ОБЪЕДИНЕННЫЙ ИНСТИТУТ ЯДЕРНЫХ ИССЛЕДОВАНИЙ

Лаборатория теоретической физики

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D-690

S-MATRIX FOR THE ONE-DIMENSIONAL SCHRÖDINGER EQUATION

Дубна 1961

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Abstract

A new equation is derived in which the kinetic energy $v = 2(E - U)$ plays the role of a variable with respect to which the differentiation is being made. This equation is equivalent to the one-dimensional Schrödinger equation. An explicit expression for the S-matrix is written and its expansion in ever-convergent series is found. In the simplest case the zero term of expansion of the matrix S corresponds to the absence of reflection and coincides with WKB approximation. The first term gives superbarrier reflection, in particular, the formula obtained by I. Goldman and A. Migdal /1/. By means of another expansion of S- matrix the correction to the connection formulae are found.

The one-dimensional non-relativistic Schrödinger equation

$$\psi''(x) + 2[E - U(x)]\psi(x) = 0 \tag{1}$$

is not the best starting-point for calculation of the scattering matrix since the amplitudes of the incident and reflected waves do not enter explicitly this equation and its structure does not reveal the fact that just the roughness of the potential $U(x)$ givesrise to the reflected wave.

In the present paper from Eq. (1) a new matrix equation is derived in which the amplitudes of the incident and reflected waves play the role of a wave function. The 'potential' $v = 2(E-U)$ becomes an independent variable with respect to which the differentiation is being made. The coordinate x becomes an auxiliary variable and transforms into an index of order in which the different parts of the potential are arranged. We introduce the notion of X -product which is similar to T -product in the quantized field theory. Although the equation thus obtained is equivalent to the Schrödinger equation (1) the first in its many properties supplements the Schrödinger equation.

In deriving the matrix equation a hitherto unknown structure of the general solution of Eq. (1) is used. The solution of the matrix equation allows us to find an explicit expression for the S -matrix and represent the latter in the form of ever-convergent series (different, of course, from those of the perturbation theory). It turns out to be possible to obtain fast convergence of these series by means of simple transformations of the S -matrix.

In the simplest case the zero term of expansion of the matrix S corresponds to the absence of reflection and coincides with quasi-classical approximation of Wentzel-Kramers-Brillouin. The first term of the expansion gives superbarrier reflection, in particular, the formula obtained by I. Goldman and A. Migdal /1/. The next terms of the expansion take into account the weakening of the incident wave and specify the reflected one.

The obtained results lead to a new estimation of the place which is occupied by quasi-classical approximation in the precise theory. The expansion with respect to the constant $\hbar$ (in fact, with respect to the smoothness of the potential $\frac{\Delta\lambda}{\lambda}$) yields a divergent series the two first terms of which (the only ones not vanishing at $\frac{\Delta\lambda}{\lambda}\to 0$) give, however, a reasonable approximation. The remaining terms vanishing at $\frac{\Delta\lambda}{\lambda}\to 0$ have no physical meaning and make the approximation worse. Owing to the fact that all the terms of the expansion in $\hbar$, except the two aforementioned terms, vanish under the same conditions as for vanishing of reflection, there arises the coincidence of WKB approximation with zero terms of expansion for the matrix S .

The phenomenon of reflection from the potential roughnesses is related deeply to the phenomenon of the non-conservation of classical adiabatic invariants in quantum mechanics. It is possible therefore, that the approach suggested here will prove expedient in the consideration of these phenomena as well. The matrix equation can also be generalized to the case of the system of coupled one-dimensional Schrödinger equations.

1. Formulation of the Problem

The variables x and v enter essentially unequally the Schrödinger equation

$$\psi''(x)+v(x)\psi(x)=0\,, \tag{1.1}$$

where $v(x)=k^2(x)=2\left(E-U(x)\right)$, namely: while the wave function $\psi(x)$ describing the state of the particle is differentiable twice with respect to x for any limited potentials $U(x)$, the derivative $\frac{d\psi}{dv}=\frac{d\psi}{dx}\frac{dx}{dv}$, generally speaking, does not exist. So, for example, $\frac{d\psi}{dv}$ turns into infinity where $v=$ const. Owing to this fact any equation containing the derivative $\frac{d\psi}{dv}$ would lose its meaning in all the regious where $v=$ const., and would possess a number of other unsuitable properties.

The aforementioned consideration does not mean at all that there exists no reasonable equation replacing the Schrödinger equation in which the 'potential' v would play the role of a variable with respect to which the differentiation is being made. On the contrary, the aim of the present paper is to constract such an equation and investigate its properties.

