Annuaire de l'Universite de Sofia "St. Kliment Ohridski", Faculte de Physique
Edition Spéciale, 2012

ON THE PROBLEM OF POTENTIAL BARRIERS AND THE SOLUTION OF THE SCHRODINGER EQUATION

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Асен Дацев. ВЪРХУ ПРОБЛЕМА ЗА ПОТЕНЦИАЛНИТЕ БАРИЕРИ И РЕШАВАНЕТО НА УРАВНЕНИЕТО НА ШРЬОДИНГЕР

Задачата за потенциалните бариери се използва активно в класическата вълнова оптика, но е особено важна за вълновата механика. Тя показва ясно разликите между класическата и вълновата механика. Много задачи от последната могат да бъдат решени приближено чрез използване на потенциални бариери. Например кривата на потенциалната енергия в областта, в която потенциалът се променя плавно, може да се замени с множество стъпаловидни бариери с проста форма, най-често – правоъгълна. В по-сложните случаи, в които имаме няколко плавни бариери, всеки от тях може да се замести с редица от прости правоъгълни бариери. Тогава решаването на задачата се свежда до многократно пресмятане на прост правоъгълен бариер.

Ние развиваме тази идея – заместването на даден плавен бариер със серия от правоъгълни бариери. Задачата се решава лесно в едномерния случай. Използвайки векторни означения, ние намираме матрицата на прехода, която свързва амплитудата на прехода от падащата вълна към отразената и преминалата вълна.

Прилагането на този метод води лесно до известното решение на вълновото уравнение за линеен потенциал, което се изразява чрез функциите на Бесел.

За задачата с n тела се получават подобни $3n$ матрици, играещи същата роля.

Накрая ние използваме този метод на приближено представяне на потенциалния бариер за решаване на едномерни задачи с релативистичното уравнение на Дирак.

Assene Datzeff. ON THE PROBLEM OF POTENTIAL BARRIERS AND THE SOLUTION OF THE SCHRÖDINGER EQUATION

The problem of potential barriers is in active use in Classical Wave Optics, but it is of particular importance in the Wave Mechanics. This problem clearly outlines certain differences between Classical Mechanics and Wave Mechanics. Many problems of the latter can be solved approximately by the use of potential barriers. One replaces, for example, the potential energy curve in a domain where the potential varies a lot by a potential wall and also a potential hill by a barrier with simple shape, mostly rectangular. In other cases, where the potential curve forms series of potential

hills, one can replace the latter with series of simple barriers. One should then repeat many times the calculations concerning a simple barrier.

We develop this idea – of replacing given barrier with a series of rectangular barriers. The problem is easy to pose in the case of motion in one dimension. Using the vector notations, we have found a transformation matrix which connects the amplitudes of the incident wave with those of the reflected and of the transmitted waves.

The application of this method in the case when the potential function is linear gave us very easily the known solution of the wave equation, expressed as Bessel series.

For the problem of *n* bodies one has to write 3*n* matrices of the same form.

In the end, we have used the method of decomposition of a potential barrier to found the solutions of the relativistic equation of Dirac for the problem in one dimension.

Keywords: solution of the Schrödinger equation, solution of the Dirac equation, potential barrier, rectangular approximation

PACS numbers: 03.65-w, 02.70.-c, 02.60.Lj

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ON THE PROBLEM OF POTENTIAL BARRIERS AND THE SOLUTION OF THE SCHRÖDINGER EQUATION

BY

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A DISSERTATION SUBMITTED IN PARTIAL FULFILLMENT OF THE

REQUIREMENTS FOR THE DEGREE OF

DOCTOR OF PHILOSOPHY

IN

FACULTY OF SCIENCES, UNIVERSITÉ DE PARIS

Université de Paris

1938

DOCTOR OF PHILOSOPHY DISSERTATION

OF

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APPROVED:

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DEAN OF THE GRADUATE SCHOOL

Université de Paris

1938

PREFACE

The problem of potential barriers is in active use in Classical Wave Optics, but it is of particular importance in the Wave Mechanics. This problem clearly outlines certain differences between Classical Mechanics and Wave Mechanics. Many problems of the latter can be solved approximately by the use of potential barriers. One replaces, for example, the potential energy curve in a domain where the potential varies rapidly by a potential wall and also a potential hill by a barrier with a simple shape, mostly rectangular. In other cases, where the potential curve forms series of potential hills, one can replace the latter with series of simple barriers. One should then repeat many times the calculations concerning a simple barrier.

On the pages that follow we develop this idea – of replacing given barrier with a series of rectangular barriers. The problem is easy to pose in the case of motion in one dimension. Using the vector notations, we have found a transformation matrix which connects the amplitudes of the incident wave with those of the reflected and of the transmitted waves. This matrix allows us to express the coefficients of reflection and the coefficients of transmission of the given barrier. As a consequence of these formulas, one obtains the solution of the Schrödinger equation in a series of multiple integrals. With the help of a dominant matrix, one proves the absolute convergence of these series in the whole interval, which does not contain the singular points of the potential function and the turning points in the Classical Mechanics. For all those points, one does separate considerations. The first approximate solution found with this method coincides with the approximate solution obtained with the method of Brillouin-Wentzel. From the study we make using the latter method, follows that the calculation of the coefficients of reflection and transmission is valid for barriers, in the interior of which, the wave function becomes infinite at the turning points.

We have then developed second method of solving the wave equation. The calculations were done with the help of matrices, as previously. The application of this method in the case when the potential function is linear, gave us very easily the known solution of the wave equation, expressed as Bessel series.

In one of the chapters that follows we have generalized the method of solving the wave equation of one independent variable, for the wave equation of multiple bodies in any motion, starting with the problem of motion of two bodies on a straight line. The integral of the equation is written with the help of two transformation matrices which have the form of the transformation matrix of the problem in one dimension. For the problem of n bodies one has to write $3n$ matrices of the same form. Almost all considerations done in the case of the one-dimensional problem can be applied easily on generalized problems and we haven't done that in detail in the last case.

In the end, we have used the method of decomposition of the potential barrier to find the solutions of the relativistic equation of Dirac for the problem in one dimension. As first approximation to this method we have found the approximate solution given by M. Pauli.

In all of the considerations that follow one had to use many facts from the theory of barriers. We have also done a brief exposé of this theory, using the principal course of M. Louis de Broglie [7]. For all this we wish to express our profound gratitude to M. Louis de Broglie, and also for the benevolent interest he granted to this work.

CHAPTER 1

1.1 The basics of potential barriers

All the problems in the Wave Mechanics consist of studying the propagation of the waves associated with material particles. Every particle with mass m and energy E, in the absence of exterior field, is associated with a de Broglie wave (matter wave) with wavelength λ:

$$\lambda = \frac{h}{\sqrt{2mE}} \tag{1}$$

where h is the Planck constant. When the particle is in exterior field defined with $U(x,y,z,t)$, the wavelength λ of the associated particle and the coefficient of refraction n are defined by:

$$\lambda = \frac{h}{\sqrt{2m(E-U)}}, \qquad n = \sqrt{\frac{E-U}{E}}, \tag{2}$$

and the wave function Φ satisfies the Schrödinger equation:

$$\Delta\Phi - \frac{8\pi^2 m}{h^2} U\Phi = \frac{4\pi i m}{h}\frac{\partial\Phi}{\partial t}. \tag{3}$$

If the exterior field does not depend on time, the equation (3) admits as solution the standing (stationary) waves $\Phi = \Psi(x,y,z)e^{\frac{2\pi i}{h}Et}$, and the amplitude Ψ satisfies the Schrödinger equation:

$$\Delta\Psi + \frac{8\pi^2 m}{h^2}[E - U(x,y,z)]\Psi = 0. \tag{4}$$

All the problems in the non-relativistic Wave Mechanics are related to the solution of the Schrödinger equation. Unfortunately, finding this solution is not easy even in simple cases. In the more complicated cases, for example, this of multiple particles interacting with each other, one cannot directly solve this problem. For the problem of Helium – two electrons moving around a nucleus – one finds approximate and qualitative results with successive approximations. Even the problem in one dimension is completely solved in the few cases, when the potential function is in the form of a polynomial with not very high degree or a ratio of such polynomials [12]. For the different cases which appear in the practice, there are approximate methods for solving the wave equation. We are going to present the often used method of Brillouin-Wentzel-Kramers.

1.2 Method of Brillouin-Wentzel [2, 15]

The Scrödinger equation (5) takes the following form in the case of motion of a particle on a straight line which we choose to be the axis OX:

$$\frac{d^2\Psi}{dx^2} + \frac{8\pi^2 m}{h^2}[E - U(x)]\Psi = 0. \tag{5}$$

One searches for a solution of (5) in the form:

$$\Psi = e^{\frac{2\pi i}{h}\int^x y dx}. \tag{6}$$

One expands the function $y(x)$ in power series of $\frac{h}{2\pi i}$:

$$y = \sum_{\nu=0}^{\infty} \left(\frac{h}{2\pi i}\right)^{\nu} y_\nu = y_0(x) + \frac{h}{2\pi i} y_1(x) + \left(\frac{h}{2\pi i}\right)^2 y_2(x) + \dots \tag{7}$$

Taking into account (7), we replace Ψ (6) in (5). By canceling the coefficients in front of the different of powers of $\frac{h}{2\pi i}$, one finds the recurrence formulas:

$$y'_{j-1} + \sum_{\nu=1}^{j} y_\nu y_{j-\nu} = 0, \qquad j = 1, 2, \dots \tag{8}$$

and explicitly the first terms of y are:

$$y_0^2 = 2m[E - U(x)], \quad y_1 = \frac{-y'_0}{2y_0}, \quad y_2 = -\frac{y'_1 + y_1^2}{2y_0}, \quad \dots \tag{9}$$

Usually one works with the first two terms y_0 and y_1:

$$\Psi = \frac{1}{\sqrt[4]{2m(E-U)}} e^{\pm \frac{2\pi i}{h} \int^x \sqrt{2m(E-U)}dx}. \tag{10}$$

The integral in the exponent of (10) is the recursive Jacobi function. One finds this function always when the approximation of geometrical optics is valid and one must expect that the form (10) of Ψ corresponds to this approximation.

Let us try to take into account the degree of the approximation that we have, by retaining only the first two terms in the series (8). For this, we have to check when the term y_2 is negligible against y_1. According to (2), y_0 is proportional to n and from (9) we obtain:

$$y_1 = -\frac{y_0'}{2y_0} = -\frac{\frac{dn}{dx}}{2n}.$$

According to (9) the value of y_2 is close to $-\frac{y_1^2}{2y_0} = -\frac{\frac{dn}{dx}}{4n^2 - y_0}$.

One sees that one can ignore y_2 against y_1 if $\frac{y_2}{y_1} << 1$ or if :

$$\frac{1}{n}\frac{dn}{dx}\lambda << 1. \tag{11}$$

Hence, it will be legitimate to use the approximate function (10) when the coefficient of refraction n varies little on the scale of the wavelength of the wave, which is to say, in the approximation of the geometrical optics.

In the domain where $E < U$ the formulas we find are analogous to the previous ones, but the wave function becomes non-periodic.

The question of the convergence of the series (8) which the Brillouin-Wentzel method introduces, is not an easy one. Often there are cases in which those series are strongly divergent. In the neighborhood of the points where $E = U$, the value of Ψ according to (10) grows indefinitely. Hence to apply the formula (10), one needs to exclude the regions around those points.

In the Kramers method [11], one searches for an approximate to (6) solution, in the form $\Psi = g(x)\cos f(x)$ in the interval $(x_1x_2)^*$. One uses the condition $f(x_2) - f(x_1) \sim n\pi$, where n is an integer. $g(x)$ is a continuous function. On arrives to a formula representing the real part of (10). The appropriate values of (6) are found with the help of the condition from the classical theory of numbers, that the phase integral is equal to $n\frac{h}{2\pi}$.

One can look for the integral of the Schrödinger equation for many particles with successive approximation [2], but already the first approximation that one finds represents the Jacobi equation for many particles and the integral of this equation is not known in general.

1.3 Potential barriers

When the wave Ψ associated with a particle crosses a surface S, on which the potential has a finite discontinuity, Ψ remains continuous as well as its first derivative along the normal to S [7]. This property is of great importance for the problem of passage of particles trough a potential barrier.

The simplest problem of discontinuity of the potential appears in the case where a plane separates two homogeneous media with constant potentials U_1 and U_2. If a monochromatic plane wave propagates in the first medium and falls on this plane, it will be partially reflected and it will partially penetrate in the second medium. One wants to determine the amplitudes of the reflected and the transmitted waves, in order to know the intensities corresponding to this waves.

Rectangular barrier – We will operate similarly to the previous case of passage of particles trough a potential barrier. We will consider a medium with a potential U. On the two sides of this medium the potential is zero. We take the axis x for normal to the parallel planes and we assume $E < U$. The plane wave

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* Translator's Note: This notation of the interval comes from the original paper. It stands for the standard notation (x_1,x_2).

which propagates following the positive direction of x, falls normally to the left side of the barrier. A part of this wave reflects, other part penetrates the barrier. Many reflections occur on the barrier and when the process becomes stationary, to the left of the barrier there is an incident wave Ψ_i and a reflected wave Ψ_r which corresponding amplitudes A and B and also two waves with amplitudes C and D with propagate to the left and to the right respectively in the interior of the barrier and also one transmitted wave Ψ_t with amplitude E to the right of the barrier. Now the fundamental problem is to find the amplitudes B and E, because $\mid B\mid^2/\mid A\mid^2 = R$ measures the number of reflected particles and $\mid E\mid^2/\mid A\mid^2 = T$ – the number of the transmitted particles (coefficient of transmission).

As we have already mentioned, the wave that crosses the discontinuity surface of the potential, remains continuous, as well as its derivative along the normal. Then, one has to write the conditions of continuity on the two parallel planes. One will have four linear equation with respect to A, B, C, D, E. Solving those equations, one finds [7] the values of B and E and ultimately of R and T:

$$R = \frac{(k_2^2 - k_1^2)^2 \sin^2 k_2 l}{4k_1^2 k_2^2 \cos^2 k_2 l + (k_1^2 + k_2^2)^2 \sin^2 k_2 l}. \tag{12}$$

$$T = \frac{4k_1^2 k_2^2}{4k_1^2 k_2^2 \cos^2 k_2 l + (k_1^2 + k_2^2)^2 \sin^2 k_2 l} = \frac{1}{1 + \frac{U^2}{4E(E-U)} \sin^2 \left[\frac{2\pi}{h}\sqrt{2m(E-U)}l\right]}. \tag{12'}$$

where:

$$k_1 = \frac{2\pi}{h}\sqrt{2mE} \qquad \text{and} \qquad k_2 = \frac{2\pi}{h}\sqrt{2m(E-U)}.$$

If $U > E$, one will have for R and T formulas similar to (12) and (12′).

The formulas (12) and (12′) show that the number of transmitted particles T is a function of the length l of the barrier and the energy E. If l is constant and E varies, T is a function of E which passes trough successive maximums of the common value $T = 1$ for a series E_n of the values of E. To all E_n correspond wavelengths λ_n of a wave which crosses the barrier completely. This choice of the wave is a resonance of a kind, which we will see manifesting always in the problem of barriers.

Triangular barrier – For rectangular barrier, the function U is constant and the solution of the wave equation is very simple. The more complicated case where U is a linear function of x was studied by Fowler and Nordheim [9]. With a convenient choice of the coordinate origin O one has: $U = 0$ for $x \leq 0$ and $U = C - Fx$ for $x > 0$ (F and C are constants). This is a barrier with the shape of a rectangular triangle. In the interior of the barrier the wave equation is:

$$\frac{d^2\Psi}{dx^2} + \frac{8\pi^2 m}{h^2}[E - C + Fx]\Psi = 0. \qquad (13)$$

The integral of (13) is expressed by the Bessel functions $J_{\frac{1}{3}}$ and $J_{-\frac{1}{3}}$. Writing the conditions of continuity on the two ends of the barrier, after long enough calculations, one obtains the following value of the coefficient of transmission T:

$$T = \frac{4[E(C-E)]^{\frac{1}{2}}}{C} e^{-\frac{8\pi}{h}\frac{\sqrt{2m}(C-E)^{\frac{3}{2}}}{3F}}. \qquad (14)$$

If one calculates now T using the approximate wave function (10), one finds [7] that the principle value of T is given by the exponential factor in (14).

When we discussed the domain of validity of equation (10), we saw that it is not always valid in a domain which contains the points for which $E = U$, because Ψ becomes infinite at those points. This is why we verify in many case, like the previous one, that the value of T evaluated according to the approximate formula (10) of the Brillouin-Wentzel gives the general phenomenon. Despite that Ψ according to (10) is discontinuous in the interval, its application for evaluating T gives sound results. We will see later the explication of this fact, when we find the solution of the wave equation using alternative approach.

Harmonic oscillator – The harmonic oscillator is formed by a material point with mass m, attracted to the point O with a force kx proportional to the distance of the origin x, $k = 4\pi^2\nu^2 m$, where ν is the frequency. Its equation is:

$$\frac{d^2\Psi}{dx^2} + \frac{8\pi^2 m}{h^2}[E - \frac{k}{2}x^2]\Psi = 0. \tag{15}$$

One finds [6, 7] that if $E = (n+\frac{1}{2})h\nu$, $(n = 0, 1, 2, \dots)$, one of the two independent solutions of (15) is an eigenfunction. If E is not in the mentioned form, then (15) does not have eigen-solutions.

Let us now consider a barrier for which the potential is with parabolic shape $U = \frac{k}{2}x^2$ in the interval $(x = -l, x = l)$ and it is zero outside this interval. If the monochromatic plane wave falls on the barrier, one can remake the usual calculations for the barrier and to find the coefficient of transmission (transparency) T. If $E \neq (n+\frac{1}{2})h\nu$, one finds:

$$T = \frac{16\mu^2}{\beta^2(1+\mu^2)^2} e^{2\lambda} e^{-4\gamma l^2}; \mu = \frac{k}{2\gamma l}, \gamma = 2\sqrt{\frac{km}{h}}, \lambda = \frac{2E}{h\nu} \tag{16}$$

If $E = (n+\frac{1}{2})h\nu$ one finds:

$$T = \frac{4\mu^2}{(1+\mu^2)^2} = 4\frac{E/Um}{(1+E/Um)^2}; U_m = \frac{kl^2}{2}. \tag{17}$$

Thus when the energy of the falling particles coincides with one of the eigenvalues of the harmonic oscillator, the number of the transmitted particles is much larger than in the case where $E \neq (n+\frac{1}{2})h\nu$. This is again a resonance phenomenon.

CHAPTER 2

2.1 Decomposition of a potential barrier into elementary barriers [5]

In the previous chapter, we presented some essential results on the problems of potential barriers in the Wave Mechanics. Certain points have been developed in detail due to their applications we will use in the following chapters.

As we have already mentioned, many problems of the passage of particles trough a barrier of any kind can be solved well enough approximately by replacing the given barrier of general shape with a barrier of simple shape where the calculations are easy to make. It is natural to pose the problem of series of simple-shape barriers, especially rectangular ones. One can hardly expect to realize in practice a series of barriers of such shape but the problem when one considers the said series on the place of a barrier with general shape, can be of interest for the approximate solutions which one can obtain. If one has to work with limited number of rectangular barriers, one repeats as many times as the given barriers the calculations done for a rectangular barrier. But if this number is too big, the calculations become too long and impractical. One can, then, make some simplifications and find handy formulas for which one can take the limit. This is what we will study.

We are to work with the problem of passage of particles trough barrier of any shape, starting with the simplest case – this of propagation of particles following a straight line OX.

The barrier extends for example from x_0 to x'. The potential curve which defines the barrier is given by its equation $U = U(x)$ and the wave equation of the

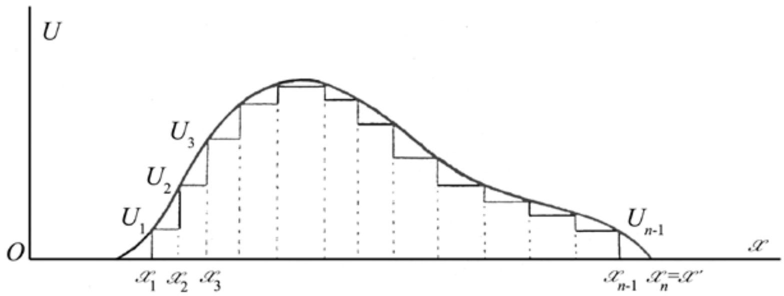

Figure 1.

particles between x_0 and x' will be:

$$\frac{d^2\Psi}{dx^2} + \frac{8\pi^2 m}{h^2}[E - U(x)]\Psi = 0. \tag{18}$$

We suppose that $U(x)$ is continuous, bounded and has first derivative for all the values of x in $(x_0 x')$, where U is composed of finite number of arcs of curves which have the listed properties.

Let us divide the interval $x_0 x'$ into n parts (n is an integer) with the points of division on the abscissa $x_0, x_1, x_2, \ldots, x_{n-1}, x_n = x'$. For this points of division we make the perpendiculars to OX which cross the curve U at the points $U_1, U_2, \ldots$. If now we draw horizontal lines from $U_1, U_2, \ldots$ until they intersect the lines perpendicular to OX and passing trough $x_2, x_3, \ldots$ we will form a broken line with the shape of a step, inscribed in the curve U. The method for studying the passage of particles trough the barrier U will consist of studying the corresponding case of a barrier formed by the broken line and taking the limit $n \to \infty$.

