SOVIET PHYSICS JETP VOLUME 13, NUMBER 6 DECEMBER, 1961

ON THE PROBLEM OF ABOVE-BARRIER REFLECTION OF HIGH-ENERGY PARTICLES

V. L. POKROVSKII and I. M. KHALATNIKOV

Institute for Physics Problems, Academy of Sciences of the U.S.S.R.

Submitted to JETP editor December 16, 1960

J. Exptl. Theoret. Phys. (U.S.S.R.) **40**, 1713-1719 (June, 1961)

A regular method is given for calculating in the quasi-classical approximation the amplitude for above-barrier reflection of a particle from a one-dimensional potential barrier, by the use of the properties of the potential in the complex plane.

In a previous paper[1] an expression has been found for the amplitude for reflection of a particle from a one-dimensional potential barrier in the quasi-classical approximation, and it was shown that in cases in which the potential U is an analytic function which has no singularities on the real axis the reflection amplitude is exponentially small and can be put in the form of an iteration series in which all the terms are of the same order. This problem has been treated earlier in a number of papers.[2-4] In these papers, however, the authors confined themselves to only the first terms of the iteration series and consequently obtained an incorrect coefficient for the exponential. For this same reason the results found in references 3 and 4 for the three-dimensional problem of the scattering of high-energy particles by centers of force in the region of classically inaccessible angles are also incorrect.

The method of reference 1 is, however, extremely cumbersome. Although it