Let us assume that the state of the particle may be described by a certain function $F(x)$ differentiable at least once with respect to v for all piecewise continuous $v\neq 0$ (even for such ones whose derivative $\frac{dv}{dx}$ exists at not a single point). Here and in the following a function is assumed to be differentiable if the derivative belongs to the class of piecewise continuous functions. The form of the function $F(x)$ and its connection with $\psi(x)$ can be established by means of the following heuristic considerations.

If $F(x)$ is differentiable in the general case not more than one time, then it may satisfy some differential equation of the order not higher then the first one. This equation can be simultaneously equivalent to Eq. (1.1) and linear only in the case the function F has two components

$$F(x)=\begin{pmatrix}F_1\ (x)\\ F_2\ (x)\end{pmatrix} \tag{1.2}$$

and is associated with $\psi(x)$ linearly

$$\psi(x)=F_1(x)\,\varphi_1(x)+F_2(x)\,\varphi_2(x)\,. \tag{1.3}$$

In order that the functions φ_1 and φ_2 be differentiable with respect to x at least once they must not contain explicitly $v(x)$ in the arguments, but they may contain there, for example, the integrals of the type $\int^x q(v,x)dx$. Taking into account that for $v=$ const. the function $\psi(x)$ must be a combination of exponents $\exp[\pm i$ (kx + const.)$]$ we get

$$\psi(x)=[F_1(x)e^{i\xi(x)}+F_2(x)e^{-i\xi(x)}]\,v^{-\frac{1}{4}} \tag{1.4}$$

where the phase $\xi(x)$ equals

$$\xi(x)=\int^x k(x)dx\,. \tag{1.5}$$

The separating out of the factor $v^{-\frac{1}{4}}$ will turn out to be convenient later. Since the requirement of the differentiability with respect to v is imposed on the functions $F_1(x)$ and $F_2(x)$, then the formula (1.4) is a certain hypotheses about the structure of the general solution of Eq. (1.1).

2. Equations for the Amplitudes

Let us derive the equations for the amplitudes $F_1(x)$ and $F_2(x)$. By calculating the derivative ψ'

$$\begin{aligned}\psi'(x)=&\,iv^{\frac{1}{4}}F_1e^{i\xi}-iv^{\frac{1}{4}}F_2e^{-i\xi}+\\ &+\frac{dv}{dx}\Big[e^{i\xi}\frac{d}{dv}\big(v^{-\frac{1}{4}}F_1\big)+e^{-i\xi}\frac{d}{dv}\big(v^{-\frac{1}{4}}F_2\big)\Big]\end{aligned} \tag{2.1}$$

we see that the existence of ψ' can be garanteed only if the expression in square brackets is zero

$$e^{i\xi}\frac{d}{dv}\big(v^{-\frac{1}{4}}F_1\big)+e^{-i\xi}\frac{d}{dv}\big(v^{-\frac{1}{4}}F_2\big)=0\,, \tag{2.2}$$

since in the opposite case the derivative v' the existence of which is not supposed, will enter the expression for ψ' .

By calculating (taking into account (2.2)) the second derivative $\psi''(x)$ we have

$$\psi''(x) = -v^{\frac{3}{4}} F_1 e^{i\xi} - v^{\frac{3}{4}} F_2 e^{-i\xi} + \\ + i\frac{dv}{dx}\left[e^{i\xi}\frac{d}{dv}\left(v^{\frac{1}{4}}F_1\right) - e^{-i\xi}\frac{d}{dv}\left(v^{\frac{1}{4}}F_2\right)\right] . \tag{2.3}$$

In a similar way for the existence of $\psi''(x)$ it is necessary that

$$e^{i\xi}\frac{d}{dv}\left(v^{\frac{1}{4}}F_1\right) - e^{-i\xi}\frac{d}{dv}\left(v^{\frac{1}{4}}F_2\right) = 0. \tag{2.4}$$

After elementary transformations the system of equations (2.2), (2.4) aquires a compact form

$$\begin{cases} \dfrac{dF_1(x)}{d\ln v(x)} = \dfrac{1}{4} F_2(x)\, e^{-2i\xi(x)} \\ \dfrac{dF_2(x)}{d\ln v(x)} = \dfrac{1}{4} F_1(x)\, e^{2i\xi(x)} \end{cases} . \tag{2.5}$$

Comparison of the expressions (1.4) and (2.3) easily shows that ψ satisfies the Schrödinger equation (1.1) as soon as the Eq. (2.2) and (2.4) are satisfied.

It is interesting to note that in deriving the Eq. (2.2) and (2.4) we have not appeal explicitly to Eq. (1.1) but used only the existence of the derivatives ψ' and ψ'' . This is connected with the fact that the Eq. (1.1) has been used already in writing $\psi(x)$ in the form (1.4).

The system of equations (2.2), (2.4) can be easily derived in a more obvious but less rigorous way, by breaking down the potential $U(x)$ into a great number of thin right-angled barriers, writing down the conditions of the continuity of ψ and ψ' at each boundary, and then by letting the thickness of these barriers tend to zero.