Let us suppose that the particles propagate in the direction OX moving uniformly. The propagation is represented by a monochromatic plane wave with amplitude A_0:

$$\Psi(x) = A_0 e^{-ikx}, \qquad k = \frac{2\pi}{h}\sqrt{2mE},$$

where we didn't write the factor $e^{2\pi i\nu t}$, which should be assumed. E is the energy of the particles. The phenomenon which will be produced from physical point of view when the wave Ψ reaches the barrier is the following. One part if the wave is reflected by the first elementary barrier of width $x_2 - x_1$ and of height $U(x_1)$, another part penetrates trough the barrier. On its turn, this part is also partially reflected from the second barrier and it partially penetrates and so on. Effectively in every barrier there will be a group of waves which propagates in the direction OX and another group moving in the opposite direction. The result will be that in every barrier there is one wave moving to the right and one moving to the left. The latter two waves will have complicated form if the barriers have finite widths but if $x_i - x_{i-1}$ is very small, one can consider the ensemble of portions of the waves in the elementary barrier $x_i - x_{i-1}$ as forming two parts of one monochromatic plane wave which propagates to the right and another which propagates to the left. Physically, one can say that in every small barrier there is certain probability to find the particles moving to the left or to the right. From purely mathematical point of view one can say that the Schrödinger equation which describes the movement of particles, admits in every elementary barrier a solution Ψ which is linear combination of two monochromatic plane waves which propagate to the left and to the right respectively. If $U(x_j)$ is the value of the potential energy in the barrier with width $x_{j+1} - x_j$, the wave equation valid in the interval (x_j, x_{j+1}) is:

$$\frac{d^2\Psi_j}{dx^2} + \frac{8\pi^2 m}{h^2}[E - U(x_j)]\Psi_j = 0 \tag{18'}$$

and its complete solution valid for the values of x between x_j and x_{j+1}:

$$\Psi_j(x) = A_j e^{-iy_j x} + B_j e^{iy_j x}, \qquad (j = 1, 2, \ldots, n-1) \tag{19}$$

with

$$y_j = \frac{2\pi}{h}\sqrt{2m[E - U(x_j)]} \tag{19'}$$

If $E > U_j$, one will have as a solution a true wave, if $E < U_j$, one will not have, strictly speaking, a wave but a real non-periodic function. Nevertheless, this does not affect the reasoning which follows. We have already seen (p.4) that the wave Ψ and its derivative should be continuous at the ends of the barrier crossed by the wave Ψ. In our case, this should be true at all ends common for two neighboring barrier. On will have then the conditions of continuity, which will be for example for $x = x_j$:

$$\Psi_j(x_{j+1}) = \Psi_{j+1}(x_{j+1}), \qquad \left(\frac{d\Psi_j}{dx}\right)_{x_{j+1}} = \left(\frac{d\Psi_{j+1}}{dx}\right)_{x_{j+1}} \tag{20}$$

where the explicit form (removing the factor i in the second equation):

$$\begin{cases} A_j e^{-iy_j x_{j+1}} + B_j e^{iy_j x_{j+1}} = A_{j+1} e^{-iy_{j+1} x_{j+1}} + B_{j+1} e^{iy_{j+1} x_{j+1}} \\ y_j (A_j e^{-iy_j x_{j+1}} - B_j e^{iy_j x_{j+1}}) = y_{j+1} (A_{j+1} e^{-iy_{j+1} x_{j+1}} - B_{j+1} e^{iy_{j+1} x_{j+1}}) \\ (j = 0, 1, 2, \dots, n-2) \end{cases} \tag{21}$$

$$\begin{cases} A_{n-1} e^{-iy_{n-1} x_n} + B_{n-1} e^{iy_{n-1} x_n} = C e^{-iy_0 x_n} \\ y_{n-1} (A_{n-1} e^{-iy_{n-1} x_n} - B_{n-1} e^{iy_{n-1} x_n}) = y_0 C e^{-iy_0 x_n} \end{cases} \tag{22}$$

The amplitude of the transmitted wave is indicated by C, this of the reflected wave – by B_0.

Since the barrier is composed of $n-1$ successive barriers, one has $2n$ conditions like (21) and (22) which allow us to eliminate the amplitudes $A_j, B_j (j = 1, 2, \dots n-1)$ and to find B_0 and C as functions of the amplitude A_0 which is arbitrary (The systems (21) and (22) contain $2n$ equations among the $2n+1$ quantities $A_j, B_j (j = 1, 2, \dots n-1)$ and C). To make this eliminations, one can proceed as follows. The system (21) takes as a value of the index $j = 0$, then one finds the A_1, B_1 as functions of A_0, B_0. One puts the values of A_1, B_1 in the two equations (21) for $j = 1$ and then one has relation between A_0, B_0 and A_2, B_2, from where one finds A_2, B_2 as functions of A_0, B_0 etc. Thus, by eliminating all amplitudes $A_j, B_j (j = 1, 2, \ldots n-1)$, one will find the two relations between A_0, B_0 and C which will give the needed formulas, expressing B_0, C as known functions of A_0.

The equations (21) are linear and non-homogeneous with respect to A_{j+1}, B_{j+1}. The determinant D_{j+1} of their coefficients is:

$$D_{j+1} = \begin{vmatrix} e^{-iy_{j+1}x_{j+1}} & e^{iy_{j+1}x_{j+1}} \\ y_{j+1}e^{-iy_{j+1}x_{j+1}} & -y_{j+1}e^{iy_{j+1}x_{j+1}} \end{vmatrix} = y_{j+1} \begin{vmatrix} 1 & 1 \\ 1 & -1 \end{vmatrix} = -2y_{j+1}. \quad (23)$$

Using the theory of linear equations, one finds

$$\begin{cases} A_{j+1} = \frac{1}{D_{j+1}} \begin{vmatrix} A_j e^{-iy_j x_{j+1}} + B_j e^{iy_j x_{j+1}} & e^{iy_{j+1}x_{j+1}} \\ A_j y_j e^{-iy_j x_{j+1}} - B_j y_j e^{iy_j x_{j+1}} & -y_{j+1}e^{iy_{j+1}x_{j+1}} \end{vmatrix} = \\ \frac{1}{2y_{j+1}} e^{i(y_{j+1}-y_j)x_{j+1}} (y_{j+1}+y_j)A_j + \frac{1}{2y_{j+1}} e^{i(y_{j+1}+y_j)x_{j+1}} (y_{j+1}-y_j)B_j \end{cases} \quad (24)$$

and similarly:

$$B_{j+1} = \frac{y_{j+1}-y_j}{2y_{j+1}} e^{-i(y_{j+1}+y_j)x_{j+1}} A_j + \frac{y_{j+1}+y_j}{2y_{j+1}} e^{-i(y_{j+1}-y_j)x_{j+1}} B_j. \quad (25)$$

It is clear that according to (23), at the points where $U(x) = E$ and thus $D_{j+1} = 0$, this method cannot be directly applied and one has to make special considerations.

It is convenient now to introduce the vector notations and language, that is to say that we consider the amplitudes A_j, B_j as the two components of a vector $\vec{a}_j$. Thus the relation (21) connects the components of the vector $\vec{a}_j$ with those of the vector $\vec{a}_{j+1}$. As we know, the transition from vector $\vec{a}_j$ to vector $\vec{a}_{j+1}$ can be performed with the help of a matrix of two rows and two columns, by considering the components of the vectors as a matrix of two lines and one column.

With this language, one can replace the two relations (24) and (25) with the following:

$$\begin{vmatrix} A_{j+1} \\ B_{j+1} \end{vmatrix} = |M_j| \begin{vmatrix} A_j \\ B_j \end{vmatrix} \quad (26)$$

or also:

$$\vec{a}_{j+1} = M_j \vec{a}_j, \qquad (j = 0, 1, 2, \ldots, n-1) \tag{27}$$

M_j being the following matrix:

$$M_j = \begin{vmatrix} e^{i(y_{j+1}-y_j)x_{j+1}} \frac{y_{j+1}+y_j}{2y_{j+1}} & e^{i(y_{j+1}+y_j)x_{j+1}} \frac{y_{j+1}-y_j}{2y_{j+1}} \\ e^{-i(y_{j+1}+y_j)x_{j+1}} \frac{y_{j+1}-y_j}{2y_{j+1}} & e^{-i(y_{j+1}-y_j)x_{j+1}} \frac{y_{j+1}+y_j}{2y_{j+1}} \end{vmatrix} \tag{28}$$

According to equation (27), the matrix M transforms the vector $\vec{a}_j$ into the vector $\vec{a}_{j+1}$. In the same manner one transforms the vector $\vec{a}_{j+1}$ into $\vec{a}_{j+2}$ with the help of the matrix M_{j+1} whose difference from M_j is that the index j is replaced with $j+1$. By performing p successive eliminations, one will arrive at the vector relation:

$$\vec{a}_{j+p} = M_{j+p} M_{j+p-1} \ldots M_{j+1} \vec{a}_j.$$

However, if we start the elimination from $j = 0$ to $p = n$, one will have:

$$\vec{a}_n = M \vec{a}_0 \tag{29}$$

$$M = M_n M_{n-1} \ldots M_1 M_0. \tag{29$'$}$$

M is a matrix with two lines and two columns, which will be calculated. The elements $m_{11} \ldots m_{22}$ of the matrix M being known, the problem of the passage of particles becomes a simple algebraic problem. The unknown amplitudes B_0 and C will be given by two linear relations coming from the following vector equation:

$$\begin{vmatrix} C \\ C \end{vmatrix} = \begin{vmatrix} m_{11} & m_{12} \\ m_{21} & m_{22} \end{vmatrix} \begin{vmatrix} A_0 \\ B_0 \end{vmatrix}. \tag{30}$$

We have divided the width of the given barrier and the barrier itself to n parts. If n is big enough, the widths of the elementary barriers are very small and the differences between the heights of each two neighboring barriers is also very small. We denote:

$$x_{j+1} - x_j = \Delta x_j, \qquad y_{j+1} - y_j = \left(\frac{dy}{dx}\right)_{x_j} \Delta x_j = \Delta y_j. \tag{31}$$

The differences Δy_j are fully determined with the assumptions on the function $U(x)$ in the interval $(x_0 x')$. One can obtain another form of M_j, by replacing in its terms y_{j+1} with $y_j + \Delta y_j$, and x_{j+1} with $x_j + \Delta x_j$. Since the Δy_j are small, we keep only the terms of the first order with respect to Δy_j in the elements of the matrix M_j. For example, the term $(m_j)_{11}$ of the matrix M_j will be:

$$\begin{cases} (m_j)_{11} = e^{i\Delta y_j x_j \frac{2y_j+\Delta y_j}{2(y_j+\Delta y_j)}} = e^{i\Delta y_j x_j \left(1+\frac{\Delta y_j}{2y_j}\right)\left(1-\frac{\Delta y_j}{y_j}\right)} \\ \qquad = e^{ix_j \Delta y_j \left(1-\frac{\Delta y_j}{2y_j}\right)} = e^{ix_j \Delta y_j - \frac{\Delta y_j}{2y_j}}. \end{cases} \tag{32}$$

In the same manner one finds, always stopping on infinitely small quantities of the first order:

$$\begin{cases} (m_j)_{12} = e^{i(2y_j+\Delta y_j)(x_j+\Delta x_j)} \frac{\Delta y_j}{2(y_j+\Delta y_j)} = \frac{\Delta y_j}{2y_j} e^{2ix_j y_j} \\ (m_j)_{21} = \frac{\Delta y_j}{2y_j} e^{-2ix_j y_j}, \qquad (m_j)_{22} = e^{-ix_j \Delta y_j - \frac{\Delta y_j}{2y_j}} \end{cases} \tag{32'}$$

and the matrix M_j can be written as:

$$M_j = \begin{vmatrix} e^{ix_j \Delta y_j - \frac{\Delta y_j}{2y_j}} & \frac{\Delta y_j}{2y_j} e^{2ix_j y_j} \\ \frac{\Delta y_j}{2y_j} e^{-2ix_j y_j} & e^{-ix_j \Delta y_j - \frac{\Delta y_j}{2y_j}} \end{vmatrix} \tag{33}$$

When Δy_k are small, the elements of the main diagonal $(m_j)_{11}$ and $(m_j)_{22}$ have values which don't differ too much from unity, while $(m_j)_{12}$ and $(m_j)_{21}$ are very small. Then M_j is an almost diagonal matrix, by calling a diagonal matrix the matrix $\|a_{ik}\delta_{ik}\|$, with any a_{ik} and:

$$\delta_{ik} = \begin{cases} 1 & \text{if} \quad i = k \\ 0 & \text{if} \quad i \neq k. \end{cases}$$

In order to evaluate more easily the multiplication of M_j in the formula (29′) and to understand clearly the law of the formation of the terms in the multiplication M, we evaluate the n^{th} of the almost diagonal matrix $A = \|a_{ik}\|(i,k = 1,2)$:

$$A = \begin{vmatrix} 1+\alpha & \alpha \\ \alpha & 1+\alpha \end{vmatrix} \tag{34}$$

where α is a positive number, very small with respect to unity, $a \ll 1$.

If one has two matrices $A = \|a_{ik}\|$ and $B = \|b_{ik}\|$, the elements x_{ik} of the matrix $C = AB$ are given, as we know, by the formula:

$$c_{ik} = \sum_l a_{il} b_{lk}$$

... *

and if n is odd, the summation index i varies from 0 to $\frac{n-1}{2}$ in the elements of B^n. If α is a complex number, with small modulus and any phase, then $\alpha = re^{i\phi}$, it is obvious that one can calculate in similar manner A^n, by formally replacing α with $re^{i\phi}$ in the elements of A^n (the same for B^n).

We are going to now calculate the matrix $M = M_n M_{n-1} \ldots M_0$ from (29′). In order to simplify the calculations we set for the elements of the matrix M_k (33) (using the index k on the place of the index j):

$$ix_k \Delta y_k = \alpha_k, \qquad 2ix_k y_k = \beta_k, \qquad \frac{\Delta y_k}{2y_k} = \rho_k, \tag{35}$$

and M_k will be written as:

$$M_k = \begin{vmatrix} e^{\alpha_k - \rho_k} & \rho_k e^{\beta_k} \\ \rho_k e^{-\beta_k} & e^{-\alpha_k - \rho_k}, \end{vmatrix} \tag{36}$$

where ρ_k enter in the elements of M_k as factors in front of the exponential functions and in the exponents of the exponential functions. One can liken the matrix M_k in the form (36) to the matrix B (2.20). ρ_k as factors in the exponential in M_k correspond to α in B. It is obvious that the terms of M_k will be composed of ρ_k, considered as factors in the exponential functions, exactly the same way as the terms of B are composed of numbers α, since the ρ_k which enter the exponents

*Translator's note: Pages 20-21 of the original thesis are missing from the document, therefore formulas (2.18), (2.19), (2.20), (2.21), appearing after (34) and before (35), are also missing. They would be referred in the text with their original numeration.

in the terms of M_k remain always in the exponents when one multiplies two exponents. As a consequence, as formula (2.21) shows, the terms $m_{rs}(r,s=1,2)$ of the matrix product M will be polynomials with respect to ρ_k. The coefficients of these polynomials will be the exponential functions which contain the ρ_k. Still comparing M with B^n (2.21) one sees that m_{11} and m_{22} will be even polynomials with respect to ρ_k, and m_{12} and m_{21} are odd polynomials.

We multiply M_k (36) with M_{k+1} according to the law of matrix multiplication. We find:

$$M_{k+1}M_k = \left| \begin{array}{cc} e^{\alpha_{k+1}+\alpha_k-\rho_{k+1}-\rho_k}+\rho_{k+1}\rho_k e^{\beta_{k+1}-\beta_k} & \rho_k e^{\alpha_{k+1}-\rho_{k+1}+\beta_k}+\rho_{k+1}e^{\beta_{k+1}-\alpha_k-\rho_k} \\ \rho_{k+1}e^{-\beta_{k+1}+\alpha_k-\rho_k}+\rho_k e^{-\beta_k-\alpha_{k+1}-\rho_{k+1}} & e^{-\alpha_{k+1}-\alpha_k-\rho_{k+1}-\rho_k}+\rho_{k+1}\rho_k e^{-\beta_{k+1}+\beta_k} \end{array} \right|. \tag{37}$$

Let us introduce notations which will be useful in what follows. Suppose we evaluated the product (37) of p successive matrices of the form M_k. In the elements of the matrix product we group the terms which contain the factor ρ_k, those with two factors ρ_k etc. . We note with $m_{11}^{2i,p}$ the sum of the elements of the first row and the first column of the matrix product, which contains $2i$ factors ρ_k. (Obviously $2i \leq p$). One will have three more, analogous to the previous, notations: $m_{22}^{2i,p}, m_{12}^{2i+1,p}, m_{21}^{2i+1,p}$. For example, one can express with those notations two elements of the matrix (37):

$$e^{\alpha_{k+1}+\alpha_k-\rho_{k+1}-\rho_k}+\rho_{k+1}\rho_k e^{\beta_{k+1}-\beta_k} = m_{11}^{0,2}+m_{11}^{2,2}$$

$$\rho_{k+1}e^{-\beta_{k+1}+\alpha_k-\rho_k}+\rho_k e^{-\beta_k-\alpha_{k+1}-\rho_{k+1}} = m_{21}^{1,2}$$

By multiplying (37) with M_{k+2}, we find the element m_{11} from the first line and the first column of the product $M_{k+2}M_{k+1}M_k$:

$$m_{11} = e^{\alpha_{k+2}+\alpha_{k+1}+\alpha_k-\rho_{k+2}-\rho_{k+1}-\rho_k}+\rho_{k-1}\rho_k e^{\alpha_{k+2}-\rho_{k+2}+\beta_{k+1}-\beta_k}$$
$$+\rho_{k+2}\rho_{k+1}e^{\alpha_k-\rho_k+\beta_{k+2}-\beta_{k+1}}+\rho_{k+2}\rho_k e^{-\alpha_{k+1}-\rho_{k+1}+\beta_{k+2}-\beta_k} = m_{11}^{0,3}+m_{11}^{2,3}.$$

The first element in the latter sum is $m_{11}^{0,3}$ which can be written as

$$m_{11}^{0,3} = e^{\sum\limits_{j=0}^{2} \alpha_{k+j} - \sum\limits_{j=0}^{2} \rho_{k+j}}.$$

The element $m_{11}^{0,4}$ will have the same form, but the sums in the exponent will have one more term. Always following the complete mathematical induction, which is immediately applicable to this case, one can see that the element $m_{11}^{0,p}$ in the matrix $M_{p-1}M_{p-2}\ldots M_2M_1$ will be:

$$m_{11}^{0,p} = e^{\sum\limits_{j=0}^{p-1} \alpha_{k+j} - \sum\limits_{j=0}^{p-1} \rho_{k+j}}$$

With the help of the notations (35) one obtains the explicit form of $m_{11}^{0,p}$. Initially, the factor in the exponents takes the following form:

$$\sum_{j=0}^{p-1} \alpha_{k+j} - \sum_{j=0}^{p-1} \rho_{k+j} = i\sum_{j=0}^{p-1} x_{k+j}\Delta y_{k+j} - \frac{1}{2}\sum_{j=0}^{p-1} \frac{\Delta y_{k+j}}{y_{k+j}}. \tag{38}$$

We divided the interval x_0x'(the width of the barrier) to n parts. If n is a very big number, thus each interval is very small, the above sums become definite integrals. In the formulas which follow, the integrations are indicated with respect to y, but one can immediately rewrite them with respect to x , since y is a known function of x (19′) and $dy = \frac{dy}{dx}dx$. For the moment, we would not deal with the question of convergence of the integrals, which will be discussed later on. By taking the limit $p \to \infty$, the right part of the last equation becomes:

$$\begin{cases} i\int_{y_k}^{y_p} xdy - \frac{1}{2}\int_{y_k}^{y_p}\frac{dy}{y} = i\int_{y_k}^{y_p} xdy - \lg\sqrt{\frac{y_p}{y_k}} \\ = i(x_py_p - x_ky_k) - i\int_{y_k}^{y_p} ydx - \lg\sqrt{\frac{y_p}{y_k}} \end{cases} \tag{37′}$$

thus with the help of (19), $m_{11}^{0,p}$ becomes:

$$\begin{cases} m_{11}^{0,p} = \sqrt{\frac{y_p}{y_k}}e^{i\int_{y_k}^{y_p} xdy} \\ = \sqrt[4]{\frac{E-U(x_k)}{E-U(x_p)}}e^{i(x_py_p - x_ky_k) - i[\Phi(x_p) - \Phi(x_k)]} \end{cases} \tag{39}$$

where we have substituted:

$$i\int_{y_k}^{y_p} y dx = \Phi(x) \qquad (37'')$$

which is not else but the classical integral of Maupertuis.

If we fix the value of x_n, the integral in $m_{11}^{0,p}$ is a function of its upper limit, thus one can consider $m_{11}^{0,p}$ as a known function of x_p, this is to say, of x. When the transition to the limit is done, we will denote this function with $m_{11}^{0}(x)$ or simply with m_{11}^{0}.

According to (36), one sees that the element m_{22} of the matrix M_k differs from m_{11} only by the sign of α_k in the exponent. Taking account of this, we repeat the reasoning of the formation of m_{11}^{0} in the matrix M. We easily see that m_{22}^{0} differs from m_{11}^{0} only by the sign of the exponent, namely:

$$\begin{cases} m_{22}^{0,p} = \sqrt{\frac{y_k}{y_p}} e^{-i\int_{y_k}^{y_p} x dy} \\ = \sqrt[4]{\frac{E-U(x_k)}{E-U(x_p)}} e^{-i(x_p y_p - x_k y_k) + i\int_{y_k}^{y_p} y dx} \end{cases} \qquad (39')$$

We mentioned above that the elements m_{12} and m_{21} of M, like the elements of the corresponding matrix B^n (2.21) are odd polynomials of ρ. Let us calculate m_{12}^{1}, the first term of m_{12}. Evaluating the products, as above, step by step we find:

$$m_{12}^{1,p} = \sum_{j=0}^{p-1} \rho_{k+j} e^{\beta_{k+j} - \sum_{l=0}^{j-1} \alpha_{k+l} + \sum_{l=j+1}^{p-1} \alpha_{k+l} - \sum_{l=0}^{p-l} \rho_{k+l}}. \qquad (40)$$

We verify immediately this relation for $p = 3$. One sees also easily that this relation is valid for the value $p = n$ if it is correct for $p = n-1$. When $p \to \infty$, the sums become integrals and one has:

$$\begin{cases} m_{12}^{1,p}(x_p) = \frac{1}{2}\int_{y_k}^{y_p} \frac{dy}{y} e^{2ixy - i\int_{y_k}^{y} x dy + i\int_{y}^{y_p} x dy - \frac{1}{2}\int_{y_k}^{y_p} \frac{dy}{y}} \\ = \frac{1}{2}\sqrt{\frac{E-U(x_k)}{E-U(x_p)}} e^{i(x_k y_k + x_p y_p)} \int_{y_k}^{y_p} \frac{dy}{y} e^{i\int_{x_k}^{x} y dx - i\int_{x}^{x_p} y dx} \end{cases} \qquad (40')$$

Likewise one can find all the terms in the polynomials which form the elements of the matrix M. This method, however, is long and painful. We will find the recurrence formulas which will allow us to write all the terms of the polynomials.

