\sigma_1}{2}\right]^{(2s)} \begin{pmatrix} C_N^{\mp} \\ D_N^{\mp} \end{pmatrix} e^{iNkr}. \end{cases} \tag{4.123}$$

Using the methods developed in chapter-3, we easily find that the outgoing amplitudes are related to the incoming amplitudes by the relation:

$$\begin{pmatrix} \Psi_s^{-,\mathrm{Pr}}(out,+\infty) \\ \Psi_s^{+,\mathrm{Pr}}(out,+\infty) \\ \Psi_s^{-,\mathrm{Pr}}(out,-\infty) \\ \Psi_s^{+,\mathrm{Pr}}(out,-\infty) \end{pmatrix} = \hat{S}_{-s}^{\mathrm{Pr}} \begin{pmatrix} \Psi_s^{-,\mathrm{Pr}}(in,-\infty) \\ \Psi_s^{+,\mathrm{Pr}}(in,-\infty) \\ \Psi_s^{-,\mathrm{Pr}}(in,+\infty) \\ \Psi_s^{+,\mathrm{Pr}}(in,+\infty) \end{pmatrix}, \tag{4.124}$$

where $\hat{S}_{-s}^{\mathrm{Pr}}$ is the resulting matrix, describing the scattering of a relativistic particle of spin-s in the presence of a series of identical barriers (periodic potential) at points $-a$, a, $-a+r$, $a+r$,...., $-a+(N-1)r$, $a+(N-1)r$. Since the potential in each cell is constant, the $\hat{S}_{-s}^{cell}-$matrix of each cell can be derived exactly. Once the individual scattering matrix for each cell is known, the overall scattering matrix $\hat{S}_{-s}^{\mathrm{Pr}}$ needed to relate the outgoing amplitudes to the incoming amplitudes is the product of the individual scattering matrices associated with each cell, i.e.,

$$\hat{S}_{-s}^{\mathrm{Pr}} = \left(\hat{S}_{-s}^{cell}\right)_N \left(\hat{S}_{-s}^{cell}\right)_{N-1} \ldots\ldots \left(\hat{S}_{-s}^{cell}\right)_2 \left(\hat{S}_{-s}^{cell}\right)_1 \tag{4.125}$$

In Equation (4.125), it is important to mutiply the individual matrices from right to left (and not the other way around) to obtain the overall transfer matrix since the individual matrices do not commute in general.

Since the periodic potential is composed of N identical cells, as a consequence, the resulting scattering matrix (4.125) can be written as follows

$$\hat{S}_{-s}^{\mathrm{Pr}} = \left(\hat{S}_{-s}^{cell}\right)^{N} \tag{4.126}$$

Let us now proceed to calculate the scattering $\hat{S}_{-s}^{cell}-$matrix of a unit cell. To do this, return to equation (4.113), rewrite the coefficients $\left(A_{n+1}^{\mp}, B_{n+1}^{\mp}, C_{n}^{\mp}, D_{n}^{\mp}\right)$ as a function of the coefficients $\left(A_{n}^{\mp}, B_{n}^{\mp}, C_{n+1}^{\mp}, D_{n+1}^{\mp}\right)$, therefore, a simple calculation gives:

$$\begin{pmatrix} A_{n+1}^{\mp} \\ B_{n+1}^{\mp} \\ C_{n}^{\mp} \\ D_{n}^{\mp} \end{pmatrix} = \hat{S}_{-s}^{cell} \begin{pmatrix} A_{n}^{\mp} \\ B_{n}^{\mp} \\ C_{n+1}^{\mp} \\ D_{n+1}^{\mp} \end{pmatrix}, \tag{4.127}$$

where $\hat{S}_{-s}^{cell}$ is the individual scattering matrix for each cell, given by

$$\hat{S}_{-s}^{cell} = \frac{1}{\left(\rho_s^{\mp}\right)^{*}} \left(\begin{pmatrix} e^{ikr} & 0 \\ 0 & e^{ikr} \end{pmatrix} \otimes \mathbb{I}_{2^{2s}(2s+1)} \right) \times$$
$$\begin{pmatrix} 1 & 0 & \sigma_s^{\mp} e^{ikr} & 0 \\ 0 & 1 & 0 & \sigma_s^{\pm} e^{ikr} \\ -\left(\sigma_s^{\pm} e^{ikr}\right)^{*} & 0 & 1 & 0 \\ 0 & -\left(\sigma_s^{\mp} e^{ikr}\right)^{*} & 0 & 1 \end{pmatrix}. \tag{4.128}$$

We now move on to the diagonalization of the $\hat{S}_{-s}^{cell}$-matrix. To illustrate this, as usual, we write the eigenvalue equation

$$\det\left(\hat{S}_{-s}^{cell} - \lambda_s \mathbb{I}_{2^{(2s+1)}(2s+1)}\right) = 0. \tag{4.129}$$

By a simple calculation, we find

$$\lambda_s^{\pm} = \frac{e^{ikr}}{\left(\rho_s^{\mp}\right)^{*}} \left(1 \pm i\sqrt{\sigma_s^{+}\left(\sigma_s^{-}\right)^{*}}\right), \tag{4.130}$$

and the diagonal matrix which represents $\hat{S}_{-s}^{cell}$ in the partial wave basis is as follows

$$\hat{S}^{cell}_{-s} = \mathbb{I}_{2^{2s(2s+1)}} \otimes \begin{pmatrix} \lambda^+_s & 0 \\ 0 & \lambda^-_s \end{pmatrix}. \tag{4.131}$$

Using the current conservation property (3.59), and introducing the phase shifts relative to even waves δ^0_s and odd waves δ^1_s, we can finally express the expression (4.131) in a more explicit form

$$\hat{S}^{cell}_{-s} = \mathbb{I}_{2^{2s(2s+1)}} \otimes \begin{pmatrix} e^{2i\delta^0_s} & 0 \\ 0 & e^{2i\delta^1_s} \end{pmatrix}, \tag{4.132}$$

with

$$e^{2i\delta^l_s} = \frac{e^{ikr}}{\left(\rho^{\mp}_s\right)^*}\left(1 + (-1)^l\, i\sqrt{\sigma^+_s\left(\sigma^-_s\right)^*}\right), \qquad l = 0, 1. \tag{4.133}$$

According to (4.126) and (4.132), the overall scattering matrix $\hat{S}^{\text{Pr}}_{-s}$ describing the entire region is then found by cascading (multiplying) the individual scattering matrices for the individual cells:

$$\hat{S}^{\text{Pr}}_{-s} = \mathbb{I}_{2^{2s(2s+1)}} \otimes \begin{pmatrix} e^{2in\delta^0_s} & 0 \\ 0 & e^{2in\delta^1_s} \end{pmatrix}. \tag{4.134}$$

Having obtained the shape of the scattering matrix, we can then calculate the reflection and transmission coefficients $\mathbb{R}^{cell}_s$ and $\mathbb{T}^{cell}_s$, as well as the cross-section $\left(\sigma^t_s\right)^{cell}$ for a unit cell.

The transmission and reflection coefficients are calculated from formulas (3.83) and (3.84) respectively, we obtain

$$\begin{aligned} \mathbb{R}^{cell}_s &= \frac{1}{4}\left|e^{2i\delta^0_s} - e^{2i\delta^1_s}\right|^2 = \frac{1}{4}\left|\frac{\sqrt{\sigma^+_s\left(\sigma^-_s\right)^*}}{\left(\rho^{\mp}_s\right)^*}\right|^2 \\ \mathbb{T}^{cell}_s &= \frac{1}{4}\left|e^{2i\delta^0_s} + e^{2i\delta^1_s}\right|^2 = \frac{1}{4}\left|\frac{1}{\left(\rho^{\mp}_s\right)^*}\right|^2 \end{aligned} \tag{4.135}$$

And for the total cross-section, we find:

$$\left(\sigma^t_s\right)^{cell} = \left|\frac{e^{ikr}}{\left(\rho^{\mp}_s\right)^*} - 1\right|^2 + \left|\frac{\sqrt{\sigma^+_s\left(\sigma^-_s\right)^*}}{\left(\rho^{\mp}_s\right)^*}\right|^2. \tag{4.136}$$

Finally, the general expressions for the transmission and reflection probabilities, as well as the total cross section, are given by:

$$\mathbb{T}_s = \left(\mathbb{T}_s^{cell}\right)^N, \quad \mathbb{R}_s = \left(\mathbb{R}_s^{cell}\right)^N, \quad \left(\sigma_s^t\right) = \left(\left(\sigma_s^t\right)^{cell}\right)^N. \tag{4.137}$$

bound states

Defined by quantum mechanics, the electrons of an isolated atom gravitate around the nucleus occupying certain energy levels. These levels being quantized can only take two electrons of opposite spin per level, according to the Pauli principle [59]. The filling of the electrons is done by shells whose energy levels are very close to each other. In the shell n, there are n^2 possible levels receiving two electrons each, in other words, $2n^2$ electrons per shell.

In a solid, where the atoms are arranged according to a periodic network, each atom gives rise to a multitude of very close levels that can be occupied by a pair of electrons of opposite spin. Given the large number of possible states, these permitted energy levels are seen as continuous bands while being separated by other forbidden ones corresponding to energy levels that an electron cannot have.

The layers closest to the nucleus that are saturated for the isolated atom thus correspond to saturated bands for the solid state. Inside these bands, all the energy levels are occupied and no additional electrons can penetrate them.

The first band of real interest is the valence band which corresponds to the valence electrons. This band is generally saturated but its electrons can leave it more or less easily depending on the nature of the solid. Finally, after the valence band we encounter the conduction band; depending on the case is empty or incomplete. The energy separation E_g between the conduction band and the valence band, called the forbidden band width, determines the electrical behavior of the body [60].

To determine the wave function $\Phi^{\mp,\mathrm{Pr}}(x)$ of the particle for a stationary state of energy E, the experience acquired in the previous sections now allows us to write, in each region where the potential is constant, a linear combination of exponential functions of real or imaginary argument depending on whether $(E - eV(x))^2 - m^2 \lessgtr 0$.

In the intervals $nr - a < x < nr + a$ where $V(x)$ is zero, the particle is free. In this case, the solution (4.99) is still valid

$$\Phi_{s,n}^{\mp,well}(x) = \begin{pmatrix} A_n^{\mp} \\ B_n^{\mp} \end{pmatrix} e^{ik(x-nr)} + \begin{pmatrix} C_n^{\mp} \\ D_n^{\mp} \end{pmatrix} e^{-ik(x-nr)}, \tag{4.138}$$

In the region $nr - a < x < nr + a$, where $V(x) = V_0$ and $(E - eV_0)^2 - m^2 < 0$. k_1 is now pure imaginary, so under the nth barrier of the potential, we can therefore obtain the solution of equation (4.89) from solution (4.101) by simply replacing ik_1 by $\kappa = \sqrt{m^2 - (E - eV_0)^2}$. Under these conditions the wave function (4.101) is now written:

$$\hat{\Phi}_{s,n}^{\mp,b}(x) = \begin{pmatrix} a_n^{\mp} \\ b_n^{\mp} \end{pmatrix} e^{\kappa(x-nr)} + \begin{pmatrix} c_n^{\mp} \\ d_n^{\mp} \end{pmatrix} e^{-\kappa(x-nr)}, \tag{4.139}$$

Finally, in the region $nr + a < x < (n+1)r - a$, and to the right of the nth barrier of the potential, as $V(x)$ is a periodic function, the periodicity conditions are applied and taking into account Bloch's theorem (4.97). The function $\Phi_s^{\mp,\mathrm{Pr}}(x)$ solution of equation (4.89) can thus be expressed as a function of $\Phi_s^{\mp,\mathrm{Pr}}(x - L)$, which written as:

$$\Phi_{s,n+1}^{\mp,well}(x) = e^{i\theta}\left(\begin{pmatrix} A_n^{\mp} \\ B_n^{\mp} \end{pmatrix} e^{ik(x-(n+1)r)} + \begin{pmatrix} C_n^{\mp} \\ D_n^{\mp} \end{pmatrix} e^{-ik(x-(n+1)r)}\right). \tag{4.140}$$

At this point, we therefore have the following three expressions for the wave function, each expression being associated with a given interval for x:

$$\Phi_s^{\mp,\mathrm{Pr}}(x) = \begin{cases} \Phi_{s,n}^{\mp,well}(x) & \text{if} \quad (n-1)r + a < x < nr - a, \\ \hat{\Phi}_{s,n}^{\mp,b}(x) & \text{if} \quad nr - a < x < nr + a, \\ e^{i\theta}\Phi_{s,n}^{\mp,well}(x - L) & \text{if} \quad nr + a < x < (n+1)r - a. \end{cases} \tag{4.141}$$

Since the potential has a finite jump, the boundary conditions (4.105), (4.106), (4.110), and (4.111) are adequate. By writing the boundary conditions of the wave function and its derivative for $x - nr = \pm a$, we obtain $2^{2(2s+1)}$ homogeneous equations relating to the coefficients $A_n^{\mp}$, $B_n^{\mp}$, $C_n^{\mp}$, $D_n^{\mp}$, $a_n^{\mp}$, $b_n^{\mp}$, $c_n^{\mp}$, and $d_n^{\mp}$. After some simple manipulations, by writing this system of equations in matrix form,

$$\widetilde{M}_s \xi_s^{\mp} = 0, \tag{4.142}$$

where $\widetilde{M}_s$ is a square matrix $\left(2^{2(2s+1)} \times 2^{2(2s+1)}\right)$ and $\xi_s^{\mp}$ is a vector with $2^{2(2s+1)}$ components.