3. Solution of Equations for the Amplitudes

We write (2.5) in a matrix form

$$dF = g(x)\, F\, d\ln v \tag{3.1}$$

where

$$g(x) = \begin{pmatrix} 0 & \frac{1}{4}e^{-2i\xi(x)} \\ \frac{1}{4}e^{2i\xi(x)} & 0 \end{pmatrix}. \qquad (3.2)$$

The matrices $g(x)$ for various x don't commute.

The solution of equation (3.1) can be written in the form of the X-exponent* /2/

$$F(x) = X\left(\exp\int_{x_0}^{x_1} g(x)\, d\ln v(x)\right) F(x_0) \qquad (3.3)$$

where the simbol of X-product implies that the matrices $g(x)$ are to be arranged in the order of increase of their arguments from the left to the right (or in the order of decrease if $x_1 < x_0$).

The matrix

$$S(x_1, x_0) = X\left(\exp\int_{x_0}^{x_1} g(x)\, d\ln v(x)\right), \qquad (3.4)$$

transforming $F(x_0)$ into $F(x_1)$ is unimodular and possesses elements

$$S_{11} = 1 + \int_{x_0}^{x_1} \frac{1}{4} e^{-2i\xi(x')} \int_{x_0}^{x'} \frac{1}{4} e^{2i\xi(x'')} d\ln v(x') d\ln v(x'') + \ldots,$$

$$S_{12} = \int_{x_0}^{x_1} \frac{1}{4} e^{-2i\xi} d\ln v +$$

$$+ \int_{x_0}^{x_1} \frac{1}{4} e^{-2i\xi} \int_{x_0}^{x'} \frac{1}{4} e^{2i\xi} \int_{x_0}^{x''} e^{-2i\xi} d\ln v(x') d\ln v(x'') d\ln v(x''') + \ldots, \qquad (3.5)$$

$$S_{22} = [S_{11}]_{\xi \to -\xi}, \quad S_{21} = [S_{12}]_{\xi \to -\xi}.$$

From (3.4) it follows that the power series of (3.5) converge provided only the integral (in the sence of Stieltjes)

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* The notion of the X-exponent coincides with that of the multiplicative integral $\int (1+f(x))dx$ introduced in 1887 by Volterra /2/ . We retain the first term as closer to the physical terminology.

$$\int_{x_0}^{x_1} e^{\pm 2i\xi(x)}\, d\ln v(x) \qquad (3.6)$$

exists. Thus, the formula

$$F(x) = S(x, x_0)\, F(x_0) \qquad (3.7)$$

yields a general solution of the Schrödinger equation. One can see it immediatley by inserting (3. 7), (3.4), (1.4) into (1.1).

We emphasize that the convergence of the series (3.5) is not connected with the smallness of any constant. From this point of view these series differ advantageously from many other series in terms of which the solution of the Schrödinger equation may be written, for example, from perturbation series.

The matrix S can be easily found in the explicit form if two independent solutions $\psi_{(1)}(x)$ and $\psi_{(2)}(x)$ of Eq. (1.1) are known. We introduce the matrices

$$W = \begin{pmatrix} \psi_{(1)} & \psi_{(2)} \\ \psi'_{(1)} & \psi'_{(2)} \end{pmatrix}; \quad Z = \begin{pmatrix} v^{-\frac{1}{4}} e^{i\xi} & v^{-\frac{1}{4}} e^{-i\xi} \\ i v^{\frac{1}{4}} e^{i\xi} & -i v^{\frac{1}{4}} e^{-i\xi} \end{pmatrix}; \quad F = \begin{pmatrix} F_{1(1)} & F_{1(2)} \\ F_{2(1)} & F_{2(2)} \end{pmatrix}. \qquad (3.8)$$

From (1.4) and (2.1) it follows

$$W(x) = Z(x)\, F(x). \qquad (3.9)$$

From (3.7), (3.9) we obtain an explicit expression for the S -matrix

$$S(x, x_0) = Z^{-1}(x)\, W(x)\, W^{-1}(x_0)\, Z(x_0). \qquad (3.10)$$

By inserting (3.10), (3.7) into (2.5) we can show that this system is satisfied as soon as Eq. (1.1) satisfies . Thus, the system (2.5) is equivalent to the Schrödinger equation (1.1) in the sense that to any solution of Eq. (1.1) there corresponds the solution of the system (2.5) and vice versa. Hence, the general solution of Eq. (1.1) has, in fact, the structure (1.4).

The phase $\xi(x)$ plays the same role in Eq. (2.5) as the potential $v(x)$ in Eq. (1.1). The wave function $F(x)$, generally speaking, is not differentiable with respect to x what is evident at least from the fact that it is expressed in terms of Stieltjes integrals. Thus, there is a certain supplementarity in the properties of the system (2.5) and the Schrödinger equation (1.1).