Let us form the product of p matrices:

$$M_{k+p}M_{k+p-1}\dots M_{k+1}M_k = M.$$

As it was already explained, $m_{11}^{2i,p}$ is the term of the first row and first column of this matrix M, term which contains $2i$ factors ρ. Let us multiply from the left this product with the matrix M_{k+p+1}. Then $m_{11}^{2i,p+1}$, the term of the first row and first column of the matrix product of $p+1$ factors, contains $2i$ factors ρ. This term will be, according to the matrix multiplication rule, the sum of the term of the first row and the first column of the preceding matrix M, which contains $2i$ factors ρ, multiplied by $e^{\alpha_{k+p+1}-\rho_{k+p+1}}$ and of the term of the second line and the first column of the same matrix M which contains $2i-1$ factors ρ, multiplied by $\rho_{k+p+1}e^{\beta_{k+p+1}}$. Explicitly, this product is:

$$m_{11}^{2i,p+1} = e^{\alpha_{k+p+1}-\rho_{k+p+1}}m_{11}^{2i,p} + \rho_{k+p+1}e^{\beta_{k+p+1}}m_{21}^{2i-1,p}. \tag{41}$$

The absolutely analogous reasoning to those above will give us three more recurrence formulas.

$$\begin{cases} m_{12}^{2i+1,p+1} = e^{\alpha_{k+p+1}-\rho_{k+p+1}}m_{12}^{2i+1,p} + \rho_{k+p+1}e^{\beta_{k+p+1}}m_{22}^{2i,p} \\ m_{21}^{2i+1,p+1} = \rho_{k+p+1}e^{-\beta_{k+p+1}}m_{11}^{2i,p} + e^{-\alpha_{k+p+1}-\rho_{k+p+1}}m_{21}^{2i+1,p} \\ m_{22}^{2i,p+1} = \rho_{k+p+1}e^{-\beta_{k+p+1}}m_{12}^{2i-1,p} + e^{-\alpha_{k+p+1}-\rho_{k+p+1}}m_{22}^{2i,p} \end{cases} \tag{41'}$$

With the help of these formulas we can write explicitly the terms of the matrix M. Let us start with $m_{11}^{2i,p+1}$. According to (41), this term is expressed with $m_{11}^{2i,p}$, thus the upper right index is decreased with one. If one expresses the term $m_{11}^{2i,p-1}$ with the help of the same formulas (41), one finds:

$$m_{11}^{2i,p+1} = \rho_{k+p+1} e^{\beta_{k+p+1}} m_{21}^{2i-1,p} + e^{\alpha_{k+p+1}-\rho_{k+p+1}} (\rho_{k+p} e^{\beta_{k+p}} m_{21}^{2i-1,p-1} + e^{\alpha_{k+p}-\rho_{k+p}} m_{11}^{2i,p-1}).$$

We can now replace $m_{11}^{2i,p-1}$ of the last equality with $m_{11}^{2i,p-2}$ using (41), the latter term with $m_{11}^{2i+1,p-3}$ and so on. We arrive this way at the term $m_{11}^{2i,2i}$. The right side of (41) will be a sum with respect to ρ. One finds easily, taking into account the formation law of the last equality:

$$m_{11}^{2i,p+1} = \rho_{k+p+1} e^{\beta_{k+p+1}} m_{21}^{2i-1,p} + \sum_{l=2i}^{p} \rho_{k+l} e^{\beta_{k+l} + \sum_{j=l+1}^{p+1} (\alpha_{k+j} - \rho_{k+j})} m_{21}^{2i-1,l}.$$

We replace in the last formula ρ, α, β with their values from (35) and we take the limit $p \to \infty$. The first term of the right side of the last equality cannot be conveniently presented as a term of the sum. On can ignore it, since it tends to zero at the same time as ρ. The term $m_{21}^{2i,l}$ of the sum depends of the index l, thus it is a function of y_l, this is to say of y, when the intervals tend to zero. This function will be noted as $m_{11}^{2i}(y)$. One finds for $m_{11}^{2i,p+1}$, taking into account (41) and (41′):

$$\begin{cases} m_{11}^{2i}(y_p) = \frac{1}{2} \int_{y_k}^{y_p} \frac{dy}{y} e^{2ixy + i\int_y^{y_p} \xi d\eta - \frac{1}{2}\int_y^{y_p} \frac{dy}{y}} m_{21}^{2i-1}(y) \\ \qquad = \frac{1}{2\sqrt{y_p}} \int_{y_k}^{y_p} \frac{dy}{\sqrt{y}} e^{2ixy + i\int_y^{y_k} \xi d\eta} m_{21}^{2i-1}(y), \end{cases} \tag{42}$$

where ξ and η replace the variables x and y. With the help of (37′) and (37″) one can put $m_{11}^{2i}(y_p)$ in the form:

$$m_{11}^{2i}(y_p) = \frac{e^{ix_p y_p - i\Phi(y_p)}}{2\sqrt{y_p}} \int_{y_k}^{y_p} \frac{dy}{\sqrt{y}} e^{ixy - i\Phi(y)} m_{21}^{2i-1}(y). \tag{42′}$$

The term $m_{11}^{2i}(y_p)$ will be a known function of y, if one knows m_{21}^{2i-1} as a function of y.

Let us take the second formula (41′). If we apply the same formula to the term $m_{21}^{2i+1,p}$ on the right side, we decrease successively the index p so that for the term $m_{21}^{2i+1,p+1}$, one obtains the following formula:

$$m_{21}^{2i+1,p+1} = \sum_{l=2i}^{p+1} \rho_{k+l} e^{-\beta_{k+l} - \sum_{i=l+1}^{p+1} (a_{k+j} - \rho_{k+j})} m_{11}^{2i,l}.$$

and by taking the limit:

$$m_{21}^{2i+1}(y_p) = \frac{1}{2\sqrt{y_p}} \int_{y_k}^{y_p} \frac{e^{-2ixy - i\int_{y}^{y_p} \xi d\eta}}{\sqrt{y}} m_{11}^{2i}(y) dy. \tag{43}$$

In equation (42) one can replace $m_{21}^{i1-2}(y)$ with the same term, taken from (43). One finds:

$$m_{11}^{2i}(y_p) = \frac{1}{2^2 y_p} \int_{y_k}^{y_p} \frac{dy}{\sqrt{y}} e^{2ixy + i\int_{y}^{y_p} \xi d\eta} \int_{y_k}^{y} \frac{e^{-2ix_1 y_1 - i\int_{y_1}^{y} \xi_1 d\eta_1}}{\sqrt{y_1}} m_{11}^{2i-2}(y_1) dy_1 \tag{44}$$

One can continue the same process on m_{2i-2}^{11} in order to decrease its upper right index to zero, this is to say, to the term m_{11}^{0} which is known from (39). The final form of m_{11}^{2i} will be:

$$\begin{cases} m_{11}^{2i}(y_p) = \frac{1}{2^2 y_p^i} \int_{y_k}^{y_p} \frac{dx}{\sqrt{y}} e^{2ixy + i\int_{y}^{y_p} \xi d\eta} \int_{y_k}^{y} \frac{dy_1}{\sqrt{y_1}} e^{-2ix_1 y_1 - i\int_{y_1}^{y_p} \xi d\eta} \int_{y_k}^{y_1} \dots \\ \qquad \int_{y_k}^{y_{2i-2}} \frac{dy_{2i-1}}{\sqrt{y_{2i-1} - 1}} e^{-2ix_{2i-1} y_{2i-1} - i\int \xi_{2i-1} d\eta_{2i-1}} m_{11}^{0}(y_{2i-1}) \end{cases} \tag{45}$$

(one should not confuse the index of the term i with the imaginary unit i).

It is clear that in the last formula, the variables with indexes which replace formally the variables x and y, and the integrals are functions of their upper limits.

The last formula expresses $m_{11}^{2i}(y)$ as a known function of y with the help of $2i$ integrations. Exactly the same way, one can find the formulas of the three other terms:

$$\begin{cases} m_{12}^{2i+1}(y_p) = \frac{1}{2^{2i+1} y_k^{i+1}} \int_{y_k}^{y_p} \frac{dy}{\sqrt{y}} e^{2ixy + i\int_{y}^{y_p} \xi d\eta} \int_{y_k}^{y} \frac{dy_1}{\sqrt{y_1}} e^{-2ix_1 y_1 - i\int_{y_1}^{y_p} \xi_1 d\eta_1} \int \dots \\ \qquad \int_{y_k}^{y_{j-1}} \frac{dy_j}{\sqrt{y_j}} e^{2ix_j y_j + \int_{y_j}^{y_p} \xi_j d\eta_j} m_{22}^{0}(y_j) \\ m_{21}^{2i+1}(y_p) = \frac{1}{2^{2i+1} y_k^{i+1}} \int_{y_k}^{y_p} \frac{dy}{\sqrt{y}} e^{-2ixy - \int_{y_k}^{y_p} \xi d\eta} \int_{y_k}^{y} \dots \int_{y_k}^{y_{j+1}} \frac{dy_j}{\sqrt{y_j}} e^{-2ix_j y_j - \int_{y_j}^{y_p} \xi_j d\eta_j} m_{11}^{0}(y_j) \\ m_{22}^{2i}(y_p) \quad = \frac{1}{2^{2i} y_k^{i}} \int_{y_k}^{y_p} \frac{dy}{\sqrt{y}} e^{-2ixy - \int_{y}^{y_p} \xi d\eta} \int_{y_k}^{y} \dots \int_{y_k}^{y_{j+1}} \frac{dy_j}{\sqrt{y_j}} e^{2ix_j y_j + \int_{y_j}^{y_p} \xi_j d\eta_j} m_{22}^{0}(y_j) \end{cases} \tag{46}$$

where one has to take for the index j of the last integral of the terms (46) $j = 2i - 1$. One can obtain another form of those formulas, like (42′), by replacing the integral $\int^x \xi d\eta$ according to (37′) and (37″) with $\Phi(x)$.

As we have said the four elements of the matrix M are polynomials of ρ. These polynomials have finite number of terms when the interval x_0x' is divided on n parts (n – finite). But if $n \to \infty$, the elements of the matrix become infinite series whose terms can be calculated according to the formulas below. The four terms of M are:

$$\begin{cases} m_{11}(x) = \sum_{i=0}^{\infty} m_{11}^{2i}(x), & m_{12} = \sum_{i=0}^{\infty} m_{12}^{2i+1}, \\ m_{21} = \sum_{i=0}^{\infty} m_{21}^{2i+1}, & m_{22} = \sum_{i=0}^{\infty} m_{22}^{2i} \end{cases} \tag{47}$$

They are known functions of y, or of x, since y is a known function of x.

The problem which we had posed in the beginning of this study was to find the proportion between the reflected particles and the transmitted particles by the barrier. This is equivalent to finding the amplitude B_0 of the reflected wave and C – that of the transmitted wave according to formula (30). Since the matrix M is known, the problem is solved in principle.

2.2 Convergence of the series (47)

We have to now discuss the question of convergence of the series $m_{11}, \ldots, m_{22}$ (47). All the integrals which enter in the terms (45) and (46) contain in the denominator $y = \sqrt{2m(E - U(x))}$. Thus the functions under the integrals become infinite for these values of x for which $E = U$, since $y = 0$. We consider firstly the case where the right side of the equation $U = E$ does not cut trough the barrier between its end points x_0x' (y does not vanish between x_0 and x'). We have seen that the matrix M_j (33) or M_k (36) is almost diagonal, this is to say that the absolute values of the main diagonal elements of M_k are almost unity, and that the absolute values of the other elements are very small. Since the function $y(x)$ is continuous and bounded between x and x', one can find a positive number α such that $1+\alpha$ will be bigger than the modules of the elements of the main diagonal of all the matrices M_k $(k=1,2,\ldots,n)$, and α bigger than the module of the two other elements of the matrices $M_k(k=1,2,\ldots,n)$. Thus the matrix:

$$M_\alpha = \begin{vmatrix} 1+\alpha & \alpha \\ \alpha & 1+\alpha \end{vmatrix}$$

is the "dominant" matrix of M_k. M_α is identical to A in (34). To the matrix M, product of n matrices, will correspond the n-th power of M_α, thus M_α^n. We already know the elements of that matrix $M_\alpha^n = A^n$ according to (2.19). We can write:

$$\begin{aligned}(a_n)_{11} &= 1+\sum_{k=1}^{n} 2^{k-1} C_n^k \alpha^k = 1+\frac{1}{2}\sum_{l=1}^{n} 2^k C_n^k \alpha^k \\ &= \frac{1}{2}(1+\sum_{k=0}^{n} 2^k C_n^k \alpha_k) = \frac{1}{2}[1+(1+2\alpha)^n]\end{aligned}$$

With the assumptions made below for the function $f(x)$, when the number n of the division of the interval x_0x' tends to infinity, the main diagonal elements of M_k tend to zero. Therefore α should tend to zero simultaneously with $\frac{1}{n}$. If we assume that $\alpha = \frac{m}{n}$, where m is a finite positive number, we will find for the limit value of $(a_n)_{11}$:

$$\lim_{n\to\infty}(a_n)_{11} = \lim_{\alpha\to 0}\frac{1}{2}\left[1+(1+2\alpha)^{\frac{m}{\alpha}}\right] = \frac{1}{2}(1+e^{2m})$$

which is finite. For the term $(a_n)_{12}$ of M one finds the same with the help of (2.19):

$$\lim_{n\to\infty}(a_n)_{12} = \frac{1}{2}(-1+e^{2m}).$$

Since $(a_n)_{11} = (a_n)_{22}$ and $(a_n)_{12} = (a_n)_{21}$ all the elements of A^n are finite. As a consequence, the sums (45) and (46) which have smaller values than the values $(a_n)_{11},\ldots,(a_n)_{22}$ are also finite.

Now let us consider the case where $y(x)$ vanishes in the interval x_0x'. Obviously the line $E = U$ crosses the barrier at two points, or, in general, in even number of points. Let us assume they are two.

The two terms m_{11}^0 and m_{22}^0 (39′), in which we have already performed an integration, contain $\sqrt{y}$ in the denominator and they will be discontinuous for $y = 0$. This discontinuity comes from the factor $e^{-\frac{1}{2}\int_{y_k}^{y_p}\frac{dy}{y}} = \sqrt{\frac{y_k}{y_p}}$. (37′), which becomes indeterminate for $y_p = 0$.

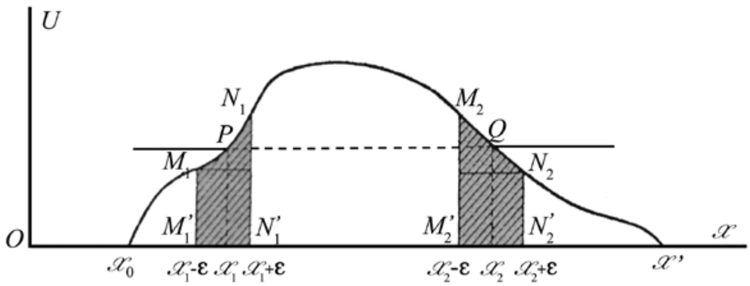

Figure 2.

This simply shows that the method of division of the barrier on a too big number of elementary barriers of rectangular shape is not applicable around the points $P(x_1)$ and $Q(x_2)$ (Fig.2), where the line $U = E$ crosses the barrier. However, we can always cut the barriers on two small barriers which contain the points P and Q and which extend from the point $M_1(x_1 - \varepsilon)$ to the point $N_1(x_1 + \varepsilon)$ and from the point $M_2(x_2 - \varepsilon)$ to the point $N_2(x_2 + \varepsilon)$ respectively (ε is a small positive number). The given barrier is thus divided to five successive barriers. The formulas (39) and (39′) are surely valid for the three barriers from x_0 to $x_1 - \varepsilon$, from $x_1 + \varepsilon$ to $x_2 + \varepsilon$ and from $x_2 + \varepsilon$ to x'.

We connect the points M_1N_1 and M_2N_2 with rectilinear segments. The two small dashed domains form two barriers where the curve U is a straight line. The passage of particles across those two barriers can be calculated as for a rectilinear barrier (triangular) with the help of the functions of Bessel $J_{\frac{1}{3}}$ and $J_{-\frac{1}{3}}$, without having the discontinuity at the points P and Q anymore. We have thus five successive barriers on the place of the given barrier and the solution of equation (18) in each of them is known. The problem is theoretically solved, but the calculations will be complicated. For the moment we will omit them, since our problem is to find the reflected wave and the transmitted wave, and we are to find them in another way.

The formulas (37) and (37′) show that the discontinuity in the terms m^0_{11} and m^0_{22} comes from those members of the second sum, for which $y_{k+j} = 0$. When one goes from M_1 to N_1 (fig.2), y varies from a real value to a purely imaginary value passing trough zero. Therefore the integration of $\int \frac{dy}{y}$ is performed along contour M_1ON in the complex plane $\xi + i\eta$ (M_1 is on $O\xi$ and N_1 is on $O\eta$). If we avoid the origin O with the help of a quarter-circle C with center O and radius ε, one has to calculate $\int \frac{dy}{y}$ along the contour following $M_1\varepsilon$; C; $i\varepsilon, N_1$:

$$\int_{M_1}^{N_1} \frac{dy}{y} = \int_{y_{M_1}}^{\varepsilon} \frac{dy}{y} + \int_C \frac{dy}{y} + \int_{i\varepsilon}^{i|y_{N_1}|} \frac{dy}{y}$$
$$= \lg \frac{|\, y_{N_1} \,|}{y_{M_1}} + i\frac{\pi}{2} = \lg \frac{y_{N_1}}{y_{M_1}}$$

since $\lg\ y_{N_1} = \lg |\, y_{N_1} \,| + i\frac{\pi}{2}$ according to the definition of the logarithm of complex variable. The same reasoning is applicable between N_2 and M_2 where y becomes real again and one has:

$$\int_{y_k}^{y_p} \frac{dy}{y} = \lg \frac{y_p}{y_k}.$$

If the line $E = U$ crosses the barrier at even number of points between (y_k) and (y_p), the preceding example is applied without change, and the integral $\int \frac{dy}{y}$ will be given with the preceding formulas.

The conclusion that one can make from the preceding results is the following:

the integral $\int \frac{dy}{y}$ has a finite value, because there is a kind of compensation of the discontinuity by the function under the integral. In analogous way one can show that all the integrals in the terms of the matrix M are finite, despite the functions under the integrals being discontinuous at even number of points. One can then always use the expressions m_{11}^0 and m_{22}^0 (39) and (39′) and the others $m_{ik}(i,k=1,2)$ (45) and (46) for the usual calculations of the passage of particles trough barrier of any kind if the potential function does not have singular points in the interval $(x_0 x')$. We will come back to that point later.

Note. – The problem of escape of particles from a potential well [7] is very analogous to the problem of passage of particles through a potential barrier. If the shape of the well is arbitrary, one can decompose it to rectangular barriers and make the eliminations of the arbitrary amplitudes with the help of almost diagonal matrices, as we have already done it for a potential barrier. We would not deal with this problem here, since in the following chapter we will give the solutions of the Schrödinger equation, and with it, the principal difficulty of the problem of escape of particles from a potential well is removed.

CHAPTER 3

3.1 Solution of the Schrödinger equation in the case of one variable [4]

We found the formulas which give the proportion of the reflected and the transmitted particles, when they fall on a potential barrier. This was the general problem of potential barriers. But those same formulas will serve us also to find one important result: the solution of the wave equation. In effect, it is easy to understand that the formulas determining the reflected and the transmitted waves must contain in some way the solution of the wave equation.

The method we used consisted of decomposing a barrier of any form to small elementary rectangular barriers. For each of them, the solution of the wave equation is known: this is a linear combination of two plane waves. When x varies for example from x_p to x_{p+1}, the solution of the equation is, according to [8]:

$$\Psi_p(x) = A_p e^{-iy_p x} + B_p e^{iy_p x}. \tag{48}$$

But if the variations of x are bigger, the wave function $\Psi_p(x)$ will not satisfy the wave equation anymore. In this moment we have to take into account that A_p and B_p cannot be considered as constants anymore. They will be functions of x. With successive eliminations we have expressed the amplitudes A_p, B_p as functions of the amplitudes A_1, B_1, in the first elementary barrier $(x_0 x_1)$ with the formula:

$$\left| \begin{matrix} A_p \\ B_p \end{matrix} \right| = M(x_1, x_p) \left| \begin{matrix} A_1 \\ B_1 \end{matrix} \right| = M_p M_{p-1} \dots M_2 M_1 \left| \begin{matrix} A_1 \\ B_1 \end{matrix} \right|$$

The elements of the matrix M, given by (46) and (47), are known functions of x_p since the upper limit in the integrals in (46) is y_p, this is to say, a function of x_p. But x_p can take all values between x_0 and x'. Consequently, if one puts in (48) the values of A_p and B_p as functions of x, one will express Ψ_p as a function of x, where x varies in the whole interval x_0x'. By taking A_p, B_p of the last relation, one has as solution of the wave equation (5):

$$\Psi(x) = [m_{11}(x)e^{-iyx} + m_{21}(x)e^{iyx}]A_1 + [m_{12}(x)e^{-iyx} + m_{22}(x)e^{iyx}]B_1. \qquad (49)$$

Here one can consider the quantities A_1 and B_1 to be arbitrary and $\Psi(x)$ will depend on two arbitrary parameters. $\Psi(x)$ (49) *is then the general integral of the wave equation* (5).

When one applies this formula to the problem of barriers and when one writes down the four conditions of continuity which connect the parameters A_1, B_1 with the amplitudes A_0, B_0, C, there will be only one arbitrary parameter: the amplitude A_0 of the incident wave, as we have seen it for the rectangular barrier.

Let us retain now in (49) only the terms m^0_{11} and m^0_{22} of M. $\Psi(x)$ will take the form:

$$\Psi(x) = m^0_{11}(x)e^{-iyx}A_1 + m^0_{22}(x)e^{iyx}B_1$$

By replacing m^0_{11} and m^0_{22} with their expressions (39) and (39′) and by setting $x_p = x$ and $x_k = x_1$, one will have:

$$\begin{cases} \Psi(x) = A_1\sqrt[4]{\frac{E-U(x_1)}{E-U(x)}}e^{-ix_1y_1 - i\int_{x_1}^{x}\sqrt{2m(E-U(x))}dx} \\ \qquad\qquad + B_1\sqrt{\frac{E-U(x_1)}{E-U(x)}}e^{ix_1y_1 + i\int_{x_1}^{x}\sqrt{2m(E-U(x))}dx} \end{cases} \qquad (50)$$

The comparison of (50) with (10) (p.3) gives immediately that each one of the two terms of $\Psi(x)$ (50) is identical up to a numerical factor, to one of the functions (10) which one finds following the method of Brillouin-Wentzel, in the most common case of its application. This was, as we know, the case where the approximation of geometrical optics is valid.

3.2 Verification that the function $\Psi(x)$ (49) satisfies the wave equation

We have to show now, in a more direct manner, that the function Ψ (49) satisfies the equation (18). But if we want to find directly the second derivative of Ψ by differentiation of (50), that will be very difficult, since the terms $m_{11},\ldots,m_{22}$ (47) are complicated functions of x.