We are in the presence of a linear system of $2^{2(2s+1)}$ equations with $2^{2(2s+1)}$ unknowns. The column of zeros to the right of this equation indicates that the only possible solution to this system of equations is that the coefficients are all zero, unless the determinant, associated with the system is zero. In this case, the $2^{2(2s+1)}$ equations are not independent. The trivial solution is not acceptable since it describes a particle that is nowhere. Acceptable solutions therefore exist in the only case where the determinant formed on the table of the matrix $\widetilde{M}_s$ is zero.

There are different ways to solve equation (4.142). Using a symbolic calculation software (Mathematica or Maple or other), we can solve this equation numerically.

For a Klein Gordon particle ($s = 0$), the $\widetilde{M}_s-$matrix reduces to a square matrix (4×4), given by

$$\widetilde{M}_0 = \begin{pmatrix} e^{-\kappa(a+nr)} & e^{\kappa(a+nr)} & -e^{-ik(a+nr)} & -e^{ik(a+nr)} \\ -e^{\kappa(a-nr)} & -e^{-\kappa(a-nr)} & e^{i\theta}e^{-ik(a+(n+1)r)} & e^{i\theta}e^{ik(a+(n+1)r)} \\ \kappa e^{-\kappa(a+nr)} & -\kappa e^{\kappa(a+nr)} & -ike^{-ik(a+nr)} & ike^{ik(a+nr)} \\ -\kappa e^{\kappa(a-nr)} & \kappa e^{-\kappa(a-nr)} & e^{i\theta}ike^{-ik(a+(n+1)r)} & -e^{i\theta}ike^{ik(a+(n+1)r)} \end{pmatrix}. \tag{4.143}$$

It remains to examine the determinant of the matrix $\widetilde{M}_0$ and impose that it vanishes. The calculation gives the condition:

$$\cos\theta = \frac{(\kappa^2 - k^2)}{2k\kappa} \sin kr \sinh 2a\kappa + \cos kr \cosh 2a\kappa. \tag{4.144}$$

This equation shows that some intervals in κ and k are excluded because the right-hand side of (4.144) can be larger than one in modulus: these areas are called forbidden bands.

The quantities κ and k are functions of E. The condition $\det \widetilde{M} = 0$ can be considered as an equation that E must satisfy.

Since the first member of (4.144) is a cosine whose modulus is always between zero and 1, the same must be true of the second member, hence

$$-1 \leq \frac{(\kappa^2 - k^2)}{2k\kappa} \sin kr \sinh 2a\kappa + \cos kr \cosh 2a\kappa \leq 1. \tag{4.145}$$

We thus obtain restrictive conditions for the energy. We will see that only the values of E contained in certain bands are possible. We can say that there is quantification, not in the form of a discrete spectrum, but in the form of a spectrum of bands (see fig-4.4).

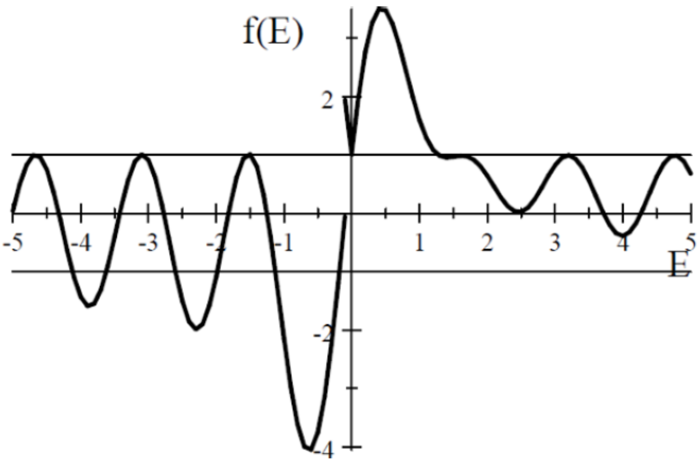

Fig-4.4: bound states

The results we have obtained are of capital importance in solid-state physics: in fact, an electron in a crystal lattice is subjected to a three-dimensional periodic potential, but the results obtained below in one dimension are generalized to three dimensions, coming from the interactions of this electron with the ions of the crystal lattice. The periodicity of the potential leads to the existence of energy bands, which, together with the Pauli principle, are the basis of our understanding of electrical conductivity.

Conclusion

The content of this manuscript generally concerns the treatment of certain problems of relativistic quantum mechanics via the diffusion matrix formalism.

In terms of form, the thesis consists of an introduction and four clearly written chapters, followed by a conclusion with bibliographic references.

The first chapter was devoted to a bibliographic analysis, in which we deal with the Klein-Gordon equation, the first candidate to simultaneously satisfy relativistic requirements and quantum postulates and an obligatory passage to arrive at another quantum and relativistic equation, the Dirac equation. The difficulties of interpreting the Klein-Gordon equation, in particular the existence of negative energy solutions, and the consequences that result from them are well recalled, as well as the passage towards an equation that takes into account the coupling with the electromagnetic field.

The second chapter was devoted to a bibliographic analysis concerning the collision theory. The notion of scattering cross-section is introduced historically in the context of classical mechanics. Then the transition to non-relativistic quantum mechanics is addressed with the introduction of the scattering matrix and the choice of the quantum representation that best reveals the diffusion problems. In particular, this chapter presents the calculation at different orders of perturbation theory concerning the scattering amplitude.

The third chapter is composed essentially of two parts. In the first part, we unified the Klein Gordon equation of spin-0 particles and the quadratic form of the Dirac equation of spin-1/2 particles into a single relativistic wave equation called the relativistic wave equation of spin-s ($s = 0.1/2$). In the second part, based on the steady states of scattering of a relativistic particle of spin-s in the presence of a localized electromagnetic field, we have constructed the formalism of the one-dimensional scattering matrix. The formalism is well exposed. and the considerations of symmetry C_s, P_s, and T_s, and the consequences that emerge from them on the wave functions and hence on the scattering matrix are recalled.

To consider the minimal changes in the exact asymptotic development of the free case, the phase shift method is used and allows us to extract the phase shifts, the scattering amplitudes, the reflection and transmission coefficients, as well as the total cross-section.

Finally, the last chapter is dedicated to the application of the scattering matrix formalism for relativistic particles of spin-s ($s = 0, 1/2$) interacting with scalar potentials having some symmetry and range properties.

This chapter is composed essentially of two parts. In the first part, we solved the relativistic wave equation of spin-s ($s = 0, 1/2$), in the Woods-Saxon potential. The exact solutions of the equation in question have been given in analytical form using the hypergeometric functions. The boundary conditions in the case of a potential jump have been determined in the general case. From the Asymptotic Behavior, we derived the scattering matrix $\hat{S}_{-s}^{WS}$. Using the partial wave basis (representation of partial waves, even and odd waves), we gave the expression of the matrix $\hat{M}_{-s}^{WS}$, the phase shifts $\delta_s^{l,WS}$ $(l = 0, 1)$, the wave function, the scattering amplitudes $f_s^{\pm,WS}$, the transmission and reflection coefficients T_s^{WS} and R_s^{WS}, as well as the total cross-section $\sigma^{t,WS}$ in the case of the Woods-Saxon potential.

The same method was adopted for the case of the barrier potential. By a limit procedure of that of Woods-Saxon when $\alpha \to 0^+$, we calculated the wave function, the scattering $\hat{S}_{-s}^{b}$-matrix, the $\hat{M}_{-s}^{b}$-matrix in the basis of the partial waves, the phase shifts $\delta_s^{l,b}$, the scattering amplitudes $f_s^{\pm,b}$, the transmission and reflection coefficients T_s^{WS} and R_s^{WS}, as well as the total cross-section $\sigma^{t,b}$.

The same method was adopted for the case of the periodic potential and allowed us to calculate the wave function, the scattering $\hat{S}_{-s}^{\mathrm{Pr}}-$matrix, the phase shifts $\delta_s^{l,\mathrm{Pr}}$, the scattering amplitudes $f_s^{\pm,\mathrm{Pr}}$, the transmission and reflection coefficients T_s^{Pr} and R_s^{Pr}, as well as the total cross-section $\sigma^{t,\mathrm{Pr}}$. Next, we addressed the problem of bound states and calculated the allowed and forbidden energy bands.

This approach proved to be rigorous and allowed us to obtain results consistent with those in the literature.

Bibliography

[1] N. Zettili, Quantum mechanics : Concepts and applications, Wiley India Pvt. Ltd, 2022.

[2] C. Joas, C. Lehner, The classical roots of wave mechanics: Schrödinger's transformations of the optical-mechanical analogy, Elsevier Ltd, Vol 40 Issue 4 338-351, 2009.

[3] C. L. Levada, H. Maceti, I. J. Lautenschleguer, Review of the Schrödinger wave equation, IOSR Journal of applied chemistry, Vol 11 Issue 4 01-07, 2018.

[4] J. H. Smith, Introduction to special relativity, Dover Publications, 2016.

[5] JP. C. Mbagwu1, Z. L. Abubakar, J. O. Ozuomba, A review article on Einstein special theory of relativity, International journal of theoretical and mathematical physics, 10(3): 65-71, 2020.

[6] A. Wachter, Relativistic Quantum Mechanics, Springer Science + Business Media B.V, 2011.

[7] M. D. Kostin, Derivation of the Hamiltonian form of the Klein-Gordon equation, Physics letters A Vol. 125, N^0 9, 1987.

[8] T. Ohlsson, Relativistic quantum mechanics from advanced quantum mechanics to introductory quantum field theory, Cambridge university press, 2011.

[9] Dirac P A M The quantum theory of the electron Proc. R. Soc. A 117 610–24, 1928.

[10] C. M. Madrid Casado, A brief history of the mathematical equivalence between the two quantum mechanics, Americain journal of physics education, Vol.2 $N^0$2, 2008.

[11] David W. Ward, How to derive the Schrödinger equation, Am.J.Phys, 2008.

[12] R. Fitzpatrick, Maxwell's equations and the principles of electromagnetism, Laxmi Publications, 2022.

[13] P. Mann, Lagrangian and hamiltonian dynamics, Oxford University Press, 2018.

[14] V. Rastogi, A. Mukherjee, A. Dasgupta, A review on extension of Lagrangian-Hamiltonian mechanics, J. Braz. Soc. Mech. Sci. & Eng. 33 (1), 2011.

[15] A. G. Rojo, Optical mechanical analogy and Hamiltonization of a nonholonomic system, Physical review E 88, 013204, 2013.

[16] V. Sahni, Xiao-Yin Pan, Schrödinger theory of electrons in electromagnetic fields: New perspectives, Academic Editor: Jianmin Tao, 2017.

[17] L. H. Buch, H. H. Denman, Solution of the Schrödinger equation for some electric field problems, : American journal of physics 42, 304, 1974.

[18] M. N. CéLérier, L. Nottale, Electromagnetic Klein Gordon and Dirac equations in scale relativity, International journal of modern physics A Vol. 25, N^0. 22 4239–4253, 2010.

[19] S. Schweber, An Introduction to Relativistic Quantum Field Theory, Dover Publications; Illustrated edition, 2005.

[20] Vladislav G. Bagrov, Dmitry Gitman, The Dirac Equation and its Solutions, Walter de Gruyter & Co, 2014.

[21] W. Pauli, V. Weisskopf, Helv, Phys. Acta, 7, 709, 1934.

[22] C. D. Anderson, and Neddermeyer, S. H. Positron from gamma rays. Phys. Rev. 43, 1933.