4. Turning Points

The direct application of the formulae (3.3) - (3.5) to the segment $[x_1, x_0]$ which contains the turning point $v=0$ * is not convenient because the rate of convergence of series (3.5) is unsatisfactory in this case. In order to get rid of the singularity at the turning point in the X - exponent we single out from the matrix $S(x_1, x_0)$ some principal part $P(x_1, x_0)$.

We make use of the identity

$$X\Big[\exp\Big(\int_{x_0}^{x_1} p(x)\,d\alpha(x) + \int_{x_0}^{x_1} e(x)\,d\beta(x)\Big)\Big] = P(x_1, x_0)\,\mathcal{E}(x_1, x_0), \tag{4.1}$$

where

$$P(x, x_0) = X\Big(\exp\int_{x_0}^{x} p\,d\alpha\Big), \tag{4.2}$$

$$\mathcal{E}(x_1, x_0) = X\Big(\exp\int_{x_0}^{x_1} P^{-1}(x, x_0)\,e(x)\,P(x, x_0)\,d\beta(x)\Big), \tag{4.3}$$

and which is easily proved by writing the exponent as an infinite product. We put

$$p = g(\bar{x}), \quad e = g(x) - g(\bar{x}), \quad d\alpha = d\beta = d\ln v, \tag{4.4}$$

where $\bar{x}$ is the turning point $v(\bar{x}) = 0$. Then instead of (3.7) we get

$$F(x_1) = P(x_1, x_0)\,\mathcal{E}(x_1, x_0)\,F(x_0). \tag{4.5}$$

The integral appearing in the X - exponent (4.3) is now regular and small for small $x_1 - x_0$, so that the matrix $\mathcal{E}$ is close to the unit one. We can write for the elements of the matrix $\mathcal{E}$ an expansion similar to (3.5) which converges fast. The matrix P is calculated explicitly

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* The integrals in Eq. (3.3), (3.5) can be understood in this case in the following sense:

$$\int f\,d\ln v = P_v\int f\,\frac{dv}{v} + i\pi\,\tfrac{1}{2}\left(\mathrm{sign}\,v^- - \mathrm{sign}\,v^+\right)\int f\,\delta(x-\bar{x})\,dx, \tag{4.1a}$$

where $\bar{x}$ is the turning point, the symbol P_v denotes omitting during integration the segment where $|v| < \varepsilon;\ \varepsilon \to 0$; v^+, v^- are the values of v at the right and the left end of the omitted segment.

$$P(x_1, x_0) = \begin{pmatrix} ch\frac{1}{4}\ln\frac{v}{v_0} & e^{-2i\xi(\bar{x})} sh\frac{1}{4}\ln\frac{v}{v_0} \\ e^{2i\xi(\bar{x})} sh\frac{1}{4}\ln\frac{v}{v_0} & ch\frac{1}{4}\ln\frac{v}{v_0} \end{pmatrix} \tag{4.6}$$

and describes the principle part of the $F(x)$ - wave function transformation, when passing through the turning point.

The singling out of the principle part of (4.6) from the S - matrix is always possible and doesn't assume the smoothness and the small curvature of the potential in the vicinity of the turning point. Thus, the turning point doesn't prevent from obtaining the S -matrix in the form of fast convergent series.

In a similar way we can single out the main part of the S -matrix not only in small neighbourhood of the turning point, but on any segment $[x_1, x_0]$ if on this segment there is the potential $\tilde{v}(x)$ which is close to $v(x)$ and for which the exact solution of Eq. (1.1) is known.

Reverting to the P-matrix it should be mentioned that the matrix (4.6) is a scattering matrix on the right-angled jump from v_0 to v at the point $\bar{x}$ (v_0 and v may have any signs).

5. Turning Point in the Quasi-Classical Case

The method of singling out the principle part of the S -matrix may be applied for obtaining corrections to usual connection formulae* for quasi-classical solutions inside and outside the potential barrier. These corrections, which arise due to the potential curvature in the neighbourhood of the turning point, are not always small and can change considerably, for example, the possibility of a particle penetration through the potential barrier.

Let the potential $v(x)$ be close to the linear one in the neighbourhood of the turning point. Then in (4.1)- (4.3) it is natural to put

$$p = e = g(x), \quad d\alpha = d\ln\left(\eta^{\frac{2}{3}} \operatorname{sign} x\right), \quad d\beta = d\ln\left|v\eta^{-\frac{2}{3}}\right|, \tag{5.1}$$

$$\eta = |\xi(x) - \xi(0)|$$

* For detailed deduction and the treatment of the usual connection formulae see paper of R. Langer /3/.