One can give some general reasons why Ψ (49) is the solution of (18). First, we have replaced the potential curve by a broken line such that the surface between the latter and the axis OX tends to the surface of the barrier. Since the broken line tends to the potential curve, in the limit when $n \to \infty$, one has to expect that the so-found solution will tend to the exact solution (18). A doubt may appear on first glance, because the first derivatives of the function which represents the broken line are discontinuous for n values of x. Nevertheless, this does not influence the result, since the wave-function Ψ and its derivatives are required to be continuous at the ends of the neighboring elementary barriers.

From another side, Ψ was constructed in such way that in each interval (x_p, x_{p+1}), its variation will be like this of the exponential function. In this interval Ψ obviously satisfies the equation, but only if we consider the potential as a constant. The function Ψ is then composed of little arcs, glued one to another in a way that Ψ and its derivative will be continuous. Since this is true for any division of the interval x_0x', in the limit the function Ψ satisfies the equation for each value of x. We have to then confirm this with calculations. But to find more directly that the function Ψ satisfies equation (18), we will calculate its second derivative. For a value x_p of x one will have the value of $\frac{d^2\Psi}{dx^2}$ if one knows the values of Ψ for three points of x: x_p, x_{p+1}, x_{p+2}, this is to say: $\Psi(x_p), \Psi(x_{p+1}), \Psi(x_{p+2})$. We have to find the two first differences:

$$\Psi(x_{p+2}) - \Psi(x_{p+1}) \qquad \text{and} \qquad \Psi(x_{p+1}) - \Psi(x_p)$$

and their difference divided by Δx_p^2, ($\Delta x_p = x_{p+1} - x_p$) will give a ratio whose limit will be the value of $\frac{d^2\Psi}{dx^2}$ for $x = x_p$. Or also one can calculate this value from the known formula:

$$\left(\frac{d^2\Psi}{dx^2}\right)_{x_p} = \lim_{\Delta x_p \to 0} \frac{\Psi(x_{p+2}) - 2\Psi(x_{p+1}) + \Psi(x_p)}{\Delta x_p^2}. \tag{51}$$

Without limiting the generality, we can consider that the points of division of the interval $x_0 x'$ are equidistant and one can write:

$$x_{p+1} = x_p + \Delta x_p, \qquad\qquad x_{p+2} = x_p + 2\Delta x_p.$$

According to formula (19), one can write for the function Ψ in the interval $x_p x_{p+1}$:

$$\Psi(x) = A_p e^{-iy_p x} + B_p e^{iy_p x}. \tag{2}$$

Let us substitute in (2) $x = x_{p+1} = x_p + \Delta x_p$ and then to expand the exponential functions, conserving the infinitesimals up to second order. We find:

$$\Psi(x_p + \Delta x_p) = A_p e^{-iy_p x_p}(1 - iy_p \Delta x_p - \frac{1}{2} y_p^2 \Delta x_p^2) + B_p e^{iy_p x_p}(1 + iy_p \Delta x_p - \frac{1}{2} y_p^2 \Delta x_p^2). \tag{52}$$

One will have for the values of Ψ in the interval (x_{p+1}, x_{p+2}):

$$\Psi(x) = A_{p+1} e^{-iy_{p+1} x} + B_{p+1} e^{iy_{p+1} x}. \tag{53}$$

This formula will give for the value $\Psi(x_{p+2})$:

$$\Psi(x_{p+2}) = A_{p+1} e^{-iy_{p+1} x_{p+2}} + B_{p+1} e^{iy_{p+1} x_{p+2}}. \tag{53'}$$

The equations (24) and (25) express the A_{p+1}, B_{p+1} as functions of A_p, B_p. One will find, for example, for A_{p+1} in (24), by substituting in it:

$$x_{p+1} = x_p + \Delta x_p \qquad \text{and} \qquad y_{p+1} = y_p + \Delta y_p :$$

$$\begin{aligned} A_{p+1} &= \frac{2y_p + \Delta y_p}{2(y_p + \Delta y_p)} e^{i\Delta y_p (x_p + \Delta x_p)} A_p + \frac{\Delta y_p}{2(y_p + \Delta y_p)} e^{i(2y_p + \Delta y_p)(x_p + \Delta x_p)} B_p \\ &= \left(1 + \frac{\Delta y_p}{2y_p}\right)\left(1 + \frac{\Delta y_p}{y_p}\right)^{-1} e^{i\Delta y_p (x_p + \Delta x_p)} A_p + \frac{\Delta y_p}{2y_p}\left(1 + \frac{\Delta y_p}{y_p}\right)^{-1} e^{i(2y_p + \Delta y_p)(x_p + \Delta x_p)} B_p. \end{aligned}$$

Let us expand the expressions in the last formula, keeping the terms up to second order on Δx_p and Δy_p. One finds after simple but little long calculations:

$$A_{p+1} = A_p\left(1 + ix_p\Delta y_p - \frac{\Delta y_p}{2y_p} + i\Delta x_p\Delta y_p - \frac{x_p^2\Delta y_p^2}{2} - \frac{ix_p\Delta y_p^2}{2y_p} + \frac{\Delta y_p^2}{2y_p^2}\right)$$
$$+B_p e^{2iy_px_p}\left(\frac{\Delta y_p}{2y_p} + i\Delta x_p\Delta y_p + \frac{ix_p\Delta y_p^2}{2y_p} - \frac{\Delta y_p^2}{2y_p^2}\right)$$

Naturally, if one keeps in the last formula only the terms of first order on Δx_p and Δy_p, the coefficients of A_p and B_p will be reduced to terms from the first row of the matrix M_j (33).

Let us calculate now the first term of the right side of (53′) by substituting in it $y_{p+1} = y_p + \Delta y_p, x_{p+2} = x_p + 2\Delta x_p$ and A_{p+1} according to the last formula. By performing operations similar to the preceding ones, one finds:

$$A_{p+1}e^{-i(y_p+\Delta y_p)(x_p+2\Delta x_p)} = A_p e^{-ix_py_p}\left(1 - \frac{\Delta y_p}{2y_p} - 2iy_p\Delta x_p - 2y_p^2\Delta x_p^2 + \frac{\Delta y_p^2}{2y_p^2}\right)$$
$$+B_p e^{ix_py_p}\left(\frac{\Delta y_p}{2y_p} - \frac{\Delta y_p^2}{2y_p^2}\right).$$

Starting from formula (25) for B_{p+1} just like we did above, we calculate the second member of (52):

$$B_{p+1}e^{i(y_p+\Delta y_p)(x_p+\Delta x_p)} = A_p e^{-ix_py_p}\left(\frac{\Delta y_p}{2y_p} - \frac{\Delta y_p^2}{2y_p^2}\right)$$
$$+B_p e^{ix_py_p}\left(1 - \frac{\Delta y_p}{2y_p} + 2iy_p\Delta x_p + \frac{\Delta y_p^2}{2y_p^2} - 2y_p^2\Delta x_p^2\right).$$

Finally, the preceding formulas allow us to find for $\Psi(x_{p+2})$(53′):

$$\begin{cases}\Psi(x_{p+2}) = \Psi(x_p + 2\Delta x_p) = A_p e^{-ix_py_p}(1 - 2iy_p\Delta x_p - 2y_p^2\Delta x_p^2) \\ \qquad +B_p e^{ix_py_p}(1 + 2iy_p\Delta x_p - 2y_p^2\Delta x_p^2).\end{cases} \tag{53''}$$

Let us substitute in (51) the value of $\Psi(x_{p+2})$ from (53″), $\Psi(x_p + \Delta x_p)$ from (52) and $\Psi(x_p)$ from (2). We find easily:

$$\begin{cases}\left(\frac{d^2\Psi}{dx^2}\right)_{x_p} = \lim_{\Delta x_p\to 0}\frac{A_p e^{-ix_py_p}(-y_p^2\Delta x_p^2) + B_p e^{iy_px_p}(-y_p^2\Delta x_p^2)}{\Delta x_p^2} \\ = -y_p^2\left(A_p e^{-iy_px_p} + B_p e^{iy_px_p}\right) = -y_p^2\Psi(x_p).\end{cases} \tag{54}$$

As a consequence, the function $\Psi(x)$ satisfies the wave equation (18).

3.3 Theorem on the coefficients of transparency and their eigenvalues

The considerations done above were valid for values of x within a bounded interval x_0x'. The series we found are convergent, if the function $U(x)$ is finite. It is not necessary for the function $U'(x) = \frac{dU}{dx}$ to be continuous in the interval x_0x', as long as it is bounded. $U(x)$ may me then composed of finite number of arcs of different curves and the solution of the wave equation will always be expressed by (49).

Let us now take the limit $x_0 \to -\infty, x' \to +\infty$. The function $\Psi(x)$ (49) still satisfies the equation (18) but it will be generally infinite for $x = \pm\infty$. If the function $U(x)$ tends to zero for $x \to \pm\infty$, the wave function remains finite for $x = \pm\infty$. One can show this just like we did for the matrix M (29′), finding a dominant matrix. But if $U(x)$ behaves differently at infinity, the wave function Ψ (49) will not be bounded. Nevertheless, in the Wave Mechanics one look for functions, which are null at infinity, which can be realized for certain values of the energy E. Obviously, it is not easy to find in the general case the eigenvalues of the energy from equation (49). We show a method permitting us to find in principle the eigenvalues and with its help we find approximate eigenvalues.

If one recalls formula (12) and (16) (Ch. 1) which give the coefficients of transmission respectively for a rectangular barrier and for a barrier of the harmonic oscillator type, one sees that the coefficient T, which measures the transparency of the barrier for incident particles, is a function of the energy E. This function admits successive maximums for a series of values of E, which are exactly the eigenvalues of the wave equation. We will see that this property remains true for any shape of the barrier.

Let us take a barrier defined by a potential function $U(x)$, between two points

M_1 and M_2 with abscissa $x_1 = -l$ and $x_2 = l$. In this interval the wave equation will be:

$$\frac{d^2\Psi}{dx^2} + \frac{8\pi^2 m}{h^2}[E - U(x)]\Psi = 0. \tag{55}$$

Let us suppose that to the left of M_1 and to the right of M_2, the potential is zero and that the incident wave propagate in the direction OX. To the left of M_1, the total wave $\Psi_1(x)$ will be a sum of the incident wave and of the reflected wave with corresponding amplitudes A and B. On can write:

$$\Psi_1(x) = Ae^{-ikx} + Be^{ikx}, \qquad k = \frac{2\pi}{h}\sqrt{2mE} \tag{56}$$

The transmitted wave Ψ_3 to the right of M_2 will be of the form:

$$\Psi_3(x) = Fe^{ikx}. \tag{57}$$

In the region M_1M_2, the general solution of the wave equation can be represented as a linear combination of two independent solutions, the waves $\phi(x)$ and $\chi(x)$:

$$\Psi_2(x) = C\phi(x) + D\chi(x) \tag{58}$$

On the two ends of the barrier one has to write the two groups of equations, expressing the continuity of the functions and their derivatives:

$$\begin{cases} Ae^{ikl} + Be^{-ikl} = C\phi(-l) + D\chi(-l) \\ -ikAe^{ikl} + ikBe^{-ikl} = C\phi' e(-l) + D\chi'(-l) \end{cases} \tag{59}$$

$$\begin{cases} C\phi(l) + D\chi(l) = Fe^{-ikl} \\ C\phi'(l) + D\chi'(l) = -ikFe^{-ikl} \end{cases} \tag{60}$$

The problem consists of determining the amplitude of the reflected wave B and that of the transmitted wave F, in order to form the coefficient of reflection R and of transmission T.

To simplify the writing we introduce the following notations:

$$\begin{cases} \phi(-l)=\phi_-, & \phi'(-l)=\phi'_-, \quad \phi(l)=\phi_+, \quad \phi'(l)=\phi'_+ \\ \chi(-l)=\chi_-, & \chi'(-l)=\chi'_-, \quad \chi(l)=\chi_+, \quad \chi'(l)=\chi'_+ \end{cases} \tag{61}$$

Let us form the determinant $\Delta(-l)$ from the coefficients C and D of (59):

$$\Delta(-l)=\Delta_-=\begin{vmatrix} \phi_- & \chi_- \\ \phi'_- & \chi'_- \end{vmatrix}=\phi_-\chi'_- -\phi'_-\phi_- \tag{62}$$

and similarly $\Delta(l)=\Delta_+$ from (60).

From (68) one easily gets:

$$\begin{cases} C=\frac{1}{\Delta_-}[Ae^{ikl}(\chi'_- +ik\chi_-)+Be^{-ikl}(\chi'_- -ik\chi_-)] \\ D=\frac{1}{\Delta_-}[-Ae^{ikl}(\phi'_- +ik\phi_-)+Be^{-ikl}(ik\phi_- -\phi'_-)] \end{cases} \tag{63}$$

Equations (60) will give for the same quantities:

$$\begin{cases} C=\frac{Fe^{-ikl}}{\Delta_+}(\chi'_+ +ik\chi_+) \\ D=\frac{-Fe^{-ikl}}{\Delta_+}(\phi'_+ +ik\phi_+) \end{cases} \tag{64}$$

By making equal the values of C and D according to (63) and (64), one finds the equations:

$$\begin{cases} \Delta_+e^{-ikl}(\chi'_- -ik\chi_-)B-\Delta_-e^{-ikl}(\chi'_+ +ik\chi_+)F=-\Delta_+e^{ikl}(\chi'_- +ik\chi_-)A \\ \Delta_+e^{-ikl}(ik\phi_- -\phi'_-)B-\Delta_-e^{-ikl}(\phi'_+ +ik\phi_+)F=\Delta_+e^{ikl}(\phi'_- +ik\phi_-)A \end{cases} \tag{65}$$

The determinant d of the coefficients B and F of (65) is then:

$$\left\{ d=\Delta_+\Delta_-e^{-2ikl}[(\chi'_- -ik\chi_-)(\phi'_+ +ik\phi_+)+(ik\phi_- -\phi'_-)(\chi'_+ +ik\chi_+)] \right. \tag{66}$$

and one will have for the values of B and F, from (65):

$$\left\{ B=\frac{\Delta_+\Delta_-}{d}A[-(\chi'_- +ik\chi_-)(\phi'_+ +ik\phi_+)+(\phi'_- +ik\phi_-)(\chi'_+ +ik\chi_+)]. \right. \tag{67}$$

$$\left\{ F = \frac{(\Delta_+)^2}{d} A[(\chi'_- - ik\chi_-)(\phi'_- + ik\phi_-) + (ik\phi_- - \phi'_-)(\chi'_- + ik\chi_-)]. \right. \tag{68}$$

We will now want to evaluate the orders of magnitude of $\mid B \mid$ and $\mid F \mid$ depending of the values of the energy E of the incident particles. Let us consider the case where l is very big, this is to say, the base of the barrier if very long. Thus, to calculate B and F from (67) and (68), we will need only the asymptotic values of ϕ and χ.

Since the wave equation (55) coincides with its conjugated one, it can be shown easily [3], that the determinant Δ (62) is constant for every value of x, where the solutions ϕ and χ are independent. But it is easy to prove this property directly. In effect, let us replace in equation (55) successively the functions χ and ϕ. We multiply the first of this equations by ϕ, the second by χ and we subtract them. One will have:

$$0 = \phi\chi'' - \chi\phi'' = \frac{d}{dx}(\phi\chi' - \phi'\chi) = \frac{d}{dx}\Delta. \tag{69}$$

As a consequence, the determinant Δ is constant:

$$\Delta = \phi\chi' - \chi\phi' = \phi\chi\left(\frac{\chi'}{\chi} - \frac{\phi'}{\phi}\right) = c^{te}. \tag{70}$$

We can now consider that the notations (61) represent the asymptotic values of ϕ and χ for $x \to -\infty$ and $x \to +\infty$ respectively. The equality (70) shows that the asymptotic values ϕ_- and χ_- for example, cannot vanish simultaneously, since Δ_- will be null in the that case. ϕ_- and χ_- cannot be also infinitely big simultaneously, since according to (70) the expression in the parentheses should tend to zero and one gets $\lg\chi = \lg\phi$, thus the asymptotic values ϕ_- and χ_- will not be independent. On the other side, ϕ_- and χ_- can be finite simultaneously, which happens when the wave equation has a known spectrum. The preceding reasoning can be repeated without change for ϕ_+ and χ_+.

Taking into account (70) and (66), one can write for F (68):

$$| F |= \left| A \frac{(\chi'_- - ik\chi_-)(ik\phi_- + \phi'_-) + (\chi'_- + ik\chi_-)(ik\phi_- - \phi'_-)}{(\chi'_- - ik\chi_-)(ik\phi_+ + \phi'_+) + (\chi'_+ + ik\chi_+)(ik\phi_- - \phi'_-)} \right| = \left| A \frac{a_1 b_1 + a_2 b_2}{a_1 b'_1 + a'_2 b_2} \right|. \tag{71}$$

where one replaces, in order to shorten the writing, the expressions in the parentheses in the numerator with the letters a_1, b_1, a_2, b_2, respectively, and the same for the denominator.

Let us suppose that the wave equation has a discrete spectrum and let us consider the case, where the energy E is not equal to one of its eigenvalues. Taking into account the preceding reasoning, one can ask, without losing the generality:

$$\begin{cases} \phi_- \to \infty, \quad \phi'_- \to \infty, \quad \chi_- \to 0, \quad \chi'_- \to 0 \\ \phi_+ \to 0, \quad \phi'_+ \to 0, \quad \chi_+ \to \infty, \quad \chi'_+ \to \infty \end{cases} \tag{72}$$

Using (71), one sees that the expressions a_1 and a_2 are of the same order of magnitude, like b_1 and b_2 from the other side, and in the numerator we keep only the expression $a_1 b_1$ which is of the order of the expression $a_2 b_2$. It also follows from the formulas (72) that the term $a_1 b'_1$ in the denominator is infinitely small compared to the term $a'_2 b_2$ and we will keep only the latter. Finally, the approximate value of $| F |$ (71) will be:

$$\left\{ | F | \sim \left| A \frac{(\chi'_- - ik\chi_-)(ik\phi_- + \phi'_-)}{(\chi'_+ + ik\chi_+)(ik\phi_- - \phi'_-)} \right| \sim \left| A \frac{\chi'_- - ik\chi_-}{\chi'_+ + ik\chi_+} \right| = \left| A \frac{a_1 b_1}{a_1 b'_1} \right| \right. \tag{73}$$

From (72), this is an extremely small value, since the numerator is infinitely small and the denominator is infinitely big.

Let us now work in the case, where E is equal to one of the eigenvalues of equation (55). If E is not a double eigenvalue, one of the functions, for example

ϕ, will be an eigenfunction. One will now have, on the place of (72):

$$\begin{cases} \bar{\phi}_- \to 0, & \bar{\phi}'_- \to 0, & \bar{\chi}_- \to \infty, & \bar{\chi}'_- \to \infty \\ \bar{\phi}_+ \to 0, & \bar{\phi}'_+ \to 0, & \bar{\chi}_+ \to \infty, & \bar{\chi}'_+ \to \infty \end{cases} \tag{72'}$$

where the bar above the functions is to distinguish their values from those in (72). But since the values (72′), like (72) are asymptotic values of the solutions of equation (55), we must have that $\bar{\phi_-}$ is of the order of χ_-, $\bar{\phi_-} \sim \chi_-$, and similarly:

$$\bar{\phi_+} \sim \phi_+, \bar{\chi_-} \sim \phi_-, \bar{\chi_+} \sim \chi_+ \tag{72''}$$

Let us now recall formula (71). There also, the terms $a_1 b_1$ and $a_2 b_2$ are of the same order, and one will have, keeping only the first one:

$$\left\{ |\ \bar{F}\ | \sim \left| A \frac{(\bar{\chi}'_- - ik\bar{\chi}_-)(ik\bar{\phi}_- + \bar{\phi}'_-)}{(\bar{\chi}'_- - ik\bar{\chi}_-)(ik\bar{\phi}_+ + \bar{\phi}'_+) + (\bar{\chi}'_+ + ik\bar{\chi}_+)(ik\bar{\phi}_- - \bar{\phi}'_+)} \right| = \left| A \frac{\bar{a}_1 \bar{b_1}}{\bar{a}_1 \bar{b_1}' + \bar{a}'_2 \bar{b_2}} \right| \right. \tag{73'}$$

With the help of (72′) and (72″) one can write:

$$\left\{ |\ \bar{F}\ | \sim \left| A \frac{(\bar{\phi}'_- - ik\bar{\phi}_-)(ik\bar{\chi}_- + \bar{\chi}'_-)}{(\bar{\phi}'_+ - ik\bar{\phi}_+)(\bar{\phi}'_- + ik\bar{\phi}_-) + (\bar{\chi}'_+ + ik\bar{\chi}_+)(ik\bar{\chi}_- - \bar{\chi}'_-)} \right| . \right. \tag{74}$$

The numerator of (74) and of (73) are of the same order, while the denominator of (73) is infinitely big compared to the two terms of the denominator of (74), like formulas (72) show. Thus the value of F (73) is infinitely small compared to the value of $\bar{F}$ (74), which can be a finite number, of the order of unity. One can, as consequence, formulate the theorem: *The coefficient of transmission $T = \frac{|F|^2}{|A|^2}$, which characterizes the transparency of the barrier, has successive maximums for these values of the energy E, which are eigenvalues of equation* (55).This is a resonance phenomenon.

The same study on the coefficients B (67), gives that B is of the order of unity, since its numerator and its denominator are of the same order. But because of the sum $R + T = \frac{|B|^2 + |F|^2}{|A|^2} = 1$, the coefficient R will have minimums for these values of

E, which are equal to the eigenvalues of equation (55). However, these minimums are much less expressed than the maximums of T.

Let us now suppose that equation (55) has a known spectrum. Then for all the values of E in the interval, finite or infinite, (55) will have at least one solution, whose asymptotic values are finite. Since the determinant Δ (62) is constant, one can have only two possibilities: either the asymptotic values ϕ_-, χ_- and ϕ_+, χ_+ are finite simultaneously, or ϕ_-, ϕ_+ are zero and χ_-, χ_+ are infinite. In the two cases, by making the same consideration as above, one finds for F (68) and thus for T, finite values. If the coefficient T, which is a function of E and of l, allows maximums and minimums with respect to E, those maximums and minimums are of the same order of magnitude, for all the fixed values of l. On the other side, if (55) has a discrete spectrum, and if l has a fixed value which is very big, the maximums of T with respect to E have finite values, while their minimums are very small and they tend to zero when l tends to infinity.

The property stated above can then serve us to search for eigenvalues of the wave equation. – For this, one has to form the coefficient of transparency T for a barrier with very long base and to search for the roots E_k of the equation $\frac{\partial}{\partial E}T = 0$. If the value of T is finite for a value of E between two arbitrary roots, E_k and E_j, those roots belong to a discrete spectrum and *vice versa*.