[23] H. Goldstein, C. Poole, J. Safko, Classical mechanics, Pearson, 2011.

[24] L. P. Fulcher, B. F. Davis, D. A. Rawe, An approximate method for classical scattering problems, Am. J. Phys. 44, 956–959, 1976.

[25] R. G. Newton, Scattering theory of waves and particles, Dover publications, 2013.

[26] M. Pijnenburg, G. Cusin, C. Pitrou, J. P. Uzan, Rutherford scattering of quantum and classical fields, Am. J. Phys. 92, 597–605, 2024.

[27] A. G. Sitenko, Scattering theory, Springer-Verlag Berlin and Heidelberg GmbH & Co. KG, 2012.

[28] Y. Tikochinsky, Variable Amplitude Equations for One-Dimensional Scattering, Annals of physics 103, 185-197, 1977.

[29] S. Selcuk Bayin, Mathemathecal methods in science and engineering, John Wiley & Sons Ltd, 2006.

[30] R. P. Shaw, N. Makris, Green's functions for Helmholtz and Laplace equations in heterogeneous media, Engineering analysis with boundary elements 10 179-183, 1992.

[31] T. S. Angell, R. E. Kleinman, Modified Green's functions and the third boundary value problem for the Helmholtz equation, Journal OURNAL of mathematical analysis and applications 97, 81-94, 1983.

[32] M. J. Ablowitz, A. S. Fokas, Introduction to complex variables and applications, Paperback publication, 2021.

[33] Y. A. Melnikov and M. Y. Melnikov, Green's functions. Construction and applications, Walter de Gruyter Berlin-Boston, 2012.

[34] V. E. Barlette, M. M. Leite, S. K Adhikari, Integral equations of scattering in one dimension, American journal of physics 69, 1010, 2001.

[35] V. E. Barlette, M. M. Leite, S. K Adhikari, Quantum scattering in one dimension, Eur. J. Phys. 21, 435–440, 2000.

[36] Hyo J. Eom, Wave scattering theory: A series approach based on the Fourier transformation, Springer, 2011.

[37] S. K. Dutta, W. A. Wilson, and A. E. S. Green, Modified Born approximation and elastic scattering by weak central potentials, Journal of mathematical physics 9, 578, 1968.

[38] K. Khounfais, T. Boudjedaa, L. Chetouani, Scattering matrix for Fehbach-Villars equation for spin 0 and 1/2 : Wods-Saxon potential, Czechoslovak J. physics. 54.7. pp. 697-792, 2004.

[39] Y. Nogami and C. K. Ross : Am. J. Phys. 64. 923, 1996.

[40] Mi. V. Moskalets, Scattering matrix approach to non-stationary quantum transport, by Imperial College Press, 2012.

[41] S. A. Hamraoui, K. Khounfais, Scattering matrix formalism for spin s (s=0, 1/2) particles, The African review of physics 14 :0020, 2019.

[42] W. Greiner, Relativistic Quantum Mecanics. Wave equations, Springer Science & Business Media, 2000.

[43] P. Boonserm, M. Visser, One dimensional scattering problems: A pedagogical presentation of the relationship between reflection and transmission amplitudes, Thai Journal of Mathematics, 83-97, 2010.

[44] A. Messiah, Quantum mechanics, volume-2, Dover Publications, 1999.

[45] Z. J. Ajaltouni, Symmetry and relativity: From classical mechanics to modern particle physics, Natural Science 6 191-197, 2014.

[46] J. H. Eberly, "Quantum scattering theory in one dimension," Am. J. Phys., vol. 33, p. 771, 1965.

[47] B. Stec, C. Jedrzejek, "Resonance scattering by a double square-well potential," Eur. J. Phys., vol. 11, p. 75, 1990.

[48] Shi-Hai Dong, Zhong-Qi Ma, The Dirac equation with a delta potential, Foundations of a physics letters, Vol 15, N^0 2, 2002.

[49] K. Heyde, The nuclear shell model: Study Edition, Springer, 2013.

[50] S. Flügge, Practical Quantum Mechanics, Vol. 1, Springer, Berlin, 1994.

[51] C. Rojas and V. M. Villalba, "Scattering of a Klein-Gordon particle by a Woods-Saxon potential," Phys. Rev., vol. A71, Art. no. 052101, 2005.

[52] H. Bíla, V. Jakubský, M. Znojil, Comment on: "Solution of the Dirac equation for the Woods–Saxon potential with spin and pseudospin symmetry", Phys. Lett. A 338, 90, 2005.

[53] M.G. Garcia, A.S. de Castro, Scattering and bound states of spinless particles in a mixed vector-scalar smooth step potential, Annals of Physics 324, 2372–2384, 2009.

[54] N. Bourouis, K. Khounfais, M. Bouatrous, Relativistic Ŝ-matrix formulation in one dimension for particles of spin-s (s = 0, 1/2), Z. Naturforsch, De Gruyter, 2023.

[55] M. Abramowitz and I. A. Stegun, Handbook of mathematical functions, New York: Dover, 1965.

[56] W. W. Bell, Special functions for scientists and engineers D. Van Nostrand Company Canada, Ltd, 1968.

[57] F. Marsiglio, R. L. Pavelich, The tight-binding formulation of the Kronig-Penney model, Scientific Reports, 2017.

[58] D. Jena, Quantum physics of semiconductor materials and devices, Oxford University Press, 2022.

[59] Ilya G. Kaplan, The Pauli exclusion principle: origin, verifications and applications Wiley, 2017.

[60] R. E. Peierls, Quantum Theory of Solids, Oxford University Press, USA, 1996.

APPENDIX

Published Paper

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Relativistic $\hat{S}$-matrix formulation in one dimension for particles of spin-s ($s = 0, 1/2$)

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Abstract: In quantum scattering theory, the time evolution of a physical system can be described as a series of unitary transformations. The operator of this transformation will be denoted $\hat{S}$; the corresponding matrix is the $\hat{S}$-matrix (scattering matrix). This last object contains all the information on the broadcast process associated with the operator $\hat{S}$ The present work has two objectives: To develop the one-dimensional formalism of the scattering matrix of relativistic particles of spin-s ($s = 0, 1/2$) in the presence of a localized electromagnetic field on the one hand and on the other hand to analyze the solutions of the problem of scattering states of relativistic particles of spin-s in interaction with some localized scalar potentials via the $\hat{S}$-matrix formalism.

Keywords: relativistic wave equation of spin-s; $\hat{S}$-matrix formalism; Woods–Saxon potential

1 Introduction

In classical scattering theory, the state of the incident particle (which is free) is entirely determined by its momentum. The same is true for the outgoing particle. At the quantum level, it is then generally not possible to predict with certainty which final state will result from a given collision; we, therefore, seek only to predict the probabilities for a certain final state. For this, we will study the evolution of the wave function associated with the incident particle in interaction with a localized field. The problem, therefore, consists in establishing the relation between the initial state Φ^{in} and the final state Φ^{out}. In quantum mechanics, if we know the scattering operator $\hat{S}$ (or $\hat{S}$-matrix) [1, 2], we can determine the final state from any initial states.

This article presents the continuity of our research work published in article [3], in which we analytically determined the solutions of the Feshbach-Villars equation, for the particles of spin-s ($s = 0, 1/2$) interacting with a symmetric scalar field, described by the Woods–Saxon potential, which is one of the most used models in nuclear physics (layer model). Then, we constructed the one-dimensional formalism of the scattering matrix for Feshbach-Villars particles, with spin-s interacting with this potential.

On the other hand, in this work, we set out to develop a general formalism of the scattering matrix for relativistic particles of spin 0 and 1/2, governed respectively by the Klein Gordon and Dirac equations in interaction with a localized external electromagnetic field.

The content of this work is organized as follows. In Section 2, we will try to find a way to bring together in a unified writing the two equations of relativistic quantum mechanics, which are the Klein–Gordon equation of spin−0 and the quadratic form of the Dirac equation of spin−1/2 subjected to the action of an electromagnetic four-potential $A_\mu = \left(A_0, \vec{A}\right)$, where A_0 is the scalar potential, and $\vec{A}$ the vector potential, into a single equation, called the relativistic wave equation of spin-s ($s = 0$, 1/2). In Section 3, we construct the one-dimensional $\hat{S}$-matrix formalism for relativistic particles of spin-s in the presence of a localized electromagnetic field. Finally, in Section 4, in order to be able to make the comparison of the results obtained in the article of reference [3] and the results of this work, as an application we study the scattering of a relativistic particle of energy E, mass m, charge e and spin-s by a localized field, composed of a time-independent scalar potential (Woods–Saxon potential, rectangular barrier potential) $A_0(x, t) = V(x)$ and a vector potential $\vec{A}(x, t) = 0$.

2 Relativistic wave equation of spin-s ($s = 0, 1/2$)

Recall that the relativistic wave equations that generalize the Schrödinger equation are the Klein–Gordon equation, which describes the dynamics of spin-0 particles, with or without mass (by setting $\hbar = c = 1$).

$$\left\{ \left(\frac{\partial}{\partial t} + ieA_0 \right)^2 - \left(\vec{\nabla} - ie\vec{A} \right)^2 + m^2 \right\} \Psi_0(x, t) = 0, \quad (1)$$

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and the Dirac equation, which describes massive spin-1/2 particles.

$$(\not{p} - e\not{A} - m)\Psi_{1/2}(x,t) = 0, \tag{2}$$

where $A_0(x,t)$ and $\vec{A}(x,t)$ are the components of the quadrivector potential A_μ. $\not{p} - e\not{A} = \gamma^\mu(i\partial_\mu - eA_\mu)$ and, γ^μ ($\mu = 0, 1, 2, 3$) are gamma matrices.

By adopting for any matrix A the following notation:

$$(A)^{2s} = \begin{cases} 1 & \text{for} \quad s = 0 \\ A & \text{for} \quad s = 1/2, \end{cases} \tag{3}$$

and introducing a new variable.

$$\Psi_s(x,t) = (\not{p} - e\not{A} + m)^{2s}\Phi_s(x,t), \quad s = 0, \frac{1}{2}, \tag{4}$$

in this case, Eqs. (1) and (2) can be expressed by a single relation, called relativistic equation of spin-s particles [3].

$$\left\{\left[\left(\frac{\partial}{\partial t} + ieA_0\right)^2 - \left(\vec{\nabla} - ie\vec{A}\right)^2 + m^2\right]\mathbb{I}_{2^{2s}(2s+1)} + se(\sigma F)^{2s}\right\}\Phi_s(x,t) = 0. \tag{5}$$

$\Phi_s(x,t)$ has $2^{2s}(2s+1)$ components, and I_d is the unity matrix of dimension d. F is the electromagnetic tensor defined by the components $F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu$ and $(\sigma F) = \sigma^{\mu\nu}F_{\mu\nu}$with $\sigma^{\mu\nu} = \frac{i}{2}[\gamma^\mu, \gamma^\nu]$.

For $s = 0$, Eq. (5) reduces to the Klein–Gordon equation (KG-0), and for $s = 1/2$ we obtain the quadratic form of the Dirac equation (or KG-1/2) [4].

Now, it is easy to check that it is possible to get from Eq. (5) the following equation of continuity:

$$\partial_\mu J^\mu = 0, \tag{6}$$

where

$$J^\mu = \frac{1}{2im}\left\{\bar{\Phi}_s\frac{\partial}{\partial x^\mu}\Phi_s - \Phi_s\frac{\partial}{\partial x^\mu}\bar{\Phi}_s\right\} + \frac{e}{m}A^\mu\bar{\Phi}_s\Phi_s, \tag{7}$$

where $\bar{\Phi}_s = \Phi_s^\dagger(\gamma^0)^{2s}$ and $\Phi_s^\dagger = (\Phi_s^*)^T$. The term $1/(2im)$ is introduced for convenience.