/ in (5.1) the turning point is taken for the origin of coordinates $v(0)=0$ and the potential barrier is assumed to be at the left sign v = sign x /. Apparently, for the linear potential $v=cx$, the differential $d\beta\equiv 0$ and $P=S$.

The main part $P(x,x_0)$ of (4.3) is easily obtained from the formula (3.10) where as solutions $\psi_{(1)}$ and $\psi_{(2)}$ we may take (cf. /4/)

$$\varphi_{\pm}=\begin{cases}\eta^{\frac{1}{3}}\frac{1}{2}\left[\mathcal{J}_{\frac{1}{3}}(\eta)\mp\mathcal{J}_{-\frac{1}{3}}(\eta)\right] \text{ at } x>0\\ -\eta^{-\frac{1}{3}}\frac{1}{2}\left[I_{\frac{1}{3}}(\eta)\pm I_{-\frac{1}{3}}(\eta)\right] \text{ at } x<0\end{cases} \tag{5.2}$$

($\mathcal{J}, I$ are Bessel functions). Taking into account that $\frac{d}{dx}=\left|\frac{d\eta}{dx}\right|\cdot$ sign $x\cdot\frac{d}{d\eta}$ and performing some linear transformation of the matrices W and Z ,

$$\widetilde{W}=LW,\quad \widetilde{Z}=LZ,\qquad L=\begin{pmatrix}\eta^{\frac{1}{6}} & 0\\ 0 & \eta^{-\frac{1}{6}}\,\mathrm{sign}\,x\end{pmatrix}$$

we obtain

$$P(x,x_0)=\widetilde{Z}^{-1}(x)\,\widetilde{W}(x)\,\widetilde{W}^{-1}(x_0)\,\widetilde{Z}(x_0)=G(x)G^{-1}(x_0), \tag{5.3}$$

where $\widetilde{Z}$ and $\widetilde{W}$ are the Vronsky's matrices with respect to $\eta\left(\dot{}=\frac{d}{d\eta}\right)$

$$\widetilde{W}=\eta^{\frac{1}{6}}\mathcal{D}(\varphi_+,\varphi_-)=\eta^{\frac{1}{6}}\begin{pmatrix}\varphi_+ & \varphi_-\\ \dot{\varphi}_+ & \dot{\varphi}_-\end{pmatrix},\quad \widetilde{Z}=\begin{matrix}\mathcal{D}(e^{i\eta},e^{-i\eta}) \text{ at } x>0\\ \bar{\gamma}\mathcal{D}(e^{\eta},e^{-\eta}) \text{ at } x<0\end{matrix} \tag{5.4}$$

det $\widetilde{W}=-\frac{\sqrt{3}}{2\pi}$ sign x .

The factor* $\bar{\gamma}=v^{-\frac{1}{4}}\left|v^{\frac{1}{4}}\right|=e^{-i\frac{\pi}{4}}$. By inserting (5. 4) into (4.3) we obtain

$$\mathcal{E}(x_1,x_0)=G(x_0)X\left[\exp\int_{x_0}^{x_1}\widetilde{W}^{-1}(x)\begin{pmatrix}1&0\\0&-1\end{pmatrix}\widetilde{W}(x)\,d\beta\right]G^{-1}(x_0), \tag{5.5}$$

$$\widetilde{W}^{-1}\begin{pmatrix}1&0\\0&-1\end{pmatrix}\widetilde{W}=-\eta^{-\frac{1}{3}}\,\frac{2\pi}{\sqrt{3}}\,\mathrm{sign}\,\frac{d}{d\eta}\begin{pmatrix}\varphi_+\varphi_- & \varphi_-^2\\ -\varphi_+^2 & -\varphi_+\varphi_-\end{pmatrix}.$$

It can be shown that for

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* Such a choice corresponds to the formula (4.1 a).

$$\left|\int_{x_0}^{x_1} d\bar{\beta}\,\frac{d}{d\eta}\left(\varphi_+\,\varphi_-\right)\right| << 1, \quad \left|\int_{x_0}^{x_1} d\bar{\beta}'\,\frac{d}{d\eta}\left(\varphi_\pm^2\right)\int_{x_0}^{x'} d\bar{\beta}''\,\frac{d}{d\eta}\left(\varphi_\mp^2\right)\right| \ll 1, \qquad (5.6)$$

where

$$d\bar{\beta} = -\eta^{\frac{1}{3}}\,\frac{\pi}{2\sqrt{3}}\,d\beta\ \mathrm{sign}\,x, \qquad (5.7)$$

in the expansion of the X- exponent in (5.5) we can restrict ourselves to the first term from which

$$S(x,x_0) \approx P(x,x_0) + G(x)\int_{x_0}^{x}\frac{d}{d\eta}\begin{pmatrix}\varphi_+\varphi_- & \varphi_-^2\\ -\varphi_+^2 & -\varphi_+\varphi_-\end{pmatrix} d\bar{\beta}\ G^{-1}(x_0). \qquad (5.8)$$

In this expression the first term in the right hand side $P(x,x_0)$ yields usual connection formulae and the second one yields a correction to these formulae.