Since in the applications one uses an approximate function, one will find approximate values for E_k.

By substituting the so found values of E_k in (49), one will find the eigenfunctions Ψ_k. If the base $(x_0 x')$ of our barrier increases infinitely, one has to expect that the Ψ_k will be finite at finite distances from the origin O and very small at infinity. The other functions Ψ (49) which are not eigenfunctions should, on the contrary, flatten on the axis OX and become null when $x_1 \to -\infty$ and $x' \to +\infty$. One will have a phenomenon analogous to the paradox of the harmonic oscillator [7].

The function (50), with whose help we often performed the approximate calculations, represents a first approximation of the wave function, and one has to take into account the degree of approximation which one is limited to by this form of the wave function. From (50) it can be seen that the exponents in the members of $\Psi(x)$ contain the integral of Maupertuis ($37''$). This indicates already that the function (50) should be valid in the approximation of geometrical optics. We have also seen that the two members of (50) coincide, up to a numerical factor, with the function (10) (p.3), given by the method of Brillouin-Wentzel. The appearance of this last function shows that the approximation of geometrical optics is realized, this-is-to-say that the condition $\frac{1}{n}\frac{dn}{dx} \ll 1$ exists.

Let us also compare directly the approximate formula (50) with the exact formula (49). To form the function (50) we retained only the terms m_{11}^0 and m_{22}^0 of the matrix M ($29'$). Recalling formulas (46) and (47), one sees that all the terms in (47) contain integrations with respect to y, or with respect to x, since $dy = y'dx$. If the barrier is rectangular, the potential is constant, $dy = 0$, thus all the integrals are null. The only terms of the matrix M ($29'$) which will be different of zero are m_{11}^0 and m_{22}^0 for which one will have: $m_{11}^0 = m_{22}^0 = 1$, as equations (39) and ($39'$) show. The matrix M will become the unity matrix, and consequently, the incident plane wave Ψ_0 will remain monochromatic after its entrance in the barrier. It is thus clear that if the potential $U(x)$ varies slowly, the terms m_{11}^0 and m_{22}^0 will dominate among all the $m_{\alpha\beta}$ $(\alpha, \beta = 1, 2)$ from equations (47). Let us take the term m_{12}^1 ($40'$) and let us substitute in the integral $dy = y'dx$. One sees easily that this term can be ignored compared to m_{11}^0 and m_{22}^0, if $\frac{y'}{y} \ll 1$, or also $\frac{1}{n}\frac{dn}{dx} \ll 1$ (since y is proportional to n), this is to say, if the index of refraction n varies slowly. Obviously it is more difficult to express using this method, than using the

Brillouin-Wentzel method, the exact condition which shows the case where the terms m^1_{12} and m^1_{21} are to be ignored compared to m^0_{11} and m^0_{22}, since m^0_{11}, m^0_{22} and m^1_{12}, m^1_{21} are not connected with a simple relation.

In the particular potential barrier problems, one uses often the form (10) (p.3) of the wave function given by the Brillouin-Wentzel method. We have seen (p.3) that this formula is not surely applicable in the neighborhood of the points $P(x)$, for which $E = U(x)$. Still this form of Ψ, applied to calculations of the coefficients of reflection and transmission, always gives the phenomenon in general, even though the barrier is cut at least at two points by the relation $U = E$. But after the considerations we did (p.25) on the terms m^0_{11} and m^0_{22} for this case, it follows that *the use of the function* (10) *or similarly of the function* (50) *is legitimate for all the usual calculations on potential barriers.*

3.4 Singular points of $\Psi(x)$. Turning points

We have seen that the points $P(x_1)$ and $Q(x_2)$ at which the relation $U = E$ cuts the barrier, represent singular points of the wave function Ψ (49). When we apply (49) to the calculation of the coefficients of reflection R and the coefficient of transmission T, this discontinuity does not bother us at all, as we have seen. But the function (49), such as it is, does not correspond to the definition of the wave function in the interval $(x_0 x')$, since it becomes infinite at the points P and Q. We have to now work out this difficulty.

The existence of discontinuity of the function $\Psi(x)$ at the points P and Q proves that in a neighborhood of the points P and Q, one cannot decompose the given barrier to elementary rectangular barriers. The wave equation shows, actually, that the wave function in a domain of the constant potential $U < E$, but very close to E $(U \sim E)$, is a periodic function varying slowly. For the limit case, $E = U$, it becomes a linear function of x and it is not anymore, strictly speaking a periodic function. The elementary rectangular barrier which contains the point P must then be replaced by another elementary barrier, formed by a curved arc, which will not be too different from the corresponding arc of the potential curve (the arc M_1N_1 on Fig. 2 2). We know [9] that the exact shape of the potential curve U around the edges of a barrier occurs much in the formulas of transparency of the barriers, if the energy E of the plane wave is close to the values of U on the edges of the barrier.

For this reason, we can replace the arc M_1N_1 (fig. 2) by a rectilinear segment M_1N_1 and make the calculations of the barrier with this elementary barrier on the place of the rectangular barrier. But if the potential U is a linear function of x, the solution of the wave equation is given by the Bessel functions $J_{\frac{1}{3}}$ and $J_{-\frac{1}{3}}$, and the calculations become more complicated. We will omit them for the moment and we will search for an approximate solution, valid in the neighborhood of P and Q, and then we will find the exact solution valid around P and Q.

Since at the points P and Q one has $E = U$, the wave equation (18) shows that $\frac{d^2\Psi}{dx^2} = 0$, this-is-to-say the function Ψ has two inflexion points $P(x_1)$ and $Q(x_2)$, and one can represent the function very approximately in the region $(x_1 - \varepsilon, x_1 + \varepsilon)$ (ε is a small positive finite number) with the linear function $\Psi(x) = ax + b$. The decomposition of the barrier to rectangular barriers is valid outside of the domain $(x_1 - \varepsilon, x_1 + \varepsilon)$. One has to write on the edges of the rectilinear barrier, with base $(x_1 - \varepsilon, x_1 + \varepsilon)$, the conditions of continuity and to eliminate the quantities a and b. This way, the amplitudes A_p, B_p which we find by decomposing the given barrier outside the interval $(x_1 - \varepsilon, x_1 + \varepsilon)$ and $(x_2 - \varepsilon, x_2 + \varepsilon)$, are related to each other by the intermediary function $ax + b$, where a and b are already known. The same operation should be performed at the point x_2.

The wave function $\Psi(x)$ constructed with the help of its transformation matrices and the matrix M is known at the points P and Q, but it is not represented by the same analytical expression in the whole domain x_0x' in which the barrier extends. It is linear in the regions $(x_1-\varepsilon, x_1+\varepsilon)$ and $(x_2-\varepsilon, x_2+\varepsilon)$ and it is given by (49) in the rest of the interval (x_0x').

3.5 A second method of solving the wave equation

Another difficulty arises at the points which are singular for the potential. We assume that those points are poles. Let the point O be a pole of order p of the function $U(x)$. Around the point O the decomposition of the barrier to elementary barriers is fictitious. One can see that if we make that decomposition near the point O, this point will be a singular point for the function $\Psi(x)$ (49), which we have learned to construct with the help of elementary barriers. We have to then change the method in neighborhood of O.

We will sketch another method to solve the equation (18). With this method, we will find the solution which remains finite in neighborhood of O.

The general integral of (18) contains two arbitrary constants. As a consequence, trough any two given points passes an integral curve, or also, trough each given point passes an integral curve, whose tangent at the point has some given angle with the axis OX. Let $P_0(x_0)$ be the given point. The function Ψ and its derivative Ψ' take arbitrary values Ψ_0 and Ψ'_0 at P_0. For an increment Δx_0 of x, one will find the values Ψ_1 and Ψ'_1 of Ψ and Ψ' given by the formulas:

$$\begin{cases} \Psi_1 = \Psi_0 + \Delta x_0 \Psi'_0 \\ \Psi'_1 = \Psi'_0 + \Delta x \Psi''_0 = \Psi'_0 - f_0 \Psi_0 \end{cases} \tag{75}$$

In the last formula we replaced Ψ''_0 by $-y_0\Psi_0$ and set $y_0^2 = f_0$. Ψ_1 and Ψ'_1 are linear functions of Ψ_0 and Ψ'_0 and one can replace (75) with the vector relation:

$$\begin{vmatrix} \Psi_1 \\ \Psi'_1 \end{vmatrix} = N_0 \begin{vmatrix} \Psi_0 \\ \Psi'_0 \end{vmatrix} = \begin{vmatrix} 1 & \Delta x_0 \\ -f_0\Delta x_0 & 1 \end{vmatrix} \begin{vmatrix} \Psi_0 \\ \Psi'_0 \end{vmatrix} \tag{76}$$

where N_0 is an almost diagonal matrix. With the same relations one finds the values:

$$\Psi_2 = \Psi(x_0 + 2\Delta x_0) \quad \text{and} \quad \Psi'_2 = \Psi'(x_0 + 2\Delta x_0)$$

as functions of Ψ_1 and Ψ'_1. Eliminating the quantities Ψ_1 and Ψ'_1 one will have a relation between Ψ_2, Ψ'_2 and Ψ_0, Ψ'_0. Like with the quantities A_j, B_j (p.13) after successive eliminations of Ψ_k, Ψ'_k, one will end with the following formula:

$$\begin{vmatrix} \Psi_p \\ \Psi'_p \end{vmatrix} = N \begin{vmatrix} \Psi_0 \\ \Psi'_0 \end{vmatrix} \tag{77}$$

where :

$$N = \prod_{i=1}^{p} N_i = \prod_{i=1}^{p} \begin{vmatrix} 1 & \Delta x_i \\ -f_i \Delta x_i & 1 \end{vmatrix} \tag{78}$$

is the transformation matrix. Since the matrix N_i resembles to the matrix B (**??**), the product N will be formed like the matrix product M ($29'$). The Δx_i from N_i correspond to the factors ρ_i in the elements of M_i (33). Therefore, the four elements $n_{\alpha\beta}(\alpha, \beta = 1, 2)$ of N will be the sums whose members contain the factors $\Delta x_i, \Delta x_i \Delta x_k, \ldots$. In the element n_{11} of the matrix N, product of p matrices N_i we indicate with $n_{11}^{2k,p}$ the term which is the sum of the terms containing $2k$ factors Δx. One finds (as in (41) and ($41'$)) the recurrence formulas:

$$\begin{cases} n_{11}^{2k,p} = n_{11}^{2k,p-1} + n_{21}^{2k-1,p-1} \Delta x_p \\ n_{12}^{2k+1,p} = n_{12}^{2k+1,p-1} + n_{22}^{2k,p-1} \Delta x_p \\ n_{21}^{2k+1,p} = -n_{11}^{2k,p-1} f_p \Delta x_p + n_{21}^{2k+1,p-1} \\ n_{22}^{2k,p} = -n_{12}^{2k-1,p-1} f_p \Delta x_p + n_{22}^{2k,p-1} \end{cases} \tag{79}$$

where $n_{12}^{2k+1,p}, n_{21}^{2k+1,p}, n_{22}^{2k,p}$ are defined the same way as the element $n_{11}^{2k,p}$. On the equations (79) one can perform the same operations which follow the equations (41) and one can represent the $n_{\alpha\beta}$ as explicit functions of x. Like for (42) one finds initially:

$$n_{11}^{2k}(x_p) = \int_{x_0}^{x_p} n_{21}^{2k-1}(x)dx \tag{80}$$

and by replacing $n_{21}^{2k-1}(x), \ldots$ one obtains the formula:

$$n_{11}^{2k}(x_p) = (-1)^k \int_{x_0}^{x_p} dx^{(2k-1)} \int_{x_0}^{x^{(2k-1)}} f(x^{(2k-2)})dx^{(2k-2)} \int_{x_0}^{x^{(2k-2)}} \ldots \int_{x_0}^{x^{(1)}} f(x)dx \tag{81}$$

where we have denoted with upper indexes the variables which replace formally the variable x. One will have also the three equations which correspond to (46):

$$\begin{cases} n_{12}^{2k+1}(x_p) = (-1)^k \int_{x_0}^{x_p} dx^{(2k)} \int_{x_0}^{x^{(2k)}} f dx^{(2k-1)} \int_{x_0}^{x^{(2k-1)}} \ldots \int_{x_0}^{x^{(1)}} dx \\ n_{21}^{2k+1}(x_p) = (-1)^k \int_{x_0}^{x_p} f dx^{(2k)} \int_{x_0}^{x^{(2k)}} dx^{(2k-1)} \int_{x_0}^{x^{(2k-1)}} \ldots \int_{x_0}^{x^{(1)}} f dx \\ n_{22}^{2k}(x_p) = (-1)^k \int_{x_0}^{x_p} f dx^{(2k-1)} \int_{x_0}^{x^{(2k-1)}} dx^{(2k-2)} \int_{x_0}^{x^{(2k-2)}} \ldots \int_{x_0}^{x^{(1)}} dx \end{cases} \tag{82}$$

and the four elements of N will be given like in (47) by:

$$n_{11} = \sum_{k=0}^{\infty} n_{11}^{2k},\, n_{12} = \sum_{k=0}^{\infty} n_{12}^{2k+1},\, n_{21} = \sum_{k=0}^{\infty} n_{21}^{2k+1},\, n_{22} = \sum_{k=0}^{\infty} n_{22}^{2k}. \tag{83}$$

Once the matrix N is known, (77) gives the values of Ψ and of Ψ' for all the values of x. From (77) one has:

$$\Psi(x) = n_{11}(x)\Psi_0 + n_{12}(x)\Psi_0'. \tag{84}$$

Since Ψ_0 and Ψ_0' are arbitrary constants, $\Psi(x)$ (84) *is the general integral of* (18).

In the whole interval of variation of x where $f(x)$ is bounded, the matrix product N (78) is finite. We can show this the same way we have done it for the matrix M (p.23): one can find a dominant matrix M_α whose power is finite. One then does not have to fear the turning points in the solution (84). Despite this, the solution (84) is not always very convenient like (49), since it does not immediately show the essential properties of the wave function. In effect, if the potential function is given, for example, by a polynomial of x, the formulas (81) and (82) show that the $n_{11}^{2k}, \ldots$(82) can be expressed easily as polynomials of x

so the $m_{\alpha\beta}$ (83) will be given by the infinite series following the powers of x , also absolutely convergent, since N is finite. We know, on the other side, that the approximate solution (50), which we found from the exact solution, gives the approximation of geometrical optics.

We supposed that the potential function has a pole of order p, which remains finite around O. We will require for the wave function and its derivatives up to at least p^{th} order, to be null at the point O:

$$\Psi_{(0)} = \Psi_{(0)}^{(1)} = \Psi_{(0)}^{(2)} = \ldots = \Psi_{(0)}^{(l)} = 0, \quad \Psi_{(0)}^{(l+1)} \neq 0, \quad l \geq p.$$

This would not, obviously, mean that the function Ψ (84) becomes identically null, because $\Psi_{(0)} = \Psi'_{(0)} = 0$, but to find the values $\Psi_1 = \Psi(\Delta x)$ and $\Psi'_1 = \Psi'(\Delta x)$ from (75), one has to start with this term in the Taylor development, which is not null for $x = 0$ and which is proportional to $\Psi^{(l+1)}$:

$$\Psi_1 = a_0(\Delta x)^{l+1}, \quad \Psi'_1 = b_0(\Delta x)^l \tag{85}$$

where a_0, b_0 are arbitrary constants. One has only to start to construct step by step the values of $\Psi(x)$ and of $\Psi(x)'$. The formula (84) remains valid when replacing in it Ψ_0 and Ψ'_0 with Ψ_1 and Ψ'_1 (85). This function is finite in the whole finite interval of variation of x, and null at the point O.

Let us now return to our potential barrier, which extends from x_0 to x', with $x_0 < 0 < x'$ and let the point O be a pole of order p for the potential. By two verticals, passing trough the points O_1 and O_2 of the abscissa $-\delta$ and δ (δ is a small positive number) we will limit a barrier which contains the pole. Between the points O_1 and O_2 the solution requires the wave equation (18) to be of the form (84) and outside of the interval O_1O_2 – of the form (49). At the points O_1 and O_2 one has to write the two conditions of continuity, in order to connect the solutions inside the interval O_1O_2 with those in its exterior. The final wave function will be then presented by different analytical expressions in the indicated parts of the interval x_0x' but it will be finite everywhere.

For the approximate calculations concerning the problem of barriers one will retain from the function (84) only the first terms in the development of $n_{\alpha\beta}$ (83).

Since the turning points P and Q are ordinary points for the function (84), we can use this to avoid the points P and Q as singular points of the function (49). But in neighborhood of the points P and Q the function (84) is essentially linear, since $f = 2m(E-U) \sim 0$, as we have seen from (75). It was exactly a linear function that we used (p.33) around the points P and Q without previously constructing the function (84).

In the problem of the solution of the wave equation for several particles, we will have to make considerations of this type for the singular points, and we will use the preceding results.

3.6 Application of the preceding method in the case of linear potential

We will apply the preceding method of solving the wave equation to the simple case, where the potential function is linear. We have seen (triangular barrier p.6), that one had to study the wave equation:

$$\frac{d^2\Psi}{d\xi^2} + \frac{8\pi^2 m}{h^2}(E - C - F\xi)\Psi = 0. \tag{86}$$

By setting:

$$x = \left(\frac{8\pi^2 m}{h^2}F\right)^{\frac{1}{3}}\left(-\frac{C-E}{F} + \xi\right) \tag{87}$$

the equation (86) becomes:

$$\frac{d^2\Psi}{dx^2} + x\Psi = 0. \tag{88}$$

The independent solutions of this equation are the functions $\sqrt{x}J_{\frac{1}{3}}\left(\frac{2}{3}x^{\frac{3}{2}}\right)$ and $\sqrt{x}J_{-\frac{1}{3}}\left(\frac{2}{3}x^{\frac{3}{2}}\right)$, where $J_{\frac{1}{3}}$ and $J_{-\frac{1}{3}}$ are the Bessel functions of order $\frac{1}{3}$ and $-\frac{1}{3}$.

The Bessel function of order γ, where γ is not a positive integer, is:

$$J_\lambda(x) = \left(\frac{x}{2}\right)^\lambda \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} \left(\frac{x}{2}\right)^{2n} \frac{1}{\Gamma(n+\lambda+1)}$$

This formula gives for $\lambda = \pm\frac{1}{3}$ the functions:

$$J_{\pm\frac{1}{3}}(x) = \left(\frac{x}{2}\right)^{\pm\frac{1}{3}} \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} \left(\frac{x}{2}\right)^{2n} \frac{1}{\Gamma(n\pm\frac{1}{3}+1)}. \tag{89}$$

As it is known, the function Γ satisfies the functional equation:

$$\Gamma(x+1) = x\Gamma(x)$$

By applying successively this formula for $x = n, n-1, \ldots$ one finds:

$$\begin{cases} \Gamma(n+\frac{1}{3}+1) = (\frac{1}{3}+n)(\frac{1}{3}+n-1)\ldots\frac{4}{3}.\frac{1}{3}.\Gamma(\frac{1}{3}) \\ \qquad = \frac{1}{3^n}[1+3n][1+3(n-1)]\ldots 7.4.1.\Gamma(\frac{1}{3}) \end{cases} \tag{90}$$

$$\begin{cases} \Gamma(n-\frac{1}{3}+1) = (-\frac{1}{3}+n)(-\frac{1}{3}+n-1)\ldots\frac{8}{3}.\frac{5}{3}.\frac{2}{3}(\frac{-1}{3}).\Gamma(-\frac{1}{3}) \\ \qquad = \frac{1}{3^n}[-1+3n][-1+3(n-1)]\ldots 5.2.(-1).\Gamma(-\frac{1}{3}) \end{cases} \tag{90'}$$

Let us now calculate $\sqrt{x}J_{\frac{1}{3}}\left(\frac{2}{3}x^{\frac{3}{2}}\right)$ using (89) and (90):

$$\begin{cases} \sqrt{x}J_{\frac{1}{3}}\left(\frac{2}{3}x^{\frac{3}{2}}\right) = \\ \sqrt{x}\left(\frac{1}{2}\right)^{\frac{1}{3}}\left(\frac{2}{3}\right)^{\frac{1}{3}}\left(x^{\frac{3}{2}}\right)^{\frac{1}{3}}\left[\frac{1}{\Gamma\left(\frac{1}{3}+1\right)} - \frac{1}{2^2}\left(\frac{2}{3}\right)^2\frac{\left(x^{\frac{3}{2}}\right)^2}{\Gamma\left(\frac{1}{3}+2\right)} + \ldots + \frac{(-1)^n}{n!}\frac{1}{2^{2n}}\left(\frac{2}{3}\right)^{2n}\frac{\left(x^{\frac{3}{2}.2n}\right)}{\Gamma\left(n+\frac{1}{3}+1\right)} + \ldots\right] \\ = \frac{\left(3^{\frac{2}{3}}\right)x}{\Gamma\left(\frac{1}{3}\right)}\left(1 - \frac{x^3}{3.4} + \frac{x^6}{2!3^2.7.4} - \frac{x^9}{3!3^3.10.7.4.1} + \ldots + \frac{(-1)^n x^{3n}}{n!3^n.[1+3n][1+3(n-1)]\ldots 7.4.1} + \ldots + \ldots\right) \end{cases} \tag{91}$$

One will also have:

$$\left\{\sqrt{x}J_{-\frac{1}{3}}\left(\frac{2}{3}x^{\frac{3}{2}}\right) = \frac{-3^{\frac{4}{3}}}{\Gamma\left(-\frac{1}{3}\right)}\left(1 - \frac{x^3}{3.2} + \frac{x^6}{2!3^2.5.2} - \ldots + \frac{(-1)^n x^{3n}}{n!3^n[-1+3n][-1+3(n-1)]\ldots 8.5.2} + \ldots\right)\right. \tag{92}$$

The general integral of (88) is a linear combination of (91) and (92).

Let us now search for a solution of equation (88) with the second method which we developed on (p.42). We have written the general integral $\Psi(x)$ of the wave equation in the form (84):

$$\Psi(x) = n_{11}(x)\Psi_0 + n_{12}(x)\Psi_0' = \sum_{k=0}^{\infty} n_{11}^{2k}(x)\Psi_0 + \sum_{k=0}^{\infty} n_{12}^{2k+1}(x)\Psi_0' \qquad (93)$$

where Ψ_0 and Ψ_0' are arbitrary constants and the terms $n_{11}^{2k}(x)$, $n_{12}^{2k+1}(x)$ are given by equations (81) and (82).