The Lorentz invariant dot product is defined as follows [5, 6],

$$\begin{aligned}\langle\Phi_s \mid \Phi_s\rangle &= \int J^0 \mathrm{d}x \\ &= \int\left\{\bar{\Phi}_s\left[\left(\frac{\partial}{\partial t} + eA^0\right)\Phi_s\right] - \left[\left(\frac{\partial}{\partial t} - eA^0\right)\bar{\Phi}_s\right]\Phi_s\right\}\mathrm{d}x.\end{aligned} \tag{8}$$

Using the Weyl representation of the gamma matrices.

$$\gamma^0 = \begin{pmatrix} 0 & \mathbb{I}_2 \\ \mathbb{I}_2 & 0 \end{pmatrix}, \ \vec{\gamma} = \begin{pmatrix} 0 & -\vec{\sigma} \\ \vec{\sigma} & 0 \end{pmatrix}, \tag{9}$$

$\vec{\sigma} = (\sigma_1, \sigma_2, \sigma_3)$ are the Pauli matrices describing the spin dynamics. Thanks to this choice of representation, eq. (5) breaks down into a system of two equations.

$$\begin{pmatrix} H_s^-(x,t) & 0 \\ 0 & H_s^+(x,t) \end{pmatrix}\begin{pmatrix} \Phi_s^-(x,t) \\ \Phi_s^+(x,t) \end{pmatrix} = 0, \tag{10}$$

where $\Phi_s(x,t) = (\Phi_s^-(x,t), \Phi_s^+(x,t))^T$. $\Phi_s^-(x,t)$ and $\Phi_s^+(x,t)$ are 2^{2s}-component wave functions. The Hamiltonians $H_s^\mp$ are given by:

$$\begin{aligned}H_s^\mp = &\left[\left(\frac{\partial}{\partial t} + ieA_0\right)^2 - \left(\vec{\nabla} - ie\vec{A}\right)^2 + m^2\right]I_{2^{2s}} \\ &\pm 2ise(\vec{\sigma})^{2s}\left(\vec{E} \pm i\vec{B}\right),\end{aligned} \tag{11}$$

$\vec{E}$ and $\vec{B}$ are the electric and magnetic fields.

3 Relativistic $\hat{S}$-matrix formulation

Let's now come to the construction of the one-dimensional scattering matrix formalism, of a relativistic particle of mass m, energy E, charge e, and spin-s ($s = 0, 1/2$) by a localized electromagnetic field $A_\mu(x,t)\xrightarrow{|x|\to+\infty}0$.

At large distance ($|x| \to \infty$), the field $A_\mu(x,t) \to 0$. Under these conditions, the hamiltonian $H_s^\mp$ can be approximated by the Hamiltonian of a free particle $H_s^{\mp,0} = \sqrt{k^2 + m^2}$ ($k^2 = E^2 - m^2$). Therefore, among all the solutions of equation (10), we will choose a particular class of solutions, called stationary states,

$$\Phi_s(x,t) = \Phi_s(x)e^{-iEt} = \begin{pmatrix} \Phi_s^-(x) \\ \Phi_s^+(x) \end{pmatrix}e^{-iEt}. \tag{12}$$

Asymptotically, the particle is considered free; the stationary solution $\Phi_s(x)$ is a linear combination of plane waves $e^{\pm ikx}$ ($k = \sqrt{E^2 - m^2} > 0$). More precisely, the wave function $\Phi_{s,L}^\mp(x)$ (arrival of $-\infty$) and $\Phi_{s,R}^\mp(x)$ (arrival of $+\infty$) behave as follows [3, 7]:

$$\begin{aligned}\Phi_{s,L}^\mp(x) &= \begin{cases} 1_s^\mp e^{ikx} + R_{s,L}^\mp e^{-ikx} & x \to -\infty, \\ T_{s,L}^\mp e^{ikx} & x \to +\infty, \end{cases} \\ \Phi_{s,R}^\mp(x) &= \begin{cases} 1_s^\mp e^{-ikx} + R_{s,R}^\mp e^{ikx} & x \to +\infty, \\ T_{s,R}^\mp e^{-ikx} & x \to -\infty. \end{cases}\end{aligned} \tag{13}$$

Here, $T^{\mp}_{s,L,R}$, $R^{\mp}_{s,L,R}$ and $1^{\mp}_{s}$ are vectors with 2^{2s} components. $\left(T^{\mp}_{s,L}, R^{\mp}_{s,L}\right)$,and $\left(T^{\mp}_{s,R}, R^{\mp}_{s,R}\right)$ represent the transmission and reflection coefficients (left) and (right) respectively, given by:

$$\mathbb{T}_s = \frac{\left(\left|T^{-}_{s,L,R}\right|^2 + \left|T^{+}_{s,L,R}\right|^2\right)}{|1^{-}_{s}|^2 + |1^{+}_{s}|^2}, \quad \mathbb{R}_s = \frac{\left(\left|R^{-}_{s,L,R}\right|^2 + \left|R^{+}_{s,L,R}\right|^2\right)}{|1^{-}_{s}|^2 + |1^{+}_{s}|^2}, \tag{14}$$

For the spin-0, $H^{-}_0 = H^{+}_0$ the equations of the system (10) are identical, and consequently, $T^{-}_{0,L,R} = T^{+}_{0,L,R}$, $R^{-}_{0,L,R} = R^{+}_{0,L,R}$ and $1^{-}_0 = 1^{+}_0$.

Let us now examine the general problem. The solution can be written as

$$\Phi^{\mp}_s(x) = \begin{cases} \Phi^{\mp}_s(\text{out}, +\infty)e^{ikx} + \Phi^{\mp}_s(\text{in}, +\infty)e^{-ikx} & x \to +\infty \\ \Phi^{\mp}_s(\text{in}, -\infty)e^{ikx} + \Phi^{\mp}_s(\text{out}, -\infty)e^{-ikx} & x \to -\infty \end{cases} \tag{15}$$

where $\Phi^{\mp}_s(\text{in, out}, \pm\infty)$ are vectors of dimension 2^{2s}. The wave function (15) can then be reformulated with an incoming and outgoing function with the Heaviside step function $\theta(x)$ as

$$\begin{cases} \Phi^{\mp,\text{in}}_s(x) = \Phi^{\mp}_s(\text{in}, -\infty)e^{ikx}\theta(-x) + \Phi^{\mp}_s(\text{in}, +\infty)e^{-ikx}\theta(x) \\ \Phi^{\mp,\text{out}}_s(x) = \Phi^{\mp}_s(\text{out}, -\infty)e^{-ikx}\theta(-x) + \Phi^{\mp}_s(\text{out}, +\infty)e^{ikx}\theta(x), \end{cases} \tag{16}$$

A suitable way to describe scattering and reactions is to introduce the scattering operator $\hat{\mathbf{S}}_{-\mathbf{s}}$, whose matrix elements form the scattering matrix $\hat{S}_{-s}$. This operator connects the initial state $\Phi^{\text{in}}_s(x)$ with the final state $\Phi^{\text{out}}_s(x)$ by means of the relation [1, 2],

$$\Phi^{\text{out}}_s(x) = \hat{\mathbf{S}}_{-\mathbf{s}}\Phi^{\text{in}}_s(x). \tag{17}$$

In matrix form,

$$\begin{pmatrix} \Phi^{-}_s(\text{out}, +\infty) \\ \Phi^{+}_s(\text{out}, +\infty) \\ \Phi^{-}_s(\text{out}, -\infty) \\ \Phi^{+}_s(\text{out}, -\infty) \end{pmatrix} = \begin{pmatrix} \hat{s}_{11} & \hat{s}_{12} & \hat{s}_{13} & \hat{s}_{14} \\ \hat{s}_{21} & \hat{s}_{22} & \hat{s}_{23} & \hat{s}_{24} \\ \hat{s}_{31} & \hat{s}_{32} & \hat{s}_{33} & \hat{s}_{34} \\ \hat{s}_{41} & \hat{s}_{42} & \hat{s}_{43} & \hat{s}_{44} \end{pmatrix} \times \begin{pmatrix} \Phi^{-}_s(\text{in}, -\infty) \\ \Phi^{+}_s(\text{in}, -\infty) \\ \Phi^{-}_s(\text{in}, +\infty) \\ \Phi^{+}_s(\text{in}, +\infty) \end{pmatrix}, \tag{18}$$

where the elements $\hat{s}_{ij}$ are block-matrices ($2^{2s} \times 2^{2s}$). In the case of spin-0 $H^{-}_0 = H^{+}_0$, the system (18) reduce to

$$\begin{pmatrix} \Phi_0(\text{out}, +\infty) \\ \Phi_0(\text{out}, -\infty) \end{pmatrix} = \begin{pmatrix} s_{11} & s_{13} \\ s_{31} & s_{33} \end{pmatrix} \begin{pmatrix} \Phi_0(\text{in}, -\infty) \\ \Phi_0(\text{in}, +\infty) \end{pmatrix}, \tag{19}$$

where $\Phi_0(\text{in, out}, \pm\infty)$ and s_{ij} $(i, j = 1, 2)$ are coefficients.

Due to the symmetry $C_sP_sT_s$ [4, 8, 9], which is the product of three fundamental symmetries: P_s, parity, C_s, charge conjugation, and T_s, time inversion, the $\hat{s}_{ij}$ matrices are not independent.

First, consider the parity operation P_s. By changing $x \to -x$, subsequently, $A_\mu(x, t)$, $\Phi_s(x, t)$ and (σF) transform as follows.

$$A_\mu \to A'_\mu = \left(A_0, -\vec{A}\right), \qquad \Phi_s(x, t) \to \Phi_s(-x, t), \\ (\sigma F) \to (\sigma F)' = -\sigma^{0i}F_{0i} + \sigma^{ij}F_{ij}, \quad i, j = 1 \to 3. \tag{20}$$

Insert (20) into (5), multiply the result on the left by P_s, and using $P_s^{-1}P_s = I_{2^{2s}(2s+1)}$, one finds:

$$P_s\left\{ \left[\left(\frac{\partial}{\partial t} + ieA_0 \right)^2 - (\vec{\nabla} - ie\vec{A})^2 + m^2 \right] \mathbb{I}_{2^{2s}(2s+1)} + se\left((\sigma F)'\right)^{2s} \right\} P_s^{-1}\Phi^{P_s}_s(x, t) = 0, \tag{21}$$

where

$$\Phi^{P_s}_s(x, t) = P_s\Phi_s(-x, t). \tag{22}$$

Compare (5) and (21), they coincide if P_s satisfies the conditions

$$P_s\left(\sigma^{0l}\right)^{2s}_s P_s^{-1} = \left(-\sigma^{0l}\right)^{2s}, \;\; P_s\left(\sigma^{ij}\right)^{2s} P_s^{-1} = \left(\sigma^{ij}\right)^{2s}. \tag{23}$$

The condition (23) is satisfied by the operator $P_s = i\left(\gamma^0\right)^{2s}$. Using (15) and (22), one can easily ensure that $\Phi^{P_s}_s(x, t)$ is obtained from $\Phi_s(x, t)$ by substituting $\Phi^{\mp}_s(\text{out, in}, +\infty) \leftrightarrow i\Phi^{\pm}_s(\text{out, in}, -\infty)$. In matrix form, we get the expression.

$$\left(\sigma_1 \otimes P_s\right)\left(\hat{S}_{-s}\right)\left(\sigma_1 \otimes P_s\right)^{-1} = \hat{S}_{-s}. \tag{24}$$

The symbol $\otimes$ is the Kronecker product of the matrices. From (24), we deduce.

$$\hat{s}_{11} = \hat{s}_{44}, \quad \hat{s}_{22} = \hat{s}_{33}, \quad \hat{s}_{13} = \hat{s}_{42}, \quad \hat{s}_{31} = \hat{s}_{24}, \\ \hat{s}_{12} = \hat{s}_{43}, \quad \hat{s}_{21} = \hat{s}_{34}, \quad \hat{s}_{23} = \hat{s}_{32}, \quad \hat{s}_{14} = \hat{s}_{41}. \tag{25}$$

Now perform the time reversal operation T_s. Thus, by reversal $t \to -t$, $A_\mu(x, t)$, $\Phi_s(x, t)$ and (σF) are transformed into.

$$A_\mu \to A'_\mu = \left(A_0, -\vec{A}\right), \; \Phi_s(x, t) \to \Phi_s(x, -t), \\ (\sigma F) \to (\sigma F)' = \sigma^{0l}F_{0l} - \sigma^{ij}F_{ij}. \tag{26}$$

Insert (26) into (5), then, take the complex conjugate and multiply the result on the left by T_s, and taking into account $T_s^{-1}T_s = I_{2^{2s}(2s+1)}$, we obtain.

$$T_s\left\{\left(\left(\frac{\partial}{\partial t}+ieA_0\right)^2-(\vec{\nabla}-ie\vec{A})^2+m^2\right)\mathbb{I}_{2^{2s}(2s+1)} + se\left(\left(\sigma^{0l}\right)^*F_{0l}-\left(\sigma^{ij}\right)^*F_{ij}\right)^{2s}\right\}T_s^{-1}\Phi_s^{T_s}(x,t)=0, \tag{27}$$

where

$$\Phi_s^{T_s}(x,t)=T_s\Phi_s^*(x,-t), \tag{28}$$

Compare (5) and (27), they coincide if T_s satisfies the conditions.