For large values of the argument η it is more convenient to express the matrices $P(x,x_0)$ and $G^{-1}(x_0)$ not in terms of functions $\varphi_\pm$ and $\dot{\varphi}_\pm$ but in terms of their combinations R , T , t - having simple asymptotic expansions (see, for ex., /5/)

$$R_\pm \backsim \sum_{m=0}^{\infty}\frac{i^m}{(2\eta)^m}\,\frac{(\frac{1}{3},m)\pm(\frac{2}{3},m)}{2}; \qquad T_\pm \backsim \sum_{m=0}^{\infty}\frac{(-i)^m}{(2\eta)^m}\,\frac{(\frac{1}{3},m)\pm(\frac{2}{3},m)}{2};$$

$$t_\pm \backsim \sum_{m=0}^{\infty}\frac{(\frac{1}{3},m)\pm(\frac{2}{3},m)}{2\cdot(2\eta)^m}; \qquad (\nu,m) = \frac{\Gamma(\nu+m+\frac{1}{2})}{m!\,\Gamma(\nu-m+\frac{1}{2})}. \qquad (5.9)$$

Then for $x > 0$, $x_0 < 0$ we have $\left(\xi = \eta(x),\ \eta = \eta(x_0)\right)$

$$P(x,x_0) = \bar{\gamma}\begin{pmatrix} e^{-i\frac{\pi}{4}} & 0\\ 0 & e^{i\frac{\pi}{4}}\end{pmatrix}\begin{pmatrix} R_+ & ie^{-2i\xi}\bar{R}\\ -ie^{2i\xi}R_- & \bar{R}_+\end{pmatrix}\begin{pmatrix} -T_-e^{2\eta}+\frac{i}{2}t_+ & T_+-\frac{i}{2}t_-e^{-2\eta}\\ -T_-e^{2\eta}-\frac{i}{2}t_+ & T_++\frac{i}{2}t_-e^{-2\eta}\end{pmatrix} \qquad (5.10)$$

$$G^{-1}(x_0) = \bar{\gamma}\sqrt{2\pi}\begin{pmatrix} -t_+ & t_-\cdot e^{-2\eta}\\ -\frac{2}{\sqrt{3}}T_-e^{2\eta} & \frac{2}{\sqrt{3}}T_+\end{pmatrix} \qquad (5.11)$$

$\bar{R}$ denotes a function complex conjugated with R) .

In most considerations only those elements of the matrices P , P^{-1} , S , S^{-1} which have a finite limit for $\eta \to \infty$ make sence. Meanwhile, the matrices P , S (as well as the matrices P^{-1} , S^{-1}) contain exponentially increasing elements. If we exclude these elements from the consideration then we obtain connection formulae which can be used either in passing from the region $v < 0$ to the region $v > 0$, or in the inverse transition only.

When using the increasing elements of the matrices S and S^{-1} it should be remembered that as follows from (5.8) these elements are very sensitive even to small non-linearity of the form of the potential.

6. Superbarrier Reflection

The superbarrier reflection has no analogue in the classical mechanics and consists in that a particle with positive kinetic energy can be reflected from the potential roughnesses. However, if pits and bumps of the potential have rather smooth slopes, then the reflection turns out to be, generally speaking, very small even for large ratio of v_{max} to v_{min} . When the ratio v_{max}/v_{min} is considerable the usual methods of approximate solution of the Schrödinger equation (1.1), for example, perturbation theory, lose efficiency . Then, the reflection coefficient is evaluated much simpler if one starts from the matrix Eq. (3.1).

The amplitude of the reflected wave (for given total current) is determined obviously by non-diagonal elements of the matrix $S(\infty,-\infty)$. So, if the current of particles fall from the left, then

$$F_2(-\infty) = S_{21}^{(-1)}(-\infty,\infty)\,F_1(\infty) = -S_{21}(\infty,-\infty)\,F_1(\infty). \qquad (6.1)$$

In order to calculate approximate calculation of the S -matrix it is convenient to break down the region where the potential is not constant into segments $[x_{i+1}, x_i]$ of such lengths that the elements of each of the matrix $S(x_{i+1}, x_i)$ would be well approximated by the first terms of series of (3.5)

$$S(x_{i+1},x_i) \approx \begin{pmatrix} 1 & \int_{x_i}^{x_{i+1}} e^{-2i\xi}\frac{1}{4}\,d\ln v \\ \int_{x_i}^{x_{i+1}} e^{2i\xi}\frac{1}{4}\,d\ln v & 1 \end{pmatrix} = \tau(x_{i+1},x_i) \qquad (6.2)$$

and then find product of matrices τ

$$S(\infty,-\infty) \approx \tau(\infty, x_{n-1}) \cdot \tau(x_{n-1}, x_{n-2}) \cdot \ldots \cdot \tau(x_1, -\infty). \tag{6.3}$$