Using (81) and (82), one can express the $n_{11}^{2k}(x)$, $n_{12}^{2k+1}(x)$ as multiple integrals (with $f(x) = x$):

$$n_{11}^{2k}(x) = (-1)^k \int_0^x dx \int_0^x xdx \int_0^x \ldots \int_0^x dx \int_0^x xdx \qquad (94)$$

$$n_{12}^{2k+1}(x) = (-1)^k \int_0^x dx \int_0^x xdx \int_0^x \ldots \int_0^x xdx \int_0^x dx \qquad (94')$$

The $2k$ successive integrations in (94) (respectively the $2k+1$ ones in (94′)) can be easily performed and one arrives at the formulas:

$$n_{11}^{2k}(x) = \frac{(-1)^k x^{3k}}{3k(3k-1)..9.8.6.5.3.2} = \frac{(-1)^k x^{3k}}{3^k k! 2.5.8.(3k-1)} \qquad (95)$$

$$n_{12}^{2k+1}(x) = \frac{(-1)^k x^{3k+1}}{(3k+1)3k..7.6.4.3.1} = \frac{(-1)^k x^{3k+1}}{3^k k! 1.4.7..(3k+1)} \qquad (95')$$

and one sees that (95) and (95′) are respectively the $k^{-\text{th}}$ term in the series (91) and (92). Thus we found, using the last method, the known solution of equation (88).

If the potential function is given by a polynomial or if it can be expanded in Taylor series in a interval $(x_0 x')$, the integral of the wave equation can be represented by the power series of x. Obviously, we found that solution using the preceding method. But this method is applicable also in the case where the integral of the wave equation cannot be expanded in power series of x. If the potential function $U(x)$ is discontinuous at finite number of points or if it is composed of arcs of different curves, remaining always bounded, the integrals (81) and (82) keep their meaning and the preceding method is still applicable.

We can find also the solutions of the equation (88) with the method of barriers (p. 27-28), but the calculations are much more complicated. The method of barriers is more convenient for search of approximate solutions of the wave equation.

Note 1 – When one studies the problem of quantification of the hydrogen atom in polar coordinates [6], the wave equation can be solved by separation of variables. The equation depends only on the vector ray r in the following form:

$$\frac{d^2R}{dr^2} + \frac{2}{r}\frac{dR}{dr} + \left(A + \frac{2B}{r} + \frac{C}{r^2}\right)R = 0 \tag{96}$$

where R is a function of r and A, B, C are constants. When the energy $E < 0$, the solution of (96) can be presented in the form $R = e^{-\rho/2}v(\rho)$, where $\rho = \frac{2r}{r_0}$ and $v(\rho)$ is a polynomial of ρ. The eigenvalues of the energy form a discrete spectrum. For $E > 0$ one finds continuous spectrum.

We can search for solution of this equation by the method of decomposition of the potential barrier.

Let us divide to n parts $(r_0 r')$ – the interval of variation of r and let us set for the interval (r_k, r_{k+1}):

$$a_k = \frac{2}{r_k}, \quad b_k = A + \frac{2B}{r_k} + \frac{C}{r_k^2}, \qquad (k = 1, 2, \ldots, n).$$

One can make a corresponding elementary barrier to each elementary interval. In the domain (r_k, r_{k+1}) one can consider the coefficients of the equation (96) as constants a_k, b_k. In the same domain, the total integral of (96) will be:

$$R_k(r) = L_k e^{-\lambda_{k_1} r} + M_k e^{+\lambda_{k_2} r} \tag{97}$$

where L_k, M_k are constants whose values change from one elementary barrier to the next, and λ_{k_1} and λ_{k_2} are the roots of the characteristic equation $\sigma^2 + a_k\sigma + b_k =$

0. λ can be real or complex, the method of solving is equally applicable. The form of the solution (97) is the same as (19) and one will have the continuity conditions as in (21). Then one will make the eliminations of L_k, M_k with the help of matrices like (28) and one will arrive at the solution $R(r)$ similar to (49). The discussion of the convergence is the same like for equation (18).

We can also apply to this equation the method of solution given on page 45. We denote $R(r_0) = R_0$ and $\left(\frac{dR}{dr}\right)_{r_0} = R'_0$, R_0 and R'_0 are arbitrary constants. The values R_1 and R'_1 of R and $\frac{dR}{dr}$ at the point $r_0 + \Delta r_0$ will be calculated with the formulas:

$$\begin{cases} R_1 = R_0 + \Delta r_0 R'_0 \\ R'_1 = R'_0 + \Delta r_0 R''_0 = -\Delta r_0 \left(A + \frac{2B}{r_0} + \frac{C}{r_0^2}\right) R_0 + \left(1 - \frac{2}{r_0}\Delta r_0\right) R'_0. \end{cases} \tag{97'}$$

The right side of the last equation can be expressed in y by replacing R'' with its value from (96).

By analogous to (97′) formulas one finds the values R_2, R'_2 etc ... R_p, R'_p. As for equation (76), one will express R_p, R'_p as functions of R_0, R'_0 with the help of a matrix in the form of N (78). One will give to the solution $R(r)$ of (96) a form similar to (84). The discussions of this solution are similar to those of the solution (84). The turning points of the Classical Mechanics are ordinary points for this solution. One can also choose the initial values R_0 and R'_0 in a way that $R(r)$ will be finite at the point $r = 0$.

Note 2 – After the preceding considerations, it is clear that the two methods of solving the wave equation developed until now, can be generalized without difficulty for solving linear differential equations of order n whose coefficients are known functions of x. One has to use almost diagonal matrices with n rows and n columns on the place of the matrices with 2 rows and 2 columns. All the considerations we have done in the case $n = 2$ apply to the case of any n.

CHAPTER 4

4.1 Generalization of the method of barriers for the solution of the wave equation in the general case [4]

We have found the solution of the wave equation in the case of a single particle moving on a straight line in any field. The essential idea of the method was the decomposition of the given barrier to successive elementary barriers. The same method of barriers will permit us to search for solution of the wave equation in the general case.

We will start with the study of the wave equation for two particles (x) and (y), of masses m_1 and m_2, which move along the straight line OX, between the two point of the abscissa x_0 and x'. Let x and y be the corresponding coordinates. The potential energy, $F(x,y)$, of the system is composed of the mutual energy of the particles, of the form $F_{12}(x-y)$, function of their relative distance and of the energy originating from the exterior field, of the form $F_1(x)+F_2(y)$. Therefore:

$$F(x,y) = F_1(x) + F_2(y) + F_{12}(x-y) \tag{98}$$

and the wave equation will be:

$$\frac{1}{m_1}\frac{\partial^2\Psi}{\partial x^2} + \frac{1}{m_2}\frac{\partial^2\Psi}{\partial y^2} + \frac{8\pi^2}{h^2}[E - F(x,y)]\Psi = 0. \tag{99}$$

When the term $F_{12}(x-y) = 0$, i.e. when the particles are without interaction, the function $\Psi(x,y)$ decomposes to a product of the function $\Psi_1(x)$ and $\Psi_2(y)$, $\Psi(x,y) = \Psi_1(x)\Psi_2(y)$. The same decomposition happens also when the exterior field is constant or null.

The equation (99) is an equation of partial derivatives of the elliptic type. Let us take in the configuration space of the variables x and y a closed contour C, which limits a region P. The integral $\Psi(x,y)$ of (99) is determined in the domain P in a unique way, if we know the values of Ψ on the contour C (a Dirichlet problem).

The integral Ψ of (99) is determined in another way in the problem of collision of two particles [1]. If the potential F tends to zero when the particles are very far from each other and from the origin O (for example x and y are very large and negative), Ψ should reduce to a linear combination of the two monochromatic plane waves, whose amplitudes tend to zero. It is this last condition which we will impose on the function Ψ, when the considered problem is that of collision.

Let us divide the interval x_0x' to n parts with the points of division of the abscissa $x_1, x_2, \ldots, x_{n-1}, x_n = x'$. We suppose that at given moment (x) and (y) are in the intervals (x_k, x_{k+1}) and (y_l, y_{l+1}) respectively. We also suppose that the value of the potential is constant, equal to $F(x_k, y_l)$ all the times when (x) is in the interval (x_k, x_{k+1}) and (y) – in the interval (y_l, y_{l+1}). Then we will reason as if the particles are without interaction and in a constant exterior field for very small displacements. But in such case the wave function $\Psi(x,y)$ decomposes to a product of a function $\Psi_1(x)$ of x and another $\Psi_2(y)$ of y. We replace in (99) $\Psi(x,y) = \Psi_1(x)\Psi_2(y)$ and we divide the equation to $\Psi_1(x)\Psi_2(y)$. Since the potential energy is supposed to be constant equal to $F(x_k, y_l) = F_1(x_k) + F_2(y_l) + F_{12}(x_k - y_l)$, the first member of the equation separates into two expressions: the first, a function of x and the second, a function of y. It follows that each of them will be equal to a constant $\lambda_{k,l}$. To simplify the calculations, we assume in the following that $\lambda_{k,l}$ has a constant value λ for all the choices of the indexes k, l. We will see that the so found solution is an integral of (99) but it is not the general integral of (99).

Then the equation (99) decomposes to two ordinary equations:

$$\begin{cases} \frac{d^2\Psi_1}{dx^2} + \frac{8\pi^2 m_1}{h^2}[E - F_1(x_k) - F_{12}(x_k - y_l) - \lambda]\Psi_1 = 0 \\ \frac{d^2\Psi_2}{dy^2} + \frac{8\pi^2 m_2}{h^2}[\lambda - F_2(y)]\Psi_2 = 0 \end{cases} \tag{100}$$

We attached the mixed term $F_{12}(x_k - y_l)$ to the first equation of (100). From (100) we will find an integral of (99), which fulfills the initial conditions, required by the problem of collision of two particles. If we attached the term $F_{12}(x_k - y_l)$ to the second equation of (100), we would have found, making the same calculations which follow, an integral of (99) which fulfills the same initial conditions in the problem of collision.

The general integral of each of the ordinary equations (100) is a linear combination of two monochromatic plane waves with amplitudes $A_{k,l}, B_{k,l}$ for the first and $C_{k,l}, D_{k,l}$ for the second. Let us introduce the notations:

$$\begin{cases} \alpha_{k,l}^2 = \frac{8\pi^2 m_1}{h^2}[E - F_1(x_k) - F_{12}(x_k - y_l) - \lambda], \\ \beta_{k,l}^2 = \frac{8\pi^2 m_2}{h^2}[\lambda - F_2(y_l)]\Psi_2 = 0 \end{cases} \tag{101}$$

Although β does not depend on x, we wrote $\beta_{k,l}$ instead of β_l because if one consider λ as a function of x and y, β will depend on x.

With $\Psi_{k,l}$ we indicate the wave function which satisfies the equation (99) for the displacements of (x) and (y) in the interval (x_k, x_{k+1}) and (y_l, y_{l+1}). We can then write:

$$\begin{cases} \Psi_{k,l}(x,y) = (A_{k,l}e^{-i\alpha_{k,l}x} + B_{k,l}e^{i\alpha_{k,l}x})(C_{k,l}e^{-i\beta_{k,l}y} + D_{k,l}e^{i\beta_{k,l}y}) \\ (k,l = 1,2,\ldots,n) \end{cases} \tag{102}$$

For the different values of the indexes k and l we will have different solutions, each valid when x and y vary in the respective defined interval. Since there are two independent indexes, there will be n^2 solutions of the form (102). The amplitudes $A_{k,l}, B_{k,l}, C_{k,l}, D_{k,l}$ are functions of x and y, which we consider as constants in the intervals mentioned above.

Let us consider the solutions $\Psi_{k+1,l}(x,y)$. The configuration of the system of two particles is the same as the configuration corresponding to the solution $\Psi_{k,l}$, except for the position of (x), which is in the interval x_{k+1}, x_{k+2} while (y) has not changed its interval. The particle (x) moves from the interval x_k, x_{k+1} where the potential has constant value, at the interval x_{k+1}, x_{k+2} where it has different constant value. The calculations go on as if we had a passage of particles trough potential barrier. When the particle (x) moves, it has to cross a sequence of barriers each with constant height. This height depends, naturally, of the position of (x) and (y). Exactly for the same reason, we can think that (y) crosses a sequence of elementary rectangular barriers with constant height, function of the position of (x) and (y). It is clear that the reasoning made for a sequence of rectangular barriers (p.4) can be applied here too. When the particle (x) switches the barrier, on the edge of two neighboring barriers, the wave function $\Psi_{k,l}(x,y)$ and its partial derivative with respect to x should be continuous, considering y as a constant.

Therefore, one can write the two following conditions:

$$\begin{cases} \Psi_{k,l}(x_{k+1}, y_l) = \Psi_{k+1,l}(x_{k+1}, y_l) \\ \left(\frac{\partial \Psi_{k,l}}{\partial x}\right)_{x_{k+1}, y_l} = \left(\frac{\partial \Psi_{k+1,l}}{\partial x}\right)_{x_{k+1}, y_l} \end{cases} \tag{103}$$

For the same reasons, $\Psi_{k,l}$ and $\frac{\partial \Psi_{k,l}}{\partial y}$ should be continuous with respect to y. One will have two conditions like (103) expressing the continuity with respect to y.

We will give the following explicit form of the conditions (103), taking into account (102):

$$\begin{cases} (A_{k,l}e^{-i\alpha_{k,l}x_{k+1}} + B_{k,l}e^{i\alpha_{k,l}x_{k+1}})(C_{k,l}e^{-i\beta_{k,l}y_l} + D_{k,l}e^{i\beta_{k,l}y_l}) \\ \qquad = (A_{k+1,l}e^{-i\alpha_{k+1,l}x_{k+1}} + B_{k+1,l}e^{i\alpha_{k+1,l}x_{k+1}})(C_{k+1,l}e^{-i\beta_{k+1,l}y_l} + D_{k+1,l}e^{i\beta_{k+1,l}y_l}) \\ i\alpha_{k,l}(-A_{k,l}e^{-i\alpha_{k,l}x_{k+1}} + B_{k,l}e^{i\alpha_{k,l}x_{k+1}})(C_{k,l}e^{-i\beta_{k,l}y_l} + D_{k,l}e^{i\beta_{k,l}y_l}) \\ \qquad = i\alpha_{k+1,l}(-A_{k+1,l}e^{-i\alpha_{k+1,l}x_{k+1}} + B_{k+1,l}e^{i\alpha_{k+1,l}x_{k+1}})(C_{k+1,l}e^{-i\beta_{k+1,l}y_l} + D_{k+1,l}e^{i\beta_{k+1,l}y_l}) \end{cases} \tag{104}$$

The two conditions (104) are linear with respect to the amplitudes $A_{k,l}, B_{k,l}, A_{k+1,l}, B_{k+1,l}$. They allow us to express $A_{k+1,l}$ and $B_{k+1,l}$ as functions of $A_{k,l}$ and $B_{k,l}$. We divide the two equalities (104) by the last factor of their right sides and we introduce the notation:

$$c_{k,k+m,l} = \frac{C_{k,l}e^{-i\beta_{k,l}y_l} + D_{k,l}e^{i\beta_{k,l}y_l}}{C_{k+m,l}e^{-i\beta_{k+m,l}y_l} + D_{k+m,l}e^{i\beta_{k+m,l}y_l}} \tag{105}$$

The equations (104) will take the form:

$$\begin{cases} c_{k,k+1,l}(A_{k,l}e^{-i\alpha_{k,l}x_{k+1}} + D_{k,l}e^{i\alpha_{k,l}x_{k+1}}) = A_{k+1,l}e^{-i\alpha_{k+1,l}x_{k+1}} + B_{k+1,l}e^{i\alpha_{k+1,l}x_{k+1}} \\ c_{k,k+1,l}\alpha_{k,l}(A_{k,l}e^{-i\alpha_{k,l}x_{k+1}} - D_{k,l}e^{i\alpha_{k,l}x_{k+1}}) = \alpha_{k+1,l}(A_{k+1,l}e^{-i\alpha_{k+1,l}x_{k+1}} - B_{k+1,l}e^{i\alpha_{k+1,l}x_{k+1}}) \end{cases} \tag{106}$$

In this form, the difference between the equations (106) and (21) is only in the factors $c_{k,k+1,l}$. Consequently the relations between $A_{k+1,l}, B_{k+1,l}$ and $A_{k,l}, B_{k,l}$ like (26) will have the form:

$$\begin{vmatrix} A_{k+1,l} \\ B_{k+1,l} \end{vmatrix} = c_{k,k+1,l} M_{k,l} \begin{vmatrix} A_{k,l} \\ B_{k,l} \end{vmatrix} \tag{107}$$

where $M_{k,l}$ is a matrix with two rows and two columns, corresponding to the matrix M_j (33), thus, we can easily write:

$$M_{k,l} = \begin{vmatrix} e^{i\Delta\alpha_{\Delta k,l}x_k - \frac{\Delta\alpha_{\Delta k,l}}{2\alpha_{k,l}}} & \frac{\Delta\alpha_{\Delta k,l}}{2\alpha_{k,l}} e^{2i\alpha_{k,l}x_k} \\ \frac{\Delta\alpha_{\Delta k,l}}{2\alpha_{k,l}} e^{-2i\alpha_{k,l}x_k} & e^{-i\Delta\alpha_{\Delta k,l}x_k - \frac{\Delta\alpha_{\Delta k,l}}{2\alpha_{k,l}}} \end{vmatrix}$$

$$\Delta\alpha_{\Delta k,l} = \alpha_{k+1,l} - \alpha_{k,l} = \left(\frac{\partial\alpha_{k,l}}{\partial x}\right)_{x_k} \Delta x_k \tag{108}$$

The index Δk indicates that the variation of α is caused only by the variation of x, while y remains a constant. The vector relation (107) is true for $k = 1, 2, \ldots, n$. By applying it for the successive values of k, one will find, like in the problem in one dimension:

$$\begin{vmatrix} A_{k+\rho,l} \\ B_{k+\rho,l} \end{vmatrix} = c_{k+\rho-1,k+\rho,l}c_{k+\rho-2,k+\rho-1,l}\ldots c_{k,k+1,l}M_{k+\rho,l}M_{k+\rho-1,l}\ldots M_{k,l} \begin{vmatrix} A_{k,l} \\ B_{k,l} \end{vmatrix} \tag{109}$$

The product of the factors c in the right part of the last equality is calculated taking into account (105). This factor product simplifies easily and one finds:

$$c_{k+\rho-1,k+\rho,l}c_{k+\rho-2,k+\rho-1,l}\cdots c_{k,k+1,l} = c_{k,k+\rho,l}. \tag{110}$$

From another side, like we have already done it, the product of the matrices $M_{k+j,l}$ in (109) gives a matrix which is calculated, obviously, like M_k (29′). In this matrix product, which we denote by $M_{k+\rho,k,l}$, the sums in its elements will be extended from x_k to x_{k+1}, y remaining a constant. One will finally have:

$$\begin{vmatrix} A_{k+\rho,l} \\ B_{k+\rho,l} \end{vmatrix} = c_{k,k+\rho,l} M_{k+\rho,k,l} \begin{vmatrix} A_{k,l} \\ B_{k,l} \end{vmatrix} \tag{111}$$

We can give the conditions of continuity with respect to y in an explicit form like (104). These conditions will give the two linear relations between $C_{k,l+1}, D_{k,l+1}$ and $C_{k,l}, D_{k,l}$ which one can write in the following vector form (like (107)):

$$\begin{vmatrix} C_{k,l+1} \\ D_{k,l+1} \end{vmatrix} = \alpha_{k,l+1,l} N_{k,l} \begin{vmatrix} C_{k,l} \\ D_{k,l} \end{vmatrix} \tag{112}$$

where the factor $\alpha_{k,l+1,l}$ is composed in an analogous to (105) way:

$$\alpha_{k,l+\sigma,l} = \frac{A_{k,l} e^{-i\alpha_{k,l} x_k} + B_{k,l} e^{i\alpha_{k,l} x_k}}{A_{k,l+\sigma} e^{-i\alpha_{k,l+\sigma} x_k} + B_{k,l+\sigma} e^{i\alpha_{k,l+\sigma} x_k}} \tag{113}$$

and $N_{k,l}$ is a matrix with two rows and two columns, like $M_{k,l}$:

$$\begin{gathered} N_{k,l} = \begin{vmatrix} e^{i\Delta\beta_{k,\Delta l} y_l - \frac{\Delta\beta_{k,\Delta l}}{2\beta_{k,l}}} & \frac{\Delta\beta_{k,\Delta l}}{2\beta_{k,l}} e^{2i\beta_{k,l} y_l} \\ \frac{\Delta\beta_{k,\Delta l}}{2\beta_{k,l}} e^{2i\beta_{k,l} y_l} & e^{-i\Delta\beta_{k,\Delta l} y_l - \frac{\Delta\beta_{k,\Delta l}}{2\beta_{k,l}}} \end{vmatrix} \\ \Delta\beta_{k,\Delta l} = \beta_{k,l+1} - \beta_{k,l} = \left(\frac{\partial \beta_{k,l}}{\partial y} \right)_{y_l} \Delta y_l . \end{gathered} \tag{114}$$

The elimination of the successive amplitudes C, D from $C_{k,l}, D_{k,l}$ to $C_{k,l+\sigma}, D_{k,l+\sigma}$ gives the relation:

$$\begin{vmatrix} C_{k,l+\sigma} \\ D_{k,l+\sigma} \end{vmatrix} = \alpha_{k,l+\sigma,l} N_{k,l+\sigma,l} \begin{vmatrix} C_{k,l} \\ D_{k,l} \end{vmatrix} \tag{115}$$

where $N_{k,l+\sigma,l}$ is the matrix product of $N_{k,l}$ and $\alpha_{k,l+\sigma,l}$ is the factor which remains from the product of α in (112).

When $n \to \infty$, the sums in the terms of $M_{k+\rho,k,l}$ and of $N_{k,l+\sigma,l}$ transform to definite integral: in the terms of $M_{k+\rho,k,l}$ the integrations are done with respect to

x, in those of $N_{k,l+\sigma,l}$ – with respect to y. The question of convergence of the sums is the same as in the case of one dimension, for the matrix M (29′). If the function $F(x,y)$ is continuous with respect to x and y and bounded in the interval x_0x', one can find a matrix M_α which is dominant to $M_{k,l}$ and whose arbitrary power is finite and a matrix N_β, dominant to $N_{k,l}$ with similar properties. Then the matrices $M_{k+\rho,k,l}$ and $N_{k,l+\sigma,l}$ are finite in the interval x_0x'.