$$T_s\left(\left(\sigma^{0l}\right)^*\right)^{2s}T_s^{-1}=\left(\sigma^{0l}\right)^{2s},\ T_s\left(\left(\sigma^{ij}\right)^*\right)^{2s}T_s^{-1} = \left(-\sigma^{ij}\right)^{2s}. \tag{29}$$

These conditions are verified by the operator $T_s = i\left(\gamma^1\gamma^3\right)^{2s}$. On the other hand, using (15) and (28), one can easily ensure that passing from $\Phi_s(x,t)$ to $\Phi_s^{T_s}(x,t)$ gives $\Phi_s^{\mp}(\text{out},\pm\infty)\leftrightarrow -\sigma_2\left(\Phi_s^{\mp}(\text{in},\pm\infty)\right)^*$. In matrix form, we get the expression.

$$\left(S_{-s}\right)\left(\sigma_1\otimes T_s\right)\left(S_{-s}^{\star}\right)\left(\sigma_1\otimes T_s\right)^{-1}=I_{2^{2s+1}(2s+1)}. \tag{30}$$

Let's now proceed to the charge conjugation operation $e\to -e$. In this case, $A_\mu(x,t)$ and (σF) are transformed into

$$A_\mu\to A'_\mu=-A_\mu,\quad (\sigma F)\to(\sigma F)'=-\sigma^{\mu\nu}F_{\mu\nu}. \tag{31}$$

In (5), we change $e\to -e$, then take the conjugate hermitic and multiply the result on the right by $\left(\gamma^0\right)^{2s}$, we get

$$\bar{\Phi}_s(x,t)\left\{\left(\left(\frac{\partial}{\partial t}+ieA_0\right)^2-(\vec{\nabla}-ie\vec{A})^2+m^2\right)\mathbb{I}_{2^{2s}(2s+1)} - se(\sigma F)^{2s}\right\}=0. \tag{32}$$

Take the transpose of (32), multiply the result on the left by C_s and with $C_s^{-1}C_s=\mathbb{I}_{2^{2s}(2s+1)}$, it comes

$$C_s\left\{\left(\left(\frac{\partial}{\partial t}+ieA_0\right)^2-(\vec{\nabla}-ie\vec{A})^2+m^2\right)\mathbb{I}_{2^{2s}(2s+1)} - se\left(\left(\sigma^{0l}\right)^TF_{0l}+\left(\sigma^{ij}\right)^TF_{ij}\right)^{2s}\right\}C_s^{-1}\Phi_s^{C_s}(x,t) = 0, \tag{33}$$

where $\bar{\Phi}_s=\Phi_s^\dagger\left(\gamma^0\right)^{2s}$

$$\Phi_s^{C_s}(x,t)=C_s\bar{\Phi}_s^T(x,t). \tag{34}$$

Compare (5) and (32), they coincide if C_s satisfies the conditions.

$$C_s\left(\left(\sigma^{0l}\right)^T\right)^{2s}C_s^{-1}=-\left(\sigma^{0l}\right)^{2s},\quad C_s\left(\left(\sigma^{ij}\right)^T\right)^{2s}C_s^{-1}=-\left(\sigma^{ij}\right)^{2s}. \tag{35}$$

Then, the conditions (35) are verified by the operator $C_s=i\left(\gamma^2\gamma^0\right)^{2s}$. On the other hand, with (15) and (34), we can easily ensure that the transition from $\Phi_s(x,t)$ to $\Phi_s^{C_s}(x,t)$ is obtained by changing $\Phi_s^{\mp}(\text{out},\pm\infty)\leftrightarrow \mp i\sigma_2\left(\Phi_s^{\pm}(\text{in},\pm\infty)\right)^*$. In matrix form, we get the expression.

$$\left(\hat{S}_{-s}\right)\left(\sigma_1\otimes C_s\right)\left(\hat{S}_{-s}^{\star}\right)\left(\sigma_1\otimes C_s\right)^{-1}=\mathbb{I}_{2^{2s+1}(2s+1)}. \tag{36}$$

Furthermore, the charge conservation of spin-s equation allows to write:

$$\langle\Phi_s^{\text{out}}|\Phi_s^{\text{out}}\rangle=\langle\Phi_s^{\text{in}}|\Phi_s^{\text{in}}\rangle. \tag{37}$$

By substituting,

$$\bar{\Phi}_s^{\text{out}}=\left(\Phi_s^{\text{in}}\right)^\dagger\hat{S}_{-s}^\dagger\left(\mathbb{I}_{2^{2s}}\otimes\left(\gamma^0\right)^{2s}\right),\quad \bar{\Phi}_s^{\text{in}}=\left(\Phi_s^{\text{in}}\right)^\dagger\left(\mathbb{I}_{2^{2s}}\otimes\left(\gamma^0\right)^{2s}\right), \tag{38}$$

in (37), we easily verify that $\hat{S}_{-s}$ satisfies:

$$\left(\mathbb{I}_{2^{2s}}\otimes\left(\gamma^0\right)^{2s}\right)\left(\hat{S}_{-s}^\dagger\right)\left(\mathbb{I}_{2^{2s}}\otimes\left(\gamma^0\right)^{2s}\right)\left(\hat{S}_{-s}\right) = \mathbb{I}_{2^{(2s+1)}(2s+1)}. \tag{39}$$

Taking into account the previous properties of the parity, the time inversion, the charge conjugation and the unitarity, we obtain:

$$\hat{s}_{12}=\hat{s}_{21}=\hat{s}_{23}=\hat{s}_{32}=\hat{s}_{14}=\hat{s}_{41}=\hat{s}_{34}=\hat{s}_{43}=0. \tag{40}$$

Combine Eqs. (25) and (40), the $\hat{S}_{-s}$ scattering matrix reduces to:

$$\hat{S}_{-s}=\begin{pmatrix}\check{T}_s^+ & 0 & \check{R}_s^+ & 0\\ 0 & \check{T}_s^- & 0 & \check{R}_s^-\\ \check{R}_s^- & 0 & \check{T}_s^- & 0\\ 0 & \check{R}_s^+ & 0 & \check{T}_s^+\end{pmatrix}, \tag{41}$$

where

$$\check{T}_s^{\pm}=\begin{pmatrix}t_s & \pm\omega_s\\ \pm\omega_s & t_s\end{pmatrix},\quad \check{R}_s^{\pm}=\begin{pmatrix}r_s & \pm\rho_s\\ \pm\rho_s & r_s\end{pmatrix}, \tag{42}$$

are blocks of matrices $\left(2^{2s}\times 2^{2s}\right)$, which represent the transmission and reflection coefficients (left) and (right) respectively. t_s, r_s, ρ_s and ω_s are functions of E, A_μ and m.

For $s = 0$, we have $\rho_0 = \omega_0 = 0$. The matrix $\hat{S}_0$ is symmetric because $\check{T}_0^+ = \check{T}_0^-$ and $\check{R}_0^+ = \check{R}_0^-$. It is pseudo-symmetric for $s = 1/2$ because we have $\sigma_3 \check{T}_{1/2}^+ \sigma_3 = \check{T}_{1/2}^-$ and $\sigma_3 \check{R}_{1/2}^+ \sigma_3 = \check{R}_{1/2}^-$. This last property is specific to the spin of the particles.

Using the charge conservation condition (39), we find

$$\begin{aligned} &\left(\check{T}_s^+\right)^\dagger \check{R}_s^- + \left(\check{R}_s^-\right)^\dagger \check{T}_s^+ = \left(\check{T}_s^-\right)^\dagger \check{R}_s^+ + \left(\check{R}_s^+\right)^\dagger \check{T}_s^- = 0, \\ &\left(\check{T}_s^+\right)^\dagger \check{T}_s^- + \left(\check{R}_s^-\right)^\dagger \check{R}_s^+ = \mathbb{I}_{2^{2s}}. \end{aligned} \tag{43}$$

Let's now express $\hat{S}_{-s}$ in the basis of even and odd waves. To illustrate this, consider the following unitary transformation:

$$\varkappa_s^{\mathrm{in}}(x) = \hat{U}_s \Phi_s^{\mathrm{in}}(x), \quad \varkappa_s^{\mathrm{out}}(x) = \hat{U}_s \Phi_s^{\mathrm{out}}(x), \tag{44}$$

where $\varkappa_s^{\mathrm{in,out}}(x) = \left(\varkappa_s^{-,\mathrm{in,out}}(x), \varkappa_s^{+,\mathrm{in,out}}(x)\right)^T$ are $2^{2s}(2s+1)$ component wave functions. $\hat{U}_s$ is the square matrix $\left(2^{(2s+1)}(2s+1) \times 2^{(2s+1)}(2s+1)\right)$, given by [3, 7]:

$$\hat{U}_s = \frac{1}{\sqrt{2}} \begin{pmatrix} \mathbb{I}_{2^{2s}} & 0 & \mathbb{I}_{2^{2s}} & 0 \\ 0 & \mathbb{I}_{2^{2s}} & 0 & \mathbb{I}_{2^{2s}} \\ i\mathbb{I}_{2^{2s}} & 0 & -i\mathbb{I}_{2^{2s}} & 0 \\ 0 & i\mathbb{I}_{2^{2s}} & 0 & -i\mathbb{I}_{2^{2s}} \end{pmatrix}. \tag{45}$$

After some manipulations of expressions (15), (17), (18), (44) and (45), we find

$$\varkappa_s^{\mathrm{out}}(x) = \hat{U}_s \hat{S}_{-s} \hat{U}_s^\dagger \varkappa_s^{\mathrm{in}}(x) = \hat{M}_{-s} \varkappa_s^{\mathrm{in}}(x). \tag{46}$$

where $\hat{M}_{-s}$ is the scattering matrix in the representation of partial waves, given by:

$$\hat{M}_{-s} = \begin{pmatrix} \bar{\check{T}}_s^+ & 0 & i\bar{\check{R}}_s^- & 0 \\ 0 & \bar{\check{T}}_s^+ & 0 & -i\bar{\check{R}}_s^- \\ i\bar{\check{R}}_s^+ & 0 & \bar{\check{T}}_s^- & 0 \\ 0 & -i\bar{\check{R}}_s^+ & 0 & \bar{\check{T}}_s^- \end{pmatrix}, \tag{47}$$

where

$$\bar{\check{T}}_s^\pm = \begin{pmatrix} t_s \pm r_s & 0 \\ 0 & t_s \pm r_s \end{pmatrix}, \quad \bar{\check{R}}_s^\pm = \begin{pmatrix} 0 & \rho_s \pm \omega_s \\ \rho_s \pm \omega_s & 0 \end{pmatrix}. \tag{48}$$

It is easy to show that when we pass to the even–odd basis, $\hat{M}_{-s}$ can be diagonalized and then get [3, 7].

$$\hat{M}_{-s} = \mathbb{I}_{2^{2s(2s+1)}} \otimes \begin{pmatrix} e^{2i\delta_s^0} & 0 \\ 0 & e^{2i\delta_s^1} \end{pmatrix}, \tag{49}$$

where δ_s^l, $l = 0, 1$, represents respectively the phase shifts of the even and odd wave functions and they are given explicitly by:

$$e^{2i\delta_s^l} = t_s + (-1)^l \sqrt{\omega_s^2 + r_s^2 - \rho_s^2}. \tag{50}$$

The wave function in the asymptotic region is given by.

$$\Phi_s^\mp(x) = \frac{1}{\sqrt{2}} \left[\varkappa_s^\mp(\mathrm{in}, -\infty) \psi_s^0(x) + \varkappa_s^\mp(\mathrm{in}, +\infty) \psi_s^1(x)\right] \tag{51}$$

with.

$$\psi_s^l(x) = (i\varepsilon)^l \left[e^{-ik|x|} + (-1)^l e^{2i\delta_s^l} e^{ik|x|}\right] \tag{52}$$

where $\varepsilon = +(-)$ for $x > 0$ ($x < 0$).