An error of the non-diagonal elements of the matrices τ is easily calculated,

$$|S_{21} - \tau_{21}| \lesssim \left(\int_{x_i}^{x_{i+1}} \frac{1}{4} |d \ln v| \right)^2 \cdot \frac{1}{2} \max \left| \int_{x_i}^{x} e^{2i\xi} \frac{1}{4} d \ln v \right|, \tag{6.4}$$

where $x_i \leqslant x \leqslant x_{i+1}$. Thus, when the number of segments is moderate, the approximation (6.3) will be good, if for all chosen segments

$$\left| \int_{x_i}^{x_{i+1}} e^{2i\xi} \frac{1}{4} d \ln v \right| \gg \left(\int_{x_i}^{x_{i+1}} \frac{1}{4} |d \ln v| \right)^2 \cdot \frac{1}{2} \max \left| \int_{x_i}^{x} e^{2i\xi} \frac{1}{4} d \ln v \right|. \tag{6.5}$$

The number of segments n which is necessary to reach desirable relative accuracy c can be roughly estimated by formula

$$n \leqslant \frac{0{,}03}{c} \left(\int |d \ln v| \right)^2. \tag{6.6}$$

For example, for one-bumped potential with $v_{max}/v_{min} = 5$ and for the accuracy $c = 0.05 = 5\%$ we get $n = 6$.

If the condition (6.5) holds for the interval $(\infty, -\infty)$, then for the superbarrier reflection amplitude we get an estimate

$$-S_{21}(\infty,-\infty) \approx -\int_{-\infty}^{\infty} e^{2i\xi} \frac{1}{4} d \ln v, \tag{6.7}$$

which coincides up to notations and normalization with the formula (9) /1/. It should be stressed that expressions (6.5), (6.7) give a total solution of the problem of the superbarrier reflection and are not connected neither with perturbation theory nor with quasi-classical approximation.

7. Superbarrier Reflection in the Quasi-Classical Case

A high smoothness of the potential

$$\left|\frac{\Delta\lambda}{\lambda}\right| \approx |\lambda'| = \left|\frac{K'}{K^2}\right| \ll 1 \quad , \quad \left|\frac{K''}{K^3}\right| \ll 1, \tag{7.1}$$

which takes place in the quasi-classical case allows to achieve by means of a simple transformation of Eq. (1.1) the fulfilment of the condition (6.5) in the interval $(\infty, -\infty)$ even for the potentials with large ratio v_{max} / v_{min} . We make use of one of the Langer transformations [3]. We put

$$\psi = K^{-\frac{1}{2}} \bar{\psi}, \; x = h(y), \quad y = \xi(x), \tag{7.2}$$

where h is a function inverse to the phase ξ . Then Eq. (1.1) takes the form

$$\frac{d^2\bar{\psi}}{d y^2} + \bar{\psi}\left(1 + \frac{3}{4}\frac{K'^2}{K^4} - \frac{1}{2}\frac{K''}{K^3}\right) = 0, \tag{7.3}$$

where the prime $'$ denotes the derivative with respect to x . According to (7.1)

$$|\bar{v} - 1| = \left|\frac{3}{4}\frac{K'^2}{K^4} - \frac{1}{2}\frac{K''}{K^3}\right| \ll 1, \tag{7.4}$$

so that for the transformed potential $\bar{v}$ $\int |d \ln v| \ll 1$ and the condition of applicability of the formula (6.7) holds.

As an example we take a particular case considered by Pokrovsky et al [6] in which $v(x)$ is of the form

$$v(x) = (x - i\sigma)\, Q(x), \tag{7.5}$$

where $Q(x)$ is the analytical function having neither zeros nor singularities in the stripe

$$-\sigma < \mathrm{Im}\, x < \sigma + c \; , \quad c \gg 1. \tag{7.6}$$

The direct calculation [6] shows that $\bar{v}(y)$ has the form

$$\bar{v}(y) = 1 + \frac{5}{36}\frac{1}{(y - i\bar{\sigma})^2}\bar{Q}(y), \quad \bar{Q}(i\bar{\sigma}) = 1, \tag{7.7}$$

where $\bar{Q}(y)$ has no singularities on the stripe

$$-\bar{\sigma} < \operatorname{Im} y < \bar{\sigma} + \bar{c}, \quad i\bar{\sigma} = \xi(i\sigma), \quad i\bar{c} = \xi(ic). \tag{7.8}$$

From (7.4) it follows that in the quasi-classical case $\bar{\sigma} \gg 1$.