Let us consider the integrals in the terms of the matrices $M_{k+\rho,k,l}$ and $N_{k,l+\sigma,l}$ as functions of their upper bounds. The elements $m_{\alpha\beta}$ and $n_{\alpha\beta}$ $(\alpha,\beta=1,2)$ of M and of N will be known functions of x and y, since they are calculated exactly like the elements $m_{\alpha\beta}$ (47) of the matrix M (29′). Then, the wave function $\Psi(x,y)$, when x varies in the interval $(x_{k+\rho},x_{k+\rho+1})$ and y – in the interval $(y_{l+\sigma},y_{l+\sigma+1})$, will be :

$$\begin{cases}\Psi_{k+\rho,l+\sigma}(x,y)=(A_{k+\rho,l+\sigma}e^{-i\alpha_{k+\rho,l+\sigma}x}+B_{k+\rho,l+\sigma}e^{i\alpha_{k+\rho,l+\sigma}x})\\ \qquad\qquad\times(C_{k+\rho,l+\sigma}e^{-i\beta_{k+\rho,l+\sigma}y}+D_{k+\rho,l+\sigma}e^{i\beta_{k+\rho,l+\sigma}y}).\end{cases}\tag{116}$$

In the formula (102) and the following, we indicated with the indexes k and l the arbitrary initial positions of the particles (x) and (y). In order to simplify the writing and without constraining the generality, we can fix the initial positions of (x) and (y) with the indexes $0,0$. All the formulas from (100) to (116) will be preserved, by substituting everywhere $k=l=0$. In the following we will use those formulas, modified in such way. Particularly, equation (116) will become:

$$\Psi_{\rho,\sigma}(x,y)=(A_{\rho,\sigma}e^{-i\alpha_{\rho,\sigma}}x+B_{\rho,\sigma}e^{i\alpha_{\rho,\sigma}x})(C_{\rho,\sigma}e^{-i\beta_{\rho,\sigma}y}+D_{\rho,\sigma}e^{i\beta_{\rho,\sigma}y})\tag{116′}$$

We can now express the amplitudes $A_{\rho,\sigma},B_{\rho,\sigma}$ from (116′) as functions of $A_{0,\sigma},B_{0,\sigma}$

with the help of (111):

$$\begin{cases}\Psi_{\rho,\sigma}(x,y) = [(m_{11}A_{0,\sigma} + m_{12}B_{0,\sigma})e^{-i\alpha_{\rho,\sigma}x} + (m_{21}A_{0,\sigma} + m_{22}B_{0,\sigma})e^{i\alpha_{\rho,\sigma}x}] \\ \times \frac{C_{0,\sigma}e^{-i\beta_{0,\sigma}y_\sigma} + D_{0,\sigma}e^{i\beta_{0,\sigma}y_\sigma}}{C_{\rho,\sigma}e^{-i\beta_{\rho,\sigma}y_\sigma} + D_{\rho,\sigma}e^{i\beta_{\rho,\sigma}y_\sigma}}(C_{\rho,\sigma}e^{-i\beta_{\rho,\sigma}y} + D_{\rho,\sigma}e^{i\beta_{\rho,\sigma}y}).\end{cases} \tag{117}$$

The last factor in the second term of (117) simplifies with the denominator of the fraction, since y becomes equal to y_σ when the intervals tend to zero. The elements $m_{11},\ldots,m_{22}$ of the matrix $M_{\rho,0,0}$ are functions of x_ρ, because y remains of the constant value y_σ.

Let us now make the elimination of the amplitudes C and D in (117) with the help of (115). One finds:

$$\begin{cases}\Psi_{\rho,\sigma}(x,y) = [(m_{11}A_{0,\sigma} + m_{12}B_{0,\sigma})e^{-i\alpha_{\rho,\sigma}x} + (m_{21}A_{0,\sigma} + m_{22}B_{0,\sigma})e^{i\alpha_{\rho,\sigma}x}] \\ \quad \times[(n_{11}C_{0,0} + n_{12}D_{0,0})e^{-i\beta_{0,\sigma}y_\sigma} + (n_{21}C_{0,0} + n_{22}D_{0,0})e^{i\beta_{0,\sigma}y_\sigma}]\frac{A_{0,0}e^{-i\alpha_{0,0}x_0} + B_{0,0}e^{i\alpha_{0,0}x_0}}{A_{0,\sigma}e^{-i\alpha_{0,\sigma}x_0} + B_{0,\sigma}e^{i\alpha_{0,\sigma}x_0}}\end{cases} \tag{118}$$

where $n_{11},\ldots,n_{22}$ are known functions of y (x in $n_{11},\ldots,n_{22}$ remains the constant x_0).

If we eliminate the $C_{\rho,\sigma}, D_{\rho,\sigma}$ of (116) with the help of (115) and (113) and the $A_{\rho,0}, B_{\rho,0}$ with the help of (111) and (105), one will find those two forms of (116′):

$$\begin{cases}\Psi_{\rho,\sigma}(x,y) = [(m_{11}A_{0,0} + m_{12}B_{0,0})e^{-i\alpha_{\rho,0}x_0} + (m_{21}A_{0,0} + m_{22}B_{0,0})e^{i\alpha_{\rho,0}x_0}] \\ \quad \times[(n_{11}C_{\rho,0} + n_{12}D_{\rho,0})e^{-i\beta_{\rho,\sigma}y} + (n_{21}C_{\rho,0} + n_{22}D_{\rho,0})e^{i\beta_{\rho,\sigma}y}]\frac{C_{0,0}e^{-i\beta_{0,0}y_0} + D_{0,0}e^{i\beta_{0,0}y_0}}{C_{\rho,0}e^{-i\beta_{\rho,0}y_0} + D_{\rho,0}e^{i\beta_{\rho,0}y_0}}\end{cases} \tag{119}$$

In the terms $m_{11},\ldots,m_{22}$, the integrals are performed with respect to x ($y = y_0$) and in the $n_{11},\ldots,n_{22}$, with respect to y ($x = x_\rho$).

We have to make a note on the singular points of the potential function $F(x,y)$, and on the points where the quantity α and β (101) cancel each other. Those last points correspond to the turning points in the Classical Mechanics for the problem of one particle. In the region P, which surrounds those points, the function $\Psi(x,y)$ is essentially linear with respect to x and y and one can make analogous considerations to those on page 42. On the edge of P one has to agree the values of the linear function with those of the wave function on the exterior of P.

The singular points of the potential function $F(x,y)$ are also singular points for the functions $\Psi(x,y)$ (117) and (118). One can use here also a method with the help of which one can construct a solution $\Psi(x,y)$ which is null at the singular points of $F(x,y)$ as we did that already in the problem of one particle (p. 40): one can take as arbitrary parameters the values of the wave function Ψ and $\frac{\partial\Psi}{\partial x}$, $\frac{\partial\Psi}{\partial y}$ at any point and little by little one can find the values of those quantities in other points. We will not go into detail on this question, since the calculations are quite long.

4.2 Verification that the function $\Psi_{k,l}(x,y)$ satisfies the wave equation

In order to construct the function $\Psi_{k,l}$ we decomposed the interval x_0x' (the domain of the variables x and y) to small elementary domains (x_k, x_{k+1}) and (y_l, y_{l+1}) $(k,l = 1,2,\ldots n)$. $\Psi_{k,l}$ is the solution of the equation in the domain above. One can consider that the function $\Psi_{k,l}$ represents a portion of certain surface $\Psi(x,y)$. $\Psi(x,y)$ is composed of small surfaces $\Psi_{k,l}$ glued on their edges so that they form a continuous surface. This is true for any choice of the intervals, also in the limit, when the intervals tend to zero. Without verifying it, we are sure that $\Psi(x,y)$ is solution of the wave equation, since it is constructed in a way so that it satisfies it. However, we will verify that in our calculations. Here, also the direct differentiation of the final formula (118) is difficult, and we will make the verification like for the linear problem, namely: we will calculate the values of Ψ for three neighboring values of x $(x_k, x_{k+1} = x_k + \Delta x_k, x_{k+2} = x_k + 2\Delta x_k)$, while y is fixed and equal to y_l. With those values we will form the derivative $\left(\frac{\partial^2\Psi}{\partial x^2}\right)_{x_k,y_l}$, following formula (51). In the same way, we will find $\left(\frac{\partial^2\Psi}{\partial y^2}\right)_{x_k,y_l}$ and the verification will be immediate.

Equation (116) gives:

$$\begin{cases} \Psi_{k,l}(x_k,y_l) = (A_{k,l}e^{-i\alpha_{k,l}x_k} + B_{k,l}e^{i\alpha_{k,l}x_k})(C_{k,l}e^{-i\beta_{k,l}y_l} + D_{k,l}e^{i\beta_{k,l}y_l}) \\ \Psi_{k,l}(x_{k+1},y_l) = (A_{k,l}e^{-i\alpha_{k,l}(x_k+\Delta x_k)} + B_{k,l}e^{i\alpha_{k,l}(x_k+\Delta x_k)})(C_{k,l}e^{-i\beta_{k,l}y_l} + D_{k,l}e^{i\beta_{k,l}y_l}) \end{cases} \tag{120}$$

Following (52) and by keeping the infinitesimals of second order one has:

$$\begin{cases} \Psi_{k,l}(x_{k+1},y_l) = [A_{k,l}e^{-i\alpha_{k,l}x_k}(1 - i\alpha_{k,l}\Delta x_k - \frac{1}{2}\alpha_{k,l}^2\Delta x_k^2) + B_{k,l}e^{i\alpha_{k,l}x_k} \\ \qquad\qquad \times(1 + i\alpha_{k,l}\Delta x_k - \frac{1}{2}\alpha_{k,l}^2\Delta x_k^2)][C_{k,l}e^{-i\beta_{k,l}y_l} + D_{k,l}e^{i\beta_{k,l}y_l})]. \end{cases} \tag{121}$$

From (116) we obtain:

$$\begin{aligned} \Psi_{k,l}(x_{k+2},y_l) &= \Psi_{k+1,l}(x_{k+2},y_l) \\ &= (A_{k+1,l}e^{-i\alpha_{k+1,l}x_{k+2}} + B_{k+1,l}e^{i\alpha_{k+1,l}x_{k+2}})(C_{k+1,l}e^{-i\beta_{k+1,l}y_l} + D_{k+1,l}e^{i\beta_{k+1,l}y_l}). \end{aligned}$$

Let us now replace $A_{k+1,l}, B_{k+1,l}$ with $A_{k,l}, B_{k,l}$ with the help of (107), x_{k+2} with $x_k + 2\Delta x_k$ and let us expand the preceding expression in the powers of Δx_k, by keeping the terms of Δx_k^2. The little long calculation, like for (53″) gives:

$$\begin{cases} \Psi_{k+1,l}(x_k+2\Delta x_k,y_l) \\ \quad = [A_{k,l}e^{-i\alpha_{k,l}x_k}(1-2i\alpha_{k,l}\Delta x_k - 2\alpha_{k,l}^2\Delta x_k^2) + B_{k,l}e^{i\alpha_{k,l}x_k}(1+2i\alpha_{k,l}\Delta x_k - 2\alpha_{k,l}^2\Delta x_k^2)] \\ \quad \times[C_{k,l}e^{-i\beta_{k,l}y_l} + D_{k,l}e^{i\beta_{k,l}y_l}]. \end{cases} \tag{122}$$

With the three expressions (120), (121), (122) one easily forms the derivative $\left(\frac{\partial^2\Psi}{\partial x^2}\right)_{x_k,y_l}$ using the formula (51). One finds:

$$\begin{aligned} \left(\frac{\partial^2\Psi}{\partial x^2}\right)_{x_k,y_l} &= (A_{k,l}e^{-i\alpha_{k,l}x_k} + B_{k,l}e^{i\alpha_{k,l}x_k})(C_{k,l}e^{-i\beta_{k,l}y_l} + D_{k,l}e^{i\beta_{k,l}y_l})(-\alpha_{k,l}^2) \\ &= \Psi_{k,l}(x_k,y_l)(-\alpha_{k,l}^2). \end{aligned} \tag{123}$$

Quite the same way, one obtains:

$$\left(\frac{\partial^2\Psi}{\partial y^2}\right)_{x_k,y_l} = \Psi_{k,l}(x_k,y_l)(-\beta_{k,l}^2). \tag{124}$$

Recalling the formulas (101) one easily sees that equation (93) is satisfied by the functions $\Psi(x,y)$ (117) and (118).

4.3 Determination of the arbitrary constants

The problem we considered of two particles in one dimensional space can be interpreted as a problem of one particle represented in the configuration space of two dimensions – a plane. In this plane, we choose the two perpendicular coordinate axes OX and OY.

Let us consider the function $\Psi_{\rho,\sigma}(x,y)$ (118). For a fixed value of the index σ, (118) will be the solution of the wave equation, valid in the horizontal band between the lines with equations $y = y_\sigma$ and $y = y_{\sigma+1}$. If we know the numerical values of $A_{0,0}, B_{0,0}, C_{0,0}, D_{0,0}$ and those of $A_{0,\sigma}, B_{0,\sigma}$, the values of the wave function Ψ will be known in the chosen band. To have the values of Ψ in the next band, between the lines $y = y_{\sigma-1}$ and $y = y_\sigma$, one has to know also the numerical values of $A_{0,\sigma-1}$ and $B_{0,\sigma-1}$. One sees that (118) contains sequence of indeterminate parameters $A_{0,\sigma}, B_{0,\sigma}$ $(\sigma = 1,2,\ldots)$. But since the equation (118) contains them linearly in the numerator and in the denominator, one can divide those last to $A_{0,\sigma}$ (supposing they are not zero) and one will have like arbitrary parameters their rations: $b_{0,\sigma} = \frac{B_{0,\sigma}}{A_{0,\sigma}}$ (Ψ is a homographic function with respect to $b_{0,\sigma}$). Then in all the horizontal bands which we have defined above, the solution Ψ will contain an arbitrary parameter $b_{0,\sigma}$ or also, in all these bands – a sequence of arbitrary parameters. Their values should be fixed, so that one can calculate the values of Ψ for all x and y.

Let us consider a horizontal band between the lines $y = y_\sigma$ and $y = y_{\sigma+1}$. With this, the values of the elements $m_{11},\ldots,m_{22}$ of the matrix $M_{\rho,0,0}$ which enter in (118), will be known as functions of x_ρ (the upper bound of the integrals in the elements $m_{11},\ldots,m_{22}$). Since we have on the above indicated band an arbitrary parameter $b_{0,\sigma}$, we can choose it in a way that $\Psi_{\rho,\sigma}(x_\rho, y_\sigma)$ takes a given value which we indicate with g_σ. In the same way we can choose the parameter $b_{0,\sigma-1}$ in the horizontal band between $y = y_\sigma$ and $y = y_{\sigma-1}$ in a way that $\Psi_{\rho,\sigma-1}(x_\rho, y_{\sigma-1}) = g_{\sigma-1}$, where $g_{\sigma-1}$ is another given value, close to g_σ. Then we can find for those arbitrary parameters $b_{0,\sigma}$ $(\sigma = 1, 2, \ldots)$ values such that the function Ψ takes sequence of given values $g_\sigma, g_{\sigma-1}, \ldots$ for a fixed value of x. In the limit, when the intervals of division $\Delta x, \Delta y$ tends to zero, the sequence of values $g_0, g_1, g_2, \ldots$ can be considered as a sequence of values of a function $g(y)$ of y for $y = y_0, y_1, y_2, \ldots$. Thus if we can determine in the indicated way the parameters $b_{0,\sigma}$, *the function* $\Psi(x,y)$*, solution of the wave equation, will merge with a given function of* y*, for a given value of* $x = x_\rho$.

$$\Psi(x_\rho, y) = g(y) \tag{125}$$

The sketched operations are easy to perform. One has to write for the horizontal band between y_σ and $y_{\sigma+1}$ the condition:

$$\Psi_{\rho,\sigma}(x_\rho, y_\sigma) = g(y_\sigma) = g_\sigma(\sigma = 1, 2, \ldots). \tag{126}$$

With the help of (118) one sees that the preceding condition expresses g_σ as a homographic function of the parameter $b_{0,\sigma}$ and one gets the value of $b_{0,\sigma}$.

The so found formula gives in principle the general solution for the parameters b. Obviously, it is not very easy to discuss, in this general case, if this formula can be used for all the given values of y_σ, this is to say, if $b_{0,\sigma}$ will have finite values for all the given g_σ. One should never, for example, choose the modulus of one of the parameters $b_{0,\sigma}$ equal to 1, $\|b_{0,\sigma}\| = 1$, because if this is realized, the denominator in the formula (118) could vanish for certain values of the variables.

We will apply the formula (118) in general to find the approximate solution of the wave equation. In the case when the potential function is slowly varying, we have already seen in the problem in one dimension that of the four terms m (47) of the matrix M (29′), one should keep in first approximation only the two elements

m^0_{11} and m^0_{22} given by (39) and (39′). By assuming that $F(x,y)$ is a function which varies slowly, here we will keep also only the elements m^0_{11} and m^0_{22} of the main diagonal of the matrix $M_{\rho,0,0}$. Again, of the terms $n_{11},\ldots,n_{22}$, one will keep only n^0_{11} and n^0_{22}. The simplified formula which we thus have found for the $b_{0,\sigma}$, by replacing in it the approximate values of m and n, shows that $b_{0,\sigma}$ are generally slowly varying functions of x and y. In the case when the mutual interaction of the two particles (x) and (y) can be ignored, one knows that the solution of the wave equation can be found by separation of the variables. We can easily find this case from formula (118) if the term F_{12} in the potential function is negligible, since in this case the conditions of continuity (103) are satisfied for $A_{0,0} = A_{0,1} = A_{0,2} = \ldots$ and $B_{0,0} = B_{0,1} = B_{0,2} = \ldots$. We will assume that in first approximation, we can take in the formula (118):

$$\begin{cases} A_{0,0} = A_{0,1} = A_{0,2} = \ldots = A_{0,\sigma} = A \\ B_{0,0} = B_{0,1} = B_{0,2} = \ldots = B_{0,\sigma} = B \end{cases} \tag{127}$$

This convention simplifies a great deal the calculations which will occur in the practical cases. This choice of the amplitudes A and B indicates only that our function Ψ takes, for $x = x_\rho$, a sequence of values which are the values of a slowly variable function $g(y)$. Vice versa, if one puts in (120) A and B according to (127), one will find this sequence of values. Thus, we will accept that (127) exists. The conditions (127) are equivalent to the unique condition:

$$b_{0,0} = b_{0,1} = \ldots = b_{0,\sigma} = b. \tag{128}$$

With this convention we write the solution (118) in the form:

$$\begin{cases} \Psi_{\rho,\sigma}(x,y) = [(m_{11} + bm_{12})e^{-i\alpha_{\rho,\sigma}x} + (m_{21} + m_{22}b)e^{i\alpha_{\rho,\sigma}x}][(n_{11}C_{0,0} + n_{12}D_{0,0})e^{-i\beta_{0,\sigma}y} \\ \qquad + (n_{21}C_{0,0} + n_{22}D_{0,0})e^{i\beta_{0,\sigma}y}] \frac{Ae^{-i\alpha_{0,0}x_0} + Be^{i\alpha_{0,0}x_0}}{e^{-i\alpha_{0,\sigma}x_0} + be^{i\alpha_{0,\sigma}x_0}} \end{cases} \tag{129}$$

When the intervals of division $\Delta x, \Delta y$ tend to zero, all the terms in (129), which depend on x_ρ and of y_σ, become known function of x and y. We can then give to (129) a final form, removing the indexes ρ and σ:

$$\begin{cases} \Psi(x,y) = [(m_{11}+bm_{12})e^{-i\alpha(x,y)x} + (m_{21}+m_{22}b)e^{i\alpha(x,y)x}] \\ \times[(n_{11}C_{0,0}+n_{12}D_{0,0})e^{-i\beta(x_0,y)y}+(n_{21}C_{0,0}+n_{22}D_{0,0})e^{i\beta(x_0,y)y}]\frac{Ae^{-i\alpha(x_0,y_0)x_0}+Be^{i\alpha(x_0,y_0)x_0}}{e^{-i\alpha(x_0,y)x_0}+be^{i\alpha(x_0,y)x_0}} \end{cases} \tag{130}$$

This formula allows us to calculate the value of Ψ for all the values of x and y. One should not forget also that the elements m in (130) are functions of x and y; $m_{11}(x,y),\ldots$, just as the n are functions only of y and $x = x_0$; $n_{11}(x_0,y),\ldots$.

Let us assume now that the studied problem is a problem of collision, this is to say, for very large values of x and y, the potential $F(x,y)$ (98) tends to zero. In this case, the terms α and β from (129) become constants. From the other side, we saw that for the linear problem, the matrix M (29′) becomes a unity matrix in a domain where the potential is constant (or null). Since the matrix $M_{k+\rho,k,l}$ (111) and $N_{k,l+\sigma,l}$ (115) have the same form as M (29′), one sees easily that with the hypothesis we used on $F(x,y)$, one has $m_{11} \sim m_{22} \sim 1$, while $m_{12} \sim m_{21} \sim 0$ and also that $n_{11} \sim n_{22} \sim 1$, while $n_{12} \sim n_{21} \sim 0$ for very large values of x and y. Recalling formula (118), one sees that each bracket will represent as an asymptotic form a linear combination of two monochromatic plane waves, and the last factor (the fraction) will become constant. Consequently, *the choice* (127) *of the amplitudes A and B determines such integral* Ψ *of the wave equation, which is required in the problem of collision,* this is to say, that these asymptotic values describe a uniform motion of the two particles.

Let us now take the form (119) which we gave to the solution (116) of the wave equation. It is clear that one can make on this formula analogous considerations to those we made for formula (118). One will have the values of Ψ at all points (x_ρ, y_σ) if one knows the constants $C_{\rho,0}, D_{\rho,0} (\rho = 1,2,\ldots)$. In each vertical band between the vertical lines $x = x_\rho, x = x_{\rho+1}$ one has two constants $C_{\rho,0}, D_{\rho,0}$ or also, if we divide the numerator and the denominator of (119) by $C_{\rho,0}$ and if we introduce the quantity $d_{\rho,0} = \frac{D_{\rho,0}}{C_{\rho,0}}$, one will have an undetermined parameter $d_{\rho,0}$ in each vertical band. One can use these parameters, like in the case of the solution (118), so that the function Ψ (119) takes a sequence of given values $r_\rho (\rho = 1, 2, \ldots)$ for given y. We will make also the simplification like (127):

$$\begin{cases} C_{0,0} = C_{1,0} = \ldots = C_{\rho,0} = C \\ D_{0,0} = D_{1,0} = \ldots = D_{\rho,0} = D \end{cases} \tag{131}$$

which one can write in another way:

$$d_{0,0} = d_{1,0} = \ldots = d_{\rho,0} = d. \tag{132}$$

We can finally give that second form of the solution, coming from (119), by removing the index ρ in the mean time:

$$\begin{cases} \Psi(x,y) = [(n_{11} + n_{12}d)e^{-i\beta(x,y)y} + (n_{21} + n_{22}d)e^{i\beta(x,y)y}] \\ \times [(m_{11}A_{0,0} + m_{12}B_{0,0})e^{-i\alpha(x,y_0)x} + (m_{21}A_{0,0} + m_{22}B_{0,0})e^{i\alpha(x,y_0)x}] \frac{Ce^{-i\beta(x_0,y_0)y_0} + De^{i\beta(x_0,y_0)y_0}}{e^{-i\beta(x,y_0)y_0} + de^{i\beta(x,y_0)y_0}} \end{cases} \tag{133}$$

where one has to write this time for the elements m and n in (133), expressed as functions of x and y: $m_{11}(x, y_0), \ldots$ and $n_{11}(x, y), \ldots$.