For the transmission problem, consider the case of a particle coming from $-\infty$. With this choice, $\varkappa_s^\mp(\mathrm{in}, +\infty) = i\varkappa_s^\mp(\mathrm{in}, -\infty)$, hence the result:

$$\Phi_{s,L}^\mp(x) = \begin{cases} \sqrt{2}\varkappa_s^\mp(\mathrm{in}, -\infty)\left[e^{ikx} + f_s^- e^{-ikx}\right] & x \to -\infty, \\ \sqrt{2}\varkappa_s^\mp(\mathrm{in}, -\infty)\left[(1 + f_s^+) e^{ikx}\right] & x \to +\infty, \end{cases} \tag{53}$$

where $f_s^\mp$ are the scattering amplitudes, given by.

$$f_s^\mp = f_s^0 \mp f_s^1, \quad f_s^l = \frac{1}{2}\left(e^{2i\delta_s^l} - 1\right), \quad l = 0, 1. \tag{54}$$

The comparison of (13) and (53), makes it possible to find the coefficients $\mathbb{T}_s$ and. $\mathbb{R}_s$

$$\begin{aligned} \mathbb{T}_s &= \left|\left(1 + f_s^+\right)\right|^2 = \frac{1}{4}\left|e^{2i\delta_s^0} + e^{2i\delta_s^1}\right|^2, \\ \mathbb{R}_s &= \left|f_s^-\right|^2 = \frac{1}{4}\left|e^{2i\delta_s^0} - e^{2i\delta_s^1}\right|^2. \end{aligned} \tag{55}$$

and we have, as expected, the relation $\mathbb{T}_s + \mathbb{R}_s = 1$.

The differential and total scattering cross-section $\sigma_s^\mp$ ($-$ for $x < 0$, $+$ for $x > 0$) and σ_s^t respectively, are given by [7, 10, 11]:

$$\sigma_s^\mp = \left|f_s^\mp\right|^2, \quad \sigma_s^t = \left|f_s^-\right|^2 + \left|f_s^+\right|^2. \tag{56}$$

4 $\hat{S}$-Matrix in the Woods–Saxon potential

As an application of this formalism, we would like to examine equation (10) in the case of one dimensional Woods–Saxon potential.

$$V_\alpha(x) = \frac{V_0}{1 + e^{\frac{|x| - L}{\alpha}}}, \tag{57}$$

V_0, α and L are positive constants. This potential is chosen for its symmetry and range properties [12, 13]. This potential admits a rectangular barrier of potential as a limit

$V_\alpha(x) \to V_0\theta(L - |x|)$ when $\alpha \to 0$. $\theta(x)$ is the Heaviside step function.

With this choice of potential, $\vec{E} = \left(-dV_\alpha(x)/\mathrm{d}x\right)\vec{i}$ and $\vec{B} = \vec{0}$, and by inserting these expressions in (10) we obtain.

$$\begin{pmatrix} H_s^{-,WS}(x,t) & 0 \\ 0 & H_s^{+,WS}(x,t) \end{pmatrix}\begin{pmatrix} \Phi_s^{-,WS}(x,t) \\ \Phi_s^{+,WS}(x,t) \end{pmatrix} = 0, \tag{58}$$

where

$$H_s^{\mp,WS}(x,t) = \left[\frac{d^2}{\mathrm{d}x^2} + \left(i\frac{\partial}{\partial t} - eV_\alpha(x)\right)^2 - m^2\right] I_{2^{2s}} \pm 2ise\sigma_1 \frac{dV_\alpha(x)}{\mathrm{d}x} \tag{59}$$

In Eq. (58), $V_\alpha(x)$ is independent of time, in this case, $\Phi_s^{\mp}(x,t) = e^{-iEt}\Phi_s^{\mp}(x)$. Consequently $\Phi_s^{\mp}(x)$ satisfies.

$$\left\{D_{KG}^2 \mathbb{I}_{2^{2s}} \pm 2ise\left(\sigma_1\right)^{2s} \frac{dV_\alpha(x)}{\mathrm{d}x}\right\}\Phi_s^{\mp,WS}(x) = 0. \tag{60}$$

$\Phi_s^{\mp,WS}(x)$ is a wave function with 2^{2s} components. $D_{KG}^2 = \frac{d^2}{\mathrm{d}x^2} + (E - eV_\alpha(x))^2 - m^2$ is the $KG-0$ operator.

In order to decouple equation (60), introduce the new variable.

$$\Phi_s^{\mp,WS}(x) = \left[\frac{\sigma_3 + \sigma_1}{2}\right]^{(2s)} \chi_s^{\mp,WS}(x). \tag{61}$$

This enables us to obtain a system of decoupled differential equations.

$$\left\{D_{KG}^2 \mathbb{I}_{2^{2s}} \pm 2ise\left(\sigma_3\right)^{(2s)} \frac{dV_\alpha(x)}{\mathrm{d}x}\right\}\chi_s^{\mp,WS}(x) = 0. \tag{62}$$

For $s = 0$, equation (62) reduces to the Klein–Gordon equation, and for $s = 1/2$ we obtain the quadratic form of the Dirac equation.

Let us now pass to the resolution of the stationary Eq. (62) in the case of the potential given by the formula (57).

We distinguish two cases depending on whether $\left(E - eV_0\right)^2 - m^2$ is greater or less than 0. We only deal here with the case $\left(E - eV_0\right)^2 - m^2 > 0$, corresponding to scattering states.

To solve Eq. (62), instead of the coordinate x, we introduce the new variable.

$$y = \frac{1}{1 + e^{\frac{|x| - L}{\alpha}}} \tag{63}$$

As there is an absolute value for the variable x, we distinguish as usual between the two regions $x < 0$ and $x > 0$.

For $x < 0$, by means of (63) the Eq. (62) becomes:

$$\left[D_y^2 I_{2^{2s}} \pm 2iesαV_0 y\left(1 - y\right)\left(\sigma_3\right)^{2s}\right]\chi_s^{\mp,WS}(x) = 0, \tag{64}$$

where D_y^2 being a second-order differential operator defined by.

$$D_y^2 = y^2\left(1 - y\right)^2\frac{d^2}{\mathrm{d}y^2} + y\left(1 - y\right)\left(1 - 2y\right)\frac{d}{\mathrm{d}y} + \alpha^2\left[\left(E - eV_0 y\right)^2 - m^2\right] \tag{65}$$

By making the new change of variable $\chi_s^{\mp,WS}(y) = y^\nu\left(1 - y\right)^\mu f_s^{\mp}\left(y\right)$, where μ and ν are two parameters that we fix later. After some elementary calculations, we obtain for the function $f_s^{\mp}\left(y\right)$ the following differential equation:

$$\left\{\left[\tilde{D}_y^2 + B\left(y\right)\right]\mathbb{I}_{2^{2s}} \pm 2iesαV_0\left(\sigma_3\right)^{2s}\right\}f_s^{\mp}\left(y\right) = 0 \tag{66}$$

where

$$\widetilde{D}_y^2 = y(1 - y)\frac{d^2}{\mathrm{d}y^2} + \left[(2\nu + 1) - 2y(\nu + \mu + 1)\right]\frac{d}{\mathrm{d}y} - \left(\mu + \nu + \frac{1}{2}\right)^2 + \frac{1}{4} - \alpha^2 e^2 V_0^2, \tag{67}$$

and

$$B\left(y\right) = \left(\frac{\nu^2}{y} + \frac{\mu^2}{1 - y}\right) + \alpha^2\left(\frac{E^2 - m^2}{y} + \frac{\left(E - eV_0\right)^2 - m^2}{1 - y}\right). \tag{68}$$

Equation (66) reduces to the standard form of a hypergeometric type equation [14, 15],

$$\left\{\tilde{D}_y^2 \mathbb{I}_{2^{2s}} \pm 2iesαV_0\left(\sigma_3\right)^{2s}\right\}f_s^{\mp}\left(y\right) = 0, \tag{69}$$

if $B\left(y\right) = 0$. Under this condition, the parameters μ and ν have the following values:

$$\begin{aligned} \mu^2 &= \alpha^2\left(m^2 - \left(E - eV_0\right)^2\right) = -\alpha^2 k_1^2, \\ \nu^2 &= \alpha^2\left(m^2 - E^2\right) = -\alpha^2 k^2. \end{aligned} \tag{70}$$

The general solution of Eq. (69) is the hypergeometric functions:

$$f_s^{\mp}\left(y\right) = \begin{pmatrix} C_1^{\mp}{}_2F_1\left(a^{\mp}, b^{\mp}, c, y\right) + C_2^{\mp} y^{-2\nu}{}_2F_1\left(a^{\mp} + 1 - c, b^{\mp} + 1 - c, 2 - c, y\right) \\ D_1^{\mp}{}_2F_1\left(a^{\pm}, b^{\pm}, c, y\right) + D_2^{\mp} y^{-2\nu}{}_2F_1\left(a^{\pm} + 1 - c, b^{\pm} + 1 - c, 2 - c, y\right) \end{pmatrix}, \tag{71}$$

with

$$a^{\mp}=\mu+\nu+\frac{1}{2}+\frac{\vartheta^{\mp}}{2},\ b^{\mp}=\mu+\nu+\frac{1}{2}-\frac{\vartheta^{\mp}}{2},\quad c=1+2\nu,\ \left(\vartheta^{\mp}\right)^2=1-4\alpha^2e^2V_0^2\pm 8ise\alpha V_0. \tag{72}$$

Now, let us consider the values of $x>0$. As we did before, let's introduce the change $\chi_s^{\mp,WS}(y)=y^{\nu}(1-y)^{\mu}g_s^{\mp}(y)$. We also get an equation similar to (69). Its solution therefore is

$$g_s^{\mp}(y)=\begin{pmatrix}C_3^{\mp}\,{}_2F_1\left(a^{\pm},b^{\pm},c,y\right)+C_4^{\mp}y^{-2\nu}\,{}_2F_1\left(a^{\pm}+1-c,b^{\pm}+1-c,2-c,y\right)\\ D_3^{\mp}\,{}_2F_1\left(a^{\mp},b^{\mp},c,y\right)+D_4^{\mp}y^{-2\nu}\,{}_2F_1\left(a^{\mp}+1-c,b^{\mp}+1-c,2-c,y\right)\end{pmatrix}. \tag{73}$$

The Eqs. (71) and (73) can be unified in the same formula as

$$\eta_s^{\mp}(y)=\theta(-x)f_s^{\mp}(y)+\theta(x)g_s^{\mp}(y) \tag{74}$$

with

$$y=\frac{1}{1+e^{\frac{|x|-L}{\alpha}}}. \tag{75}$$

Including all these last results, we will write the stationary solutions like.

$$\Phi_s^{\mp,W-S}(x)=y^{\nu}(1-y)^{\mu}\left[\frac{\sigma_3+\sigma_1}{2}\right]^{(2s)}\eta_s^{\mp}(y). \tag{76}$$

The coefficients $\left(C_j^{\mp},D_j^{\mp},j=1\rightarrow 4\right)$ are not independent of each other. They are determined by the connection conditions of the wave function and its derivative at the point $x=0$ or $y=\lambda=\left[1+e^{-\frac{L}{\alpha}}\right]^{-1}$. Effectively, by imposing the conditions.

$$\chi_s^{\mp,WS}(0^-)=\chi_s^{\mp,WS}(0^+),\quad \frac{d\chi_s^{\mp,WS}(0^-)}{dx}=\frac{d\chi_s^{\mp,WS}(0^+)}{dx}, \tag{77}$$

which make it possible to fix the coefficients by the following relations:

$$C_1^{\mp}=C_2^{\mp}W_{12}^{\mp}+C_4^{\mp}W_{14}^{\mp},\ C_3^{\mp}=C_2^{\mp}W_{32}^{\mp}+C_4^{\mp}W_{34}^{\mp},\quad D_1^{\mp}=D_2^{\mp}W_{12}^{\pm}+D_4^{\mp}W_{14}^{\pm},\ D_3^{\mp}=D_2^{\mp}W_{32}^{\pm}+D_4^{\mp}W_{34}^{\pm}, \tag{78}$$

where

$$W_{12}^{\mp}=W_{34}^{\pm}=-\frac{F_1^{\pm}\left(F_2^{\mp}\right)'+F_2^{\mp}\left(F_1^{\pm}\right)'}{F_1^{\pm}\left(F_1^{\mp}\right)'+F_1^{\mp}\left(F_1^{\pm}\right)'},\quad W_{32}^{\mp}=W_{14}^{\pm}=\frac{F_2^{\mp}\left(F_1^{\mp}\right)'-F_1^{\mp}\left(F_2^{\mp}\right)'}{F_1^{\pm}\left(F_1^{\mp}\right)'+F_1^{\mp}\left(F_1^{\pm}\right)'} \tag{79}$$

and $F_1^{\mp}$, $F_2^{\mp}$, $\left(F_1^{\mp}\right)'$ et $\left(F_2^{\mp}\right)'$ are defined by

$$\begin{aligned}\left(F_1^{\mp}\right)&=\left[y^{\nu}(1-y)^{\mu}\,{}_2F_1\left(a^{\mp},b^{\mp},c,y\right)\right]_{y=\lambda},\\ \left(F_2^{\mp}\right)&=\left[y^{-\nu}(1-y)^{\mu}\,{}_2F_1\left(a^{\mp}+1-c,b^{\mp}+1-c,2-c,y\right)\right]_{y=\lambda},\\ \left(F_1^{\mp}\right)'&=\frac{d}{dx}\left[y^{\nu}(1-y)^{\mu}\,{}_2F_1\left(a^{\mp},b^{\mp},c,y\right)\right]_{y=\lambda},\\ \left(F_2^{\mp}\right)'&=\frac{d}{dx}\left[y^{-\nu}(1-y)^{\mu}\,{}_2F_1\left(a^{\mp}+1-c,b^{\mp}+1-c,2-c,y\right)\right]_{y=\lambda}.\end{aligned} \tag{80}$$