By inserting (7.7) into (6.7) and integrating over the contour closed in the upper half-plane we see that the singularities of the function $Q(y)$ give an exponentially small contribution which may be neglected if these singularities are not too numerous. By substituting a unit for $\bar{Q}(y)$ for the amplitude of the superbarrier reflection we have

$$R = -S_{21}(\infty, -\infty) =$$
$$= -\int \exp\left\{2i\int^{y}\left[1+\frac{5}{36}(z-i\bar{\sigma})^{-2}\right]^{1/2}dz\right\}\frac{1}{4}d\ln\left[1+\frac{5}{36}(y-i\bar{\sigma})^{-2}\right] = -ie^{-2\bar{\sigma}} \tag{7.9}$$

(the calculation of the integral (7.9) is discussed in the Appendix).

The same estimate for R has been obtained in [6] by means of the complicated summation of perturbation series and the comparison of the result with the known exact solution (for $V = 1 + \beta\, ch^{-2}(\alpha, x)$).

It should be mentioned that the papers by V. Pokrovsky et al [6,7] contain a wrong assertion that the formula (6.7) derived first by I.Goldman and A.Migdal [1] coincides with the first term of the perturbation series. In fact substitution of the Pokrovsky potential (7.7) into the integral (6.7) of Goldman and Migdal leads to the exact result (7.9), while the first term of the perturbation series for discussed example gives [6]

$$R \approx -i\frac{5}{18}\pi e^{-2\bar{\sigma}} = -i\ 0{,}87\, e^{-2\bar{\sigma}}.$$

In conclusion the author would like to express its deep gratitude to Ja.A. Smorodinsky for multiple discussions, S.S. Gerstein for the constant assistance during the work and L.D. Zastavenko for friendly encouragement at the early stage of work.

Appendix

The integral (7.9) can be easily calculated by expanding entering exponent square root in power series in β

$$\beta(z-i\bar{\sigma}) = \frac{5}{36}(z-i\bar{\sigma})^{-2}, \quad \sqrt{1+\beta} = 1+\frac{1}{2}\beta - \frac{1}{8}\beta^2 + \frac{1}{16}\beta^3 - \ldots, \tag{A.1}$$

and integrating this series term by term. In the lower half-plane (for any $\bar{\sigma}$) there is always a line on which the series

$$\frac{1}{2i} B(y - i\bar{\sigma}) = \frac{1}{2}\int^{y} \beta\, dz - \frac{1}{8}\int^{y} \beta^2 dz + \frac{1}{16}\int^{y} \beta^3 dz - \dots \qquad (A.2)$$

converges everywhere absolutely so that such a procedure is valid. Further we expand in power series $\exp B = 1 + B + \dots$. Calculating explicitly $\frac{d}{dy} \ln(1+\beta)$, we have

$$R = -\int e^{2iy}\left(1 + B + \dots\right)\left(-\frac{1/2}{y - i\bar{\sigma}} + \frac{1/4}{y - i\left(\bar{\sigma} + \frac{\sqrt{5}}{6}\right)} + \frac{1/4}{y - i\left(\bar{\sigma} - \frac{\sqrt{5}}{6}\right)}\right) dy. \qquad (A.3)$$

The expression (A.3) allows the integration term by term. Making the substitution $y - i\bar{\sigma} = x$ we have $R = -\rho \exp(-2\bar{\sigma})$, where ρ doesn't depend on $\bar{\sigma}$:

$$\rho = \int e^{2ix}\left(1 + B(x) + \dots\right)\left(-\frac{1/2}{x} + \frac{1/4}{x - i\frac{\sqrt{5}}{6}} + \frac{1/4}{x + i\frac{\sqrt{5}}{6}}\right) dx . \qquad (A.4)$$

It is easy to obtain a numerical value of the constant ρ which turns out to be equal to i . So, the first four terms of the series in B, β give:

$$\rho_0 = \int e^{2ix} d\ln(1 + \beta(x)) = i\pi\left(\mathrm{ch}\frac{\sqrt{5}}{3} - 1\right) = i \cdot 0{,}91$$

$$\rho_1 = \rho_0 + \int e^{2ix}\left(\frac{-i5}{36x}\right) d\ln(1+\beta) = i \cdot 0{,}997$$

$$\rho_2 = \rho_1 + \int e^{2ix}\left(\frac{5}{36}\right)^2\left(\frac{-1}{2x^2}\right) d\ln(1+\beta) = i \cdot 0{,}9998$$

$$\rho_3 = \qquad\qquad = i \cdot 0{,}999998 .$$

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Received by Publishing Department
on March, 8, 1961.