We can now generalize the preceding solution of the Schrödinger equation in the case of any number of particles in any field. The wave equation in this configuration space is:

$$\sum_{i=1}^{N} \frac{1}{m_i} \Delta_i \Psi + \frac{8\pi^2}{h^2} [E - F(x_1, \ldots, x_{3N})] \Psi = 0 \tag{134}$$

We can consider that $x_1, \ldots, x_{3N}$ vary in the given interval $x_0 x'$. Let us divide this interval to n parts, assuming that the potential has a constant value when each particle moves in the elementary interval. The solution of the wave equation for these small variations of the variables will be the product of $3N$ functions, each function being a linear combination of two exponential functions of one variable. For a determined choice of intervals, one can write the corresponding solution in the form:

$$\Psi_{k,l,\ldots,p}(x_1,x_2,\ldots,x_{3N}) = \prod_{j=1}^{N}[(A_j)_{k,l,\ldots,p}e^{-i(\alpha_j)_{k,l,\ldots,p}x_j} + (B_j)_{k,l,\ldots,p}e^{i(\alpha_j)_{k,l,\ldots,p}x_j}]. \quad (135)$$

One should write $2.3N$ continuity conditions like (103) on the edges of the neighboring elementary barriers. Of these conditions, one can eliminate the amplitudes with the help of $3N$ matrices of two rows and two columns, and one will finally arrive at a form of the wave function Ψ like (118). The question of convergence in the elements of the matrices does not differ from that in the already studied cases.

One can determine the amplitudes A_j, B_j in a way such that the wave function takes a sequence of given values: values of one function of x_k, when the other variables $x_i\,(i \neq k)$ have fixed values. If we assume that all the amplitudes A_j are equal to a quantity A, and the same for the other amplitudes, this will be equivalent to assuming that if the particles are far enough from each other, so that one can neglect their mutual interactions, the wave function will be decomposed to a product of monochromatic plane waves. This is the condition in the limit for the problem of collision of particles.

CHAPTER 5

5.1 The problem of barriers in the relativistic case

The problem of relativistic passage of particles trough a potential barrier will be treated with the Dirac equation as a departure point. We will give in the beginning some basic concepts of the theory of Dirac.

The Schrödinger equation is not relativistic. It does not contain other effect than the spin of the electron. One knows that this equation can be found in a formal manner starting from the classical equation of Hamilton. To this end, one has to replace in the latter equation in rectangular coordinates the conjugated moments p_k of the coordinates q_k with the operators $-\frac{h}{2\pi i}\frac{\partial}{\partial x_k}$, and the Hamilton function S with the wave function.

It has been tried to find the relativistic wave equation following the same path. In the special relativity one has the following relation:

$$\frac{1}{c^2}(W-\varepsilon V)^2 - \sum_{x,y,z}(p_x - \frac{\varepsilon}{c}A_x)^2 - m^2c^2 = 0 \tag{136}$$

where W is the total energy of the electron, V is its potential energy and $A(A_x, A_y, A_z)$ – the vector potential. By introducing the operators:

$$\begin{cases} P_1 = -\frac{h}{2\pi i}\frac{\partial}{\partial x} + \frac{\varepsilon A_x}{c}, P_2 = -\frac{h}{2\pi i}\frac{\partial}{\partial y} + \frac{\varepsilon A_y}{c}, \\ P_3 = -\frac{h}{2\pi i}\frac{\partial}{\partial z} + \frac{\varepsilon A_z}{c}, P_4 = \frac{1}{c}\frac{h}{2\pi i}\frac{\partial}{\partial t} + \frac{\varepsilon V}{c}, \end{cases} \tag{137}$$

one finds an operator, which applied to the wave function, gives the equation:

$$(P_4^2 - \sum_{i=1}^{3} P_i^2 - m_0^2c^2)\Psi = 0 \tag{138}$$

which has been considered as the relativistic wave equation. But this equation has some serious defects like M. Dirac has showed. First, it does not allow to define a probability density of the presence which will be always positive. Second the equation (138) is of second order with respect to t and in order to know the function Ψ in each moment, one has to have the initial values of Ψ and $\frac{\partial\Psi}{\partial t}$. To avoid this last difficulty, one has to take an equation, which will be of first order with respect to t, and in principle, the relativity requires that it should be the same for x, y and z. Dirac admits that the equation (138) is a consequence from an equation of first order of many wave functions, which one finds by decomposing (138) to two factors of first order. This equation is [8]:

$$(P_4 + \sum_{i=1}^{3} d_i P_i + \alpha_4 m_0 c)\Psi_k = 0, \qquad (k = 1,2,3,4). \tag{139}$$

The α_i are Hermitian matrices of four rows and four columns, which have the anticommutative property:

$$\alpha_i\alpha_k + \alpha_k\alpha_i = 0\,(i \neq k), \quad \alpha_i^2 = 1\,(k = 1,2,3,4)$$

and it acts on the functions $\Psi_k\,(k = 1,\ldots,4)$ following the relation: $\alpha_i\Psi_k = \sum_{l=1}^{4}(\alpha_i)_{kl}\Psi_l$.

The explicit form of (139) is:

$$\begin{cases}
\left(\frac{1}{c}\frac{h}{2\pi i}\frac{\partial}{\partial t} + \frac{\varepsilon V}{c} + m_0 c\right)\Psi_1 - \left(\frac{h}{2\pi i}\frac{\partial}{\partial x} + i\frac{h}{2\pi i}\frac{\partial}{\partial y} - \frac{\varepsilon A_x}{c} - i\frac{\varepsilon A_y}{c}\right)\Psi_4 \\
-\left(\frac{h}{2\pi i}\frac{\partial}{\partial z} - \frac{\varepsilon A_z}{c}\right)\Psi_3 = 0 \\
\left(\frac{1}{c}\frac{h}{2\pi i}\frac{\partial}{\partial t} + \frac{\varepsilon V}{c} + m_0 c\right)\Psi_2 - \left(\frac{h}{2\pi i}\frac{\partial}{\partial x} - i\frac{h}{2\pi i}\frac{\partial}{\partial y} - \frac{\varepsilon A_x}{c} + i\frac{\varepsilon A_y}{c}\right)\Psi_3 \\
-\left(\frac{h}{2\pi i}\frac{\partial}{\partial z} - \frac{\varepsilon A_z}{c}\right)\Psi_4 = 0 \\
\left(\frac{1}{c}\frac{h}{2\pi i}\frac{\partial}{\partial t} + \frac{\varepsilon V}{c} - m_0 c\right)\Psi_3 - \left(\frac{h}{2\pi i}\frac{\partial}{\partial x} + i\frac{h}{2\pi i}\frac{\partial}{\partial y} - \frac{\varepsilon A_x}{c} - i\frac{\varepsilon A_y}{c}\right)\Psi_2 \\
-\left(\frac{h}{2\pi i}\frac{\partial}{\partial z} - \frac{\varepsilon A_z}{c}\right)\Psi_1 = 0 \\
\left(\frac{1}{c}\frac{h}{2\pi i}\frac{\partial}{\partial t} + \frac{\varepsilon V}{c} - m_0 c\right)\Psi_4 - \left(\frac{h}{2\pi i}\frac{\partial}{\partial x} - i\frac{h}{2\pi i}\frac{\partial}{\partial y} - \frac{\varepsilon A_x}{c} + i\frac{\varepsilon A_y}{c}\right)\Psi_1 \\
-\left(\frac{h}{2\pi i}\frac{\partial}{\partial z} - \frac{\varepsilon A_z}{c}\right)\Psi_2 = 0
\end{cases} \tag{140}$$

Knowing the system of functions Ψ_k which satisfy the equation (140), the presence probability of the particles in the volume $dxdydz$ is $\sum_{i=1}^{4}\Psi_i\Psi_i^* dxdydz$. But the determination of such solution is not easy if the fields are arbitrary. In the case when $\vec{A}=0$ and V is function of one of the variables, there is the method of Pauli [13] of solution of the Dirac equation.

5.2 Passage of particles trough a rectangular potential barrier

We will study now the passage of particles, whose motion is described by the Dirac equation, trough a potential barrier. This problem is treated by O. Klein [10].

Let us take the case in which the motion of the particles is done following the given direction OX. We suppose that the potential energy is null to the left of a point M with abscissa x_0 and that it has a constant value P to the right of M.

The potential vector is null everywhere. The particles which propagate from left to right with constant speed, come and hit the separation surface at M. One part of the particles is reflected, and another enters in the second medium. The equation of propagation to the left of M is:

$$\left(\frac{1}{c}\frac{h}{2\pi i}\frac{\partial}{\partial t}+\alpha_4 m_0 c-\frac{h}{2\pi i}\alpha_1\frac{\partial}{\partial x}\right)\Psi_k=0 \tag{141}$$

and to the right of M:

$$\left(\frac{1}{c}\frac{h}{2\pi i}\frac{\partial}{\partial t}+\frac{P}{c}+\alpha_4 m_0 c-\frac{h}{2\pi i}\frac{\partial}{\partial x}\right)\Psi_k=0. \tag{142}$$

We will look for a solution of (141) in the form of a monochromatic plane wave represented by the system of four functions $(\Psi_i)_k$ $(k=1,\ldots,4)$.

$$(\Psi_i)_k=(a_i)_k e^{\frac{2\pi i}{h}(Et-px)} \tag{143}$$

where all the amplitudes $(a_i)_k$ are constants. By substituting (143) in (141), we will find the conditions of existence of the solution in the form of a determinant equal to zero. By expanding it, one finds:

$$\left(\frac{E^2}{c^2} - m_0^2c^2 - p^2\right)^2 = 0. \tag{144}$$

We know that (144) is realized always according to (136). One verifies also that all the subdeterminants of three rows and three columns of the above mentioned determinant are null. Thus, of the four quantities $(a_i)_k (k = 1,2,3,4)$ only two are independent, for example $(a_i)_3$ and $(a_i)_4$. Let us set $(a_i)_3 = A, (a_i)_4 = B$. The equations (141) give:

$$(a_i)_1 = -\frac{pA}{\frac{E}{c} + m_0c}, \quad (a_i)_2 = \frac{pB}{\frac{E}{c} + m_0c}. \tag{145}$$

We know thus the incident wave Ψ_i. For the reflected wave Ψ_r, we can set:

$$(\Psi_r)_k = (a_r)_k e^{\frac{2\pi i}{h}(Et+px)}, \quad (k = 1,2,3,4). \tag{146}$$

For the $(a_r)_k$ we will have the same condition (144). Two of the $(a_r)_k$ will be independent, for example $(a_r)_3 = C, (a_r)_4 = D$. One will find similarly for the other amplitudes:

$$(a_r)_1 = \frac{pC}{\frac{E}{c} + m_0c}, \quad (a_r)_2 = -\frac{pD}{\frac{E}{c} + m_0c}. \tag{147}$$

In the interior of the second medium, the wave equation for the transmitted wave Ψ_t will be equation (142), whose solution is the wave Ψ_t:

$$(\Psi_t)_k = (a_t)_k e^{\frac{2\pi i}{h}(\frac{E-P}{c}t - p_1x)}. \tag{148}$$

In the same way we will find that there are two independent amplitudes $(a_t)_3 = C_1, (a_t)_4 = D_1$ and the two other amplitudes are:

$$(a_t)_1 = \frac{-p_1C_1}{\frac{E-P}{c} + m_0c}, \quad (a_t)_2 = \frac{p_1D_1}{\frac{E-P}{c} + m_0c}. \tag{149}$$

When the wave in the Dirac Mechanics crosses a potential wall, it remains continuous. It was proved in [10] the same way as for the wave Ψ in the Shcrödinger equation. Let us apply this in our problem. The wave function which exists on the left of the point M is a superposition of the incident wave and of the reflected wave. On the surface of separation, it should be equal to the transmitted wave. This gives the conditions of continuity:

$$(\Psi_i)_k + (\Psi_r)_k = (\Psi_t)_k \qquad (k = 1,2,3,5). \tag{150}$$

Of these four linear equalities, one can get the amplitudes C, D, C_1, D_1 as functions of A and B, which are considered as given.

5.3 Solution of the relativistic problem of barriers using the method of decomposition of barriers

Let us assume that the electrons which propagate following the positive direction of OX have to cross a potential barrier which extends from x_0 to x'. The potential is supposed to be null on the two sides of the barrier. The problem consists of finding the ratio of reflected and transmitted particles. If the form of the barrier is rectangular (P is constant inside the barrier), the problem is easy, since one knows the solution of the Dirac equation in the interior of the barrier. The solution of the equation between x_0 and x' is a sum of the two waves propagating to the left and to the right. One has to write the conditions of continuity, similarly to (150), which exist on the two edges of the barrier. For each wave one will have two independent amplitudes. In short, one will have ten amplitudes and eight conditions of continuity, from where one will express eight of the amplitudes as functions of those of the incident wave.

Let us take a barrier which extends from x_0 to x', of any form, this is to say, the potential is a given function $P(x)$ of x, which we assume continuous and bounded.

We divide the interval x_0x' to n parts, and the barrier to small elementary barriers of base (x_{l+1}, x_l), the potential will have constant values $P(x_l)$, thus we will have as a solution of the Dirac equation in (x_{l+1}, x_l) a sum of two monochromatic plane waves. Indicating with ψ_l the wave which propagates to the right and with ϕ_l th e one which propagates to the left, their respective components will be given by:

$$\psi_{l,k} = a_{l,k}e^{\frac{2\pi i}{h}(Et-p_lx)}, \quad \phi_{l,k} = b_{l,k}e^{\frac{2\pi i}{h}(Et+p_lx)}, \quad (k = 1,\ldots n; l = 1,\ldots n) \quad (151)$$

On the common edge of the barrier (x_{l-1}, x_l) and $(x_l, x_l + 1)$ one will have the four conditions of continuity:

$$\psi_{l,k}(x_l) + \phi_{l,k}(x_l) = \psi_{l+1,k}(x_l) + \phi_{l+1,k}(x_l), (k = 1,2,3,4) \quad (152)$$

The four amplitudes which characterize each wave will be then expressed by two of them, connected by an equality of the form (144), there will be only two independent among the four amplitudes. We indicate by:

$$A_l = a_{l,3}, \qquad B_l = a_{l,4} \quad (153)$$

the independent amplitudes of the wave which propagates to the right and by:

$$C_l = b_{l,3}, \qquad D_l = a_{l,4} \quad (154)$$

those of the wave propagating to the left. By setting:

$$g_l = \frac{p_l}{\frac{E-P_l}{c} + m_0c} \quad (155)$$

we will have, exactly as we had for the formulas (145):

$$\begin{cases} a_{l,1} = -g_lA_l, & a_{l,2} = g_lB_l, \\ b_{l,1} = g_lC_l, & b_{l,2} = -g_lD_l \end{cases} \quad (156)$$

since one has, in short, always the same problem as on page 74 – the plane wave in Dirac's theory. With the help of the preceding notations, we can now write explicitly the conditions (152):

$$\begin{cases} g_l(A_l e^{-ip_l x_l} - C_l e^{ip_l x_l}) = g_{l+1}(A_{l+1} e^{-ip_{l+1} x_l} - C_{l+1} e^{ip_{l+1} x_l}) \\ A_l e^{-ip_l x_l} + C_l e^{ip_l x_l} = A_{l+1} e^{-ip_{l+1} x_l} + C_{l+1} e^{ip_{l+1} x_l} \\ g_l(B_l e^{-ip_l x_l} - D_l e^{ip_l x_l}) = g_{l+1}(B_{l+1} e^{-ip_{l+1} x_l} - D_{l+1} e^{ip_{l+1} x_l}) \\ B_l e^{-ip_l x_l} + D_l e^{ip_l x_l} = B_{l+1} e^{-ip_{l+1} x_l} + D_{l+1} e^{ip_{l+1} x_l} \end{cases} \tag{157}$$

From this system of linear equations with respect to the four quantities A, B, C, D, one can express the amplitudes with index $l+1$ as functions of those with index l. The determinant Δ_{l+1} of the coefficients of the amplitudes of the right part of equations (157) has the value 4. One can consider the amplitudes $A_{l+1}, B_{l+1}, C_{l+1}, D_{l+1}$ as the components of a vector $\vec{r}_{l+1}$. The equations (157) express a transformation of the vector $\vec{r}_{l+1}$ to the vector $\vec{r}_l$ with the help of a matrix M_l of four rows and four columns:

$$\vec{r}_{l+1} = M_l \vec{r}_l. \tag{158}$$

It is easy to solve the equations (157) and one finds for $M_l = \|(m_l)_{\alpha\beta}\|$, $(\alpha, \beta = 1,2,3,4)$:

$$\begin{cases} (m_l)_{11} = (1+\rho_l) e^{-i(p_{l+1}-p_l)x_l}, (m_l)_{12} = (1-\rho_l) e^{i(p_{l+1}+p_l)x_l}, \\ (m_l)_{21} = (1-\rho_l) e^{-i(p_{l+1}+p_l)x_l}, (m_l)_{22} = (1+\rho_l) e^{-i(p_{l+1}-p_l)x_l}, \\ (m_l)_{33} = (1+\rho_l) e^{i(p_{l+1}-p_l)x_l}, (m_l)_{34} = (1-\rho_l) e^{i(p_{l+1}+p_l)x_l}, \\ (m_l)_{43} = (1-\rho_l) e^{-i(p_{l+1}+p_l)x_l}, (m_l)_{44} = (1+\rho_l) e^{-i(p_{l+1}-p_l)x_l}, \\ (m_l)_{13} = (m_l)_{14} = (m_l)_{23} = (m_l)_{24} = (m_l)_{31} = (m_l)_{32} = (m_l)_{41} = (m_l)_{42} = 0 \end{cases} \tag{159}$$

where one sets $\rho_l = \frac{g_l}{g_{l+1}}$. From (155), g_l and g_{l+1} have close values, consequently, the value of ρ_l is close to unity. The difference $p_{l+1} - p_l$ is very small. Since all the terms of M_l are divided by $\frac{1}{2}$, it follows that all the terms of the main diagonal have values close to unity and the other terms are very small, thus M_l is almost diagonal. Making the successive eliminations of the amplitudes, one will find the relation:

$$r_{l+j} = M_{l+j-1} M_{l+j-2} \dots M_l \vec{r}_l = M_{l,j} \vec{r}_l \tag{160}$$

where $M_{l,j}$ is the matrix product. If we introduce the two matrices σ_l and τ_l, to which the matrix M_l decomposes, it can be written:

$$M_l = \begin{vmatrix} \sigma_l & 0 \\ 0 & \tau_l \end{vmatrix}. \tag{161}$$

Because of this form of M_l, the matrix $M_{l,j}$ (160) will be formed by two matrices σ and τ such that $\sigma = \sigma_{l+j-1}\sigma_{l+j-2}\dots\sigma_l$ and $\tau = \tau_{l+j-1}\tau_{l+j-2}\dots\tau_l$. From the other side we asked that $\rho_l = \frac{g_l}{g_{l+1}}$, where g (155) is a known function of x. One can then write:

$$\rho_l = \frac{g_l}{g_l + \Delta g_l} = 1 - \frac{\Delta g_l}{g_l}$$

$$\frac{1}{2}(1+\rho_l) = 1 - \frac{\Delta g_l}{2g_l} = e^{-\frac{\Delta g_l}{2g_l}}; \quad \frac{1}{2}(1-\rho_l) = \frac{\Delta g_l}{2g_l}.$$

By stopping always on the infinitesimals from the first order, one can represent the matrix σ_l in the following way:

$$\sigma_l = \begin{vmatrix} e^{i\Delta p_l x_l - \frac{\Delta g_l}{2g_l}} & \frac{\Delta g_l}{2g_l} e^{2ip_l x_l} \\ \frac{\Delta g_l}{2g_l} e^{-2ip_l x_l} & e^{-i\Delta p_l x_l - \frac{\Delta g_l}{2g_l}} \end{vmatrix} \tag{162}$$

and the same way for the matrix τ_l. Now σ_l and τ_l are in the same form as the matrix M_j (33). Then, there is no difficulty in forming the products σ and τ, since the elements of the matrices σ and τ are composed of those of the matrix M (29′). The elements $\sigma_{\alpha\beta}$, $(\alpha, \beta = 1, 2)$ will be given by infinite series as (47). One will thus have $\sigma_{11} = \sum_{i=0}^{\infty} \sigma_{11}^{2i}, \dots$ and also $\tau_{11} = \sum_{i=0}^{\infty} \tau_{11}^{2i}, \dots$. The integrals in $\sigma_{\alpha\beta}$ and $\tau_{\alpha\beta}$ will be known functions of x. With the help of the so-found matrices σ and

τ, one immediately writes the matrix $M_{l,j}$. To know the matrix $M_{l,j}$ is to know the solution of the Dirac equation, since this solution was given in each interval (x_{l+1}, x_l) by the functions (151) and to find this solution in the whole interval x_0x', one needs only the coefficients $a_{l,k}, b_{l,k}$ as functions of x, which are given to us by the knowledge of the matrix $M_{l,j}$. By keeping only the elements σ^0_{11} and σ^0_{22} of the main diagonal of σ and in analogous way – the elements τ^0_{11} and τ^0_{22} of τ, the solution of the Dirac equation which one finds this way, coincides with the solution of Pauli [13] in the case, where the geometric optics is valid.

Since the two first equations (157) contain only the amplitudes A and C, one can determine from these two equations only A_{l+1} and C_{l+1} as functions of A_l and C_l with the help of the matrix σ_l. In the same way, one will determine B_{l+1} and D_{l+1} from the two last equations (157) with the help of the matrix τ_l. One could then do without the matrix M_l (159), but we used it, because there are cases where the system (157) does not decompose to two groups of equations, each containing only two of the amplitudes.

In the case where the potential vector is not null, and where the scalar potential is a function of all the coordinates, the solution of the Dirac equation presents much more difficulties and we would not pursue it here.

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