Since for $|x|\rightarrow\infty$ the argument $y\rightarrow 0$. Using the relation ${}_2F_1(a,b,c,0)=1$ and

$$\lim_{|x|\rightarrow\infty}y^{\pm\nu}=e^{\pm ik(|x|-L)},\quad \lim_{|x|\rightarrow\infty}(1-y)^{\mu}=1, \tag{81}$$

we obtain the asymptotic expression of the function (76)

$$\Phi_s^{\mp,WS}(x)=\begin{cases}\left[\frac{\sigma_3+\sigma_1}{2}\right]^{(2s)}\left[\begin{pmatrix}C_3^{\mp}\\ D_3^{\mp}\end{pmatrix}e^{ik(x-L)}+\begin{pmatrix}C_4^{\mp}\\ D_4^{\mp}\end{pmatrix}e^{-ik(x-L)}\right] & x\rightarrow+\infty\\ \left[\frac{\sigma_3+\sigma_1}{2}\right]^{(2s)}\left[\begin{pmatrix}C_2^{\mp}\\ D_2^{\mp}\end{pmatrix}e^{ik(x+L)}+\begin{pmatrix}C_1^{\mp}\\ D_1^{\mp}\end{pmatrix}e^{-ik(x+L)}\right] & x\rightarrow-\infty\end{cases} \tag{82}$$

Compare (82) with (15), it comes

$$\begin{aligned}
\Phi_s^{\mp,W-S}(\text{out},+\infty) &= \left[\frac{\sigma_3+\sigma_1}{2}\right]^{(2s)}\begin{pmatrix}C_3^{\mp}\\ D_3^{\mp}\end{pmatrix}e^{-ikL},\\
\Phi_s^{\mp,W-S}(\text{out},-\infty) &= \left[\frac{\sigma_3+\sigma_1}{2}\right]^{(2s)}\begin{pmatrix}C_1^{\mp}\\ D_1^{\mp}\end{pmatrix}e^{-ikL},\\
\Phi_s^{\mp,W-S}(\text{in},-\infty) &= \left[\frac{\sigma_3+\sigma_1}{2}\right]^{(2s)}\begin{pmatrix}C_2^{\mp}\\ D_2^{\mp}\end{pmatrix}e^{ikL},\\
\Phi_s^{\mp,W-S}(\text{in},+\infty) &= \left[\frac{\sigma_3+\sigma_1}{2}\right]^{(2s)}\begin{pmatrix}C_4^{\mp}\\ D_4^{\mp}\end{pmatrix}e^{ikL}.
\end{aligned} \tag{83}$$

To determine the matrix $\hat{S}_{-s}^{WS}$, replace $C_1^{\mp}$, $D_1^{\mp}$, $C_3^{\mp}$ and $D_3^{\mp}$ by their expressions in terms of $C_2^{\mp}$, $D_2^{\mp}$, $C_4^{\mp}$ and $D_4^{\mp}$. Let's rewrite $\Phi_s^{\mp,W-S}(\text{out},\mp\infty)$ in terms of $\Phi_s^{\mp,W-S}(\text{in},\mp\infty)$, it comes:

$$\begin{pmatrix}\Phi_s^{-,WS}(\text{out},+\infty)\\ \Phi_s^{+,WS}(\text{out},+\infty)\\ \Phi_s^{-,WS}(\text{out},-\infty)\\ \Phi_s^{+,WS}(\text{out},-\infty)\end{pmatrix} = \hat{S}_{-s}^{WS}\begin{pmatrix}\Phi_s^{-,WS}(\text{in},-\infty)\\ \Phi_s^{+,WS}(\text{in},-\infty)\\ \Phi_s^{-,WS}(\text{in},+\infty)\\ \Phi_s^{+,WS}(\text{in},+\infty)\end{pmatrix}. \tag{84}$$

where

$$\hat{S}_{-s}^{WS} = \begin{pmatrix}\check{T}_s^{+,WS} & 0 & \check{R}_s^{+,WS} & 0\\ 0 & \check{T}_s^{-,WS} & 0 & \check{R}_s^{-,WS}\\ \check{R}_s^{-,WS} & 0 & \check{T}_s^{-,WS} & 0\\ 0 & \check{R}_s^{+,WS} & 0 & \check{T}_s^{+,WS}\end{pmatrix}, \tag{85}$$

with

$$\begin{aligned}
\check{T}_s^{\pm,WS} &= \begin{pmatrix}t_s^{WS} & \pm\omega_s^{WS}\\ \pm\omega_s^{WS} & t_s^{WS}\end{pmatrix},\\
\check{R}_s^{\pm,WS} &= \begin{pmatrix}r_s^{WS} & \pm\rho_s^{WS}\\ \pm\rho_s^{WS} & r_s^{WS}\end{pmatrix},
\end{aligned} \tag{86}$$

and

$$\begin{aligned}
t_s^{WS} &= \frac{1}{2}\left(W_{14}^{+}+W_{14}^{-}\right)e^{2ikL},\\
\omega_s^{WS} &= \frac{1}{2}\left(W_{14}^{+}-W_{14}^{-}\right)e^{2ikL},\\
r_s^{WS} &= \frac{1}{2}\left(W_{12}^{+}+W_{12}^{-}\right)e^{2ikL},\\
\rho_s^{WS} &= \frac{1}{2}\left(W_{12}^{+}-W_{12}^{-}\right)e^{2ikL}.
\end{aligned} \tag{87}$$

From (49), the $\hat{M}_{-s}^{WS}$-matrix is

$$\hat{M}_{-s}^{WS} = \mathbb{I}_{2^{2s(2s+1)}} \otimes \begin{pmatrix}e^{2i\delta_s^{0,WS}} & 0\\ 0 & e^{2i\delta_s^{1,WS}}\end{pmatrix}, \tag{88}$$

where

$$e^{2i\delta_s^{l,WS}} = t_s^{WS} + (-1)^l\sqrt{\left(\omega_s^{WS}\right)^2+\left(r_s^{WS}\right)^2-\left(\rho_s^{WS}\right)^2}. \tag{89}$$

Finally, for the transmission problem in the case of the Woods–Saxon potential, we have

$$\begin{aligned}
\mathbb{T}_s^{WS} &= \mid 1+f_s^{+,WS}\mid^2 = \frac{1}{4}\left|e^{2i\delta_s^{0,WS}}+e^{2i\delta_s^{1,WS}}\right|^2,\\
\mathbb{R}_s^{WS} &= \mid f_s^{-,WS}\mid^2 = \frac{1}{4}\mid e^{2i\delta_s^{0,WS}}-e^{2i\delta_s^{1,WS}}\mid^2
\end{aligned} \tag{90}$$

and

$$\begin{aligned}
\sigma_s^{t,WS} &= \left|f_s^{+,WS}\right|^2+\left|f_s^{-,WS}\right|^2\\
&= 2\left(\sin^2\delta_s^{0,WS}+\sin^2\delta_s^{1,WS}\right).
\end{aligned} \tag{91}$$

5 $\hat{S}$-Matrix in the rectangular barrier potential

Now consider the limiting case when the smooth potential tends towards the rectangular barrier. The latter is found as a limiting case of the Woods–Saxon potential for $\alpha \to 0^+$,

$$V^b(x) = \lim_{\alpha\to0^+}\frac{V_0}{1+e^{\frac{|x|-L}{\alpha}}} = V_0\theta\left(L-\mid x\mid\right). \tag{92}$$

For $|x| > L$, we have

$$\begin{aligned}
&\lim_{\alpha\to0^+}(1-\lambda)^{-2\mu} = e^{-2ik_1L},\ \lim_{\alpha\to0^+}\frac{1}{\alpha}(1-\lambda) = 0,\\
&\lim_{\alpha\to0^+}\lambda = 1,\ \lim_{\alpha\to0^+}y^{\nu} = e^{ik(|x|-L)},\quad \lim_{\alpha\to0^+}y = 0,\\
&\lim_{\alpha\to0^+}y^{-2\nu} = e^{-2ik(|x|-L)},\ \lim_{\alpha\to0^+}(1-y)^{\mu} = 1,
\end{aligned} \tag{93}$$

where $\mu = -i\alpha k_1$, $\nu = -i\alpha k$. By using (93) and the relations to the hypergeometric functions, as well as the properties of the functions Γ [14, 15].

$$\begin{aligned}
&{}_2F_1(a,b,c,0) = 1,\\
&\frac{d}{dz}\left[{}_2F_1(a,b,c,z)\right] = \frac{ab}{c}\,{}_2F_1(a+1,b+1,c+1,z),\\
&z\Gamma(z) = \Gamma(z+1),\quad \lim_{z\to0^+}\Gamma(z) = \frac{1}{z},
\end{aligned} \tag{94}$$

we easily check that

$$\begin{aligned}
&\lim_{\alpha\to0^+}W_{32}^{\mp} = \lim_{\alpha\to0^+}W_{32}^{\pm} = \lim_{\alpha\to0^+}W_{14}^{\mp} = \lim_{\alpha\to0^+}W_{14}^{\pm} = \varrho_s,\\
&\lim_{\alpha\to0^+}W_{12}^{\mp} = \lim_{\alpha\to0^+}W_{34}^{\pm} = \varsigma_s^{\mp},
\end{aligned} \tag{95}$$

with

$$\varrho_s = \frac{(2k_1k)}{(2k_1k)\cos(2k_1L) - i(k_1^2 + k^2 - 4s^2e^2V_0^2)\sin(2k_1L)}$$

$$\varsigma_s^{\mp} = \frac{i\left(k_1^2 - (k \mp 2seV_0)^2\right)\sin(2k_1L)}{(2k_1k)\cos(2k_1L) - i(k_1^2 + k^2 - 4s^2e^2V_0^2)\sin(2k_1L)} \quad (96)$$

Insert all these expressions into equation (76),

$$\Phi_s^{\mp,b}(x) = \lim_{\alpha\to 0^+}\Phi_s^{\mp,W-S}(x) = \left[\frac{\sigma_3+\sigma_1}{2}\right]^{(2s)}\eta_s^{\mp,b}(x). \quad (97)$$

where

$$\eta_s^{\mp,b}(x) = \left\{\begin{pmatrix} C_2^{\mp}\varsigma_s^{\mp} + C_4^{\mp}\varrho_s \\ D_2^{\mp}\varsigma_s^{\pm} + D_4^{\mp}\varrho_s\end{pmatrix}e^{-ik(x+L)} + \begin{pmatrix} C_2^{\mp} \\ D_2^{\mp}\end{pmatrix}e^{ik(x+L)}\right\}\theta(-x-L) + \left\{\begin{pmatrix} C_2^{\mp}\varrho_s + C_4^{\mp}\varsigma_s^{\pm} \\ D_2^{\mp}\varrho_s + D_4^{\mp}\varsigma_s^{\mp}\end{pmatrix}e^{ik(x-L)} + \begin{pmatrix} C_4^{\mp} \\ D_4^{\mp}\end{pmatrix}e^{-ik(x-L)}\right\}\theta(x-L). \quad (98)$$

For $|\,x\,| < L$, using

$$\lim_{\alpha\to 0^+}(1-y)^{-2\mu} = e^{2ik_1(|x|-L)},$$
$$\lim_{\alpha\to 0^+}(1-y)^{\mu} = e^{-ik_1(|x|-L)} \quad (99)$$
$$\lim_{\alpha\to 0^+} y^{\nu} = \lim_{\alpha\to 0^+} y^{-2\nu} = 1, \quad \lim_{\alpha\to 0^+} y = 1$$

and the formula relating the hypergeometric functions of arguments z and $1-z$ [14, 15], we find

$$\lim_{\alpha\to 0^+} {}_2F_1(a^{\mp}+1-c, b^{\mp}+1-c, 2-c, y) = \overline{B}^{\mp} + \overline{A}^{\pm}e^{2ik_1(|x|-L)}, \quad (100)$$
$$\lim_{\alpha\to 0^+} {}_2F_1(a^{\mp}, b^{\mp}, c, y) = \overline{A}^{\mp} + \overline{B}^{\pm}e^{2ik_1(|x|-L)},$$

where

$$\overline{A}^{\mp} = \frac{k_1 - k \mp 2seV_0}{2k_1}, \quad \overline{B}^{\pm} = \frac{k_1 + k \pm 2seV_0}{2k_1}. \quad (101)$$

These relations reported in (76), give the following result:

$$\Phi_s^{\mp,b}(x) = \lim_{\alpha\to 0^+}\Phi_s^{\mp,W-S}(x) = \left[\frac{\sigma_3+\sigma_1}{2}\right]^{(2s)}\overline{\eta}_s^{\mp}(x)\theta(L-|x|) \quad (102)$$

where

$$\overline{\eta}_s^{\mp}(x) = f_s^{\mp,b}(y)\theta(-x) + g_s^{\mp,b}(y)\theta(x) \quad (103)$$

with

$$f_s^{\mp,b}(y) = \begin{pmatrix} (C_2^{\mp}\varsigma_s^{\mp} + C_4^{\mp}\varrho_s)\overline{A}^{\mp} + C_2^{\mp}\overline{B}^{\mp} \\ (D_2^{\mp}\varsigma_s^{\pm} + D_4^{\mp}\varrho_s)\overline{A}^{\pm} + D_2^{\mp}\overline{B}^{\pm}\end{pmatrix}e^{ik_1(x+L)} + \begin{pmatrix} (C_2^{\mp}\varsigma_s^{\mp} + C_4^{\mp}\varrho_s)\overline{B}^{\pm} + C_2^{\mp}\overline{A}^{\pm} \\ (D_2^{\mp}\varsigma_s^{\pm} + D_4^{\mp}\varrho_s)\overline{B}^{\mp} + D_2^{\mp}\overline{A}^{\mp}\end{pmatrix}e^{-ik_1(x+L)} \quad (104)$$

and

$$g_s^{\mp,b}(y) = \begin{pmatrix} (C_2^{\mp}\varrho_s + C_4^{\mp}\varsigma_s^{\pm})\overline{A}^{\pm} + C_4^{\mp}\overline{B}^{\pm} \\ (D_2^{\mp}\varrho_s + D_4^{\mp}\varsigma_s^{\mp})\overline{A}^{\mp} + D_4^{\mp}\overline{B}^{\mp}\end{pmatrix}e^{-ik_1(x-L)} + \begin{pmatrix} (C_2^{\mp}\varrho_s + C_4^{\mp}\varsigma_s^{\pm})\overline{B}^{\mp} + C_4^{\mp}\overline{A}^{\mp} \\ (D_2^{\mp}\varrho_s + D_4^{\mp}\varsigma_s^{\mp})\overline{B}^{\pm} + D_4^{\mp}\overline{A}^{\pm}\end{pmatrix}e^{ik_1(x-L)} \quad (105)$$

We can also give the scattering matrices $\hat{S}_{-s}^{b}$ and $\hat{M}_{-s}^{b}$, the phase shifts $\delta_s^{l,b}$ $(l=0,1)$, the transmission and reflection coefficients $\mathbb{T}_s^b$ and $\mathbb{R}_s^b$, as well as the total scattering cross-section $\sigma_s^{t,b}$ by a limit case $\alpha \to 0^+$.

$$\hat{S}_{-s}^{b} = \lim_{\alpha\to 0^+}\hat{S}_{-s}^{WS} = \begin{pmatrix} \check{T}_s^{+,b} & 0 & \check{R}_s^{+,b} & 0 \\ 0 & \check{T}_s^{-,b} & 0 & \check{R}_s^{-,b} \\ \check{R}_s^{-,b} & 0 & \check{T}_s^{-,b} & 0 \\ 0 & \check{R}_s^{+,b} & 0 & \check{T}_s^{+,b}\end{pmatrix}, \quad (106)$$

with

$$\check{T}_s^{\pm,b} = \begin{pmatrix} t_s^b & \pm\omega_s^b \\ \pm\omega_s^b & t_s^b\end{pmatrix}, \quad \check{R}_s^{\pm,b} = \begin{pmatrix} r_s^b & \pm\rho_s^b \\ \pm\rho_s^b & r_s^b\end{pmatrix}, \quad (107)$$

and

$$r_s^b = \lim_{\alpha\to 0^+} r_s^{WS} = \frac{1}{2}(\varsigma_s^+ + \varsigma_s^-)e^{2ikL},$$
$$\rho_s^b = \lim_{\alpha\to 0^+}\rho_s^{WS} = \frac{1}{2}(\varsigma_s^+ - \varsigma_s^-)e^{2ikL} \quad (108)$$
$$t_s^b = \lim_{\alpha\to 0^+} t_s^{WS} = \varrho_s e^{2ikL}, \quad \omega_s^b = \lim_{\alpha\to 0^+}\omega_s^{WS} = 0.$$

$$\hat{M}_{-s}^{b} = \lim_{\alpha\to 0^+}\hat{M}_{-s}^{WS} = \mathbb{I}_{2^{2s(2s+1)}} \otimes \begin{pmatrix} e^{2i\delta_s^{0,b}} & 0 \\ 0 & e^{2i\delta_s^{1,b}}\end{pmatrix}, \quad (109)$$

where

$$e^{2i\delta_s^{l,b}} = \left(\varrho_s + (-1)^l\sqrt{\varsigma_s^+\varsigma_s^-}\right)e^{2ikL} \quad (110)$$

For the coefficients $\mathbb{T}_s^b$ and $\mathbb{R}_s^b$, we have

$$\mathbb{T}_s^b = \lim_{\alpha\to0^+}\mathbb{T}_s^{WS} = |\varrho_s|^2 = \frac{4k_1^2k^2}{4k_1^2k^2 + \left[k_1^2 - \left(k+2seV_0\right)^2\right]\left[k_1^2 - \left(k-2seV_0\right)^2\right]\sin^2(2k_1L)} \tag{111}$$

$$\mathbb{R}_s^b = \lim_{\alpha\to0^+}\mathbb{R}_s^{WS} = \varsigma_s^-\left(\varsigma_s^+\right)^\star = \frac{\left[k_1^2 - \left(k+2seV_0\right)^2\right]\left[k_1^2 - \left(k-2seV_0\right)^2\right]\sin^2(2k_1L)}{4k_1^2k^2 + \left[k_1^2 - \left(k+2seV_0\right)^2\right]\left[k_1^2 - \left(k-2seV_0\right)^2\right]\sin^2(2k_1L)} \tag{112}$$

And for the total scattering cross-section for the barrier, we have.

$$\sigma_s^{t,b} = \lim_{\alpha\to0^+}\sigma_s^{t,WS} = \left|f_s^{+,b}\right|^2 + \left|f_s^{-,b}\right|^2 = 2\left(\sin^2\delta_s^{0,b} + \sin^2\delta_s^{1,b}\right). \tag{113}$$

6 Conclusions

In the context of relativistic quantum mechanics, our work is articulated around three main parts. In the first part, we unified the Klein- Gordon equation and the second-order Dirac equation into a single wave equation, called the relativistic wave equation of spin-s ($s = 0, 1/2$). The second part was dedicated to the scattering matrix. The $\hat{S}_{-s}$-matrix formalism of a relativistic particle of energie E, masse m, charge e and spin-s governed by the one-dimensionnel relativistic wave equation of spin-s in the presence of a localized electromagnetic field has been well exposed and the symmetry considerations C_s, P_s and T_s and the consequences which emerge on both the wave functions and the scattering matrix were recalled. The phase shift method was used that allowed us to extract the phase shifts δ_s^l ($l = 0, 1$), the scattering amplitudes $f_s^{\mp}$, the $\hat{M}_{-s}$-matrix expression in the basis of even and odd waves, the reflection and transmission coefficients $\mathbb{R}_s$ and $\mathbb{T}_s$, as well as the total cross-section σ_s^t.

In order to be able to compare the results obtained in the article [3] and the results of this work, the last part of this manuscript was devoted to the application of this formalism of the $\hat{S}_{-s}$−matrix for relativistic particles spin-s interacting with a localized field, composed of a time-independent scalar potential (Woods−Saxon potential, rectangular barrier potential) $A_0(x,t) = V(x)$ and a vector potential $\vec{A}(x,t) = \vec{0}$.

For the Woods−Saxon potential, we solved the relativistic wave equation of spin-s in the case of a Woods−Saxon potential. The exact solutions of the equation were given as hypergeometric functions. The conditions of continuity of the wave function and its derivative were determined. From the asymptotic behavior of the wave function and the continuity conditions, we derived the $\hat{S}_{-s}^{WS}$−matrix. Then, using the methods developed above, we calculated the phase shifts $\delta_s^{l,WS}$, the scattering amplitudes $f_s^{\mp,WS}$, the $\hat{M}_{-s}^{WS}$-matrix, the transmission and reflection coefficients $\mathbb{R}_s^{WS}$ and $\mathbb{T}_s^{WS}$ and the total scattering cross-section $\sigma_s^{t,WS}$.

The same method was adopted for the case of the barrier potential. By a limit procedure of that of Woods−Saxon when $\alpha \to 0$, we calculated the wave function, the scattering $\hat{S}_{-s}^b$−matrix, the $\hat{M}_{-s}^{WS}$−matrix in the basis of the partial waves, the phase shifts $\delta_s^{l,b}$, the scattering amplitudes $f_s^{\mp,b}$, the transmission or reflection coefficients $\mathbb{T}_s^b$ and $\mathbb{R}_s^b$, as well as the total cross section $\sigma_s^{t,b}$.

This approach proved to be rigorous where we found convergence between the results of reference [3] and those of our work, and allowed us to have results in agreement with those of the literature.

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References

[1] R. G. Newton, *Scattering Theory of Waves and Particles*, New York Heidelberg Berlin, Springer-verlag, 1982.
[2] F. J. Dyson, "The S matrix in quantum electrodynamics," *Phys. Rev.*, vol. 75, pp. 486; 1736, 1949.
[3] K. Khounfais, T. Boudjedaa, and L. Chetouani, "Scattering matrix for Feshbach-Villars equation for spin 0 and 1/2: Woods−Saxon potential," *Czechoslov. J. Phys.*, vol. 54, no. 7, p. 697, 2004.
[4] A. Wachter, *Relativistic Quantum Mechanics*, Berlin, Springer Science + Business Media B.V, 2011.
[5] L. Mario and O. Benhar, *Relativistic Quantum Mechanics, An Introduction to Relativistic Quantum Fields*, USA, CRC Press Taylor&Francis Group, 2016.

[6] V. G. Bagrov and D. Gitman, *The Dirac Equation And its Solutions*, Berlin, Walter de Gruyter & Co, 2014.
[7] Y. Nogami and C. K. Ross, “Scattering from a nonsymmetric potential in one dimension as a coupled-channel problem,” *Am. J. Phys.*, vol. 64, p. 923, 1996.
[8] L. B. Okun, *Weak Interaction of Elementary Particles*, Oxford, Pergamon Press, 1965.
[9] W. Greiner, *Relativistic Quantum Mechanics*, Berlin, Springer, 2000.
[10] J. H. Eberly, “Quantum scattering theory in one dimension,” *Am. J. Phys.*, vol. 33, p. 771, 1965.
[11] B. Stec and C. Jedrzejek, “Resonance scattering by a double square-well potential,” *Eur. J. Phys.*, vol. 11, p. 75, 1990.
[12] C. Rojas and V. M. Villalba, “Scattering of a Klein-Gordon particle by a Woods—Saxon potential,” *Phys. Rev.*, vol. A71, 2005, Art. no. 052101.
[13] P. Kennedy, “The Woods—Saxon potential in the Dirac equation,” *J. Phys. A: Math. Gen.*, vol. 35, pp. 689—698, 2002.
[14] M. Abramowitz and I. A. Stegun, *Handbook of Mathematical Functions*, New York, Dover, 1965.
[15] W. W. Bell, *Special Functions for Scientists and Engineers*, D. Van Nostrand Company Canada, Ltd, 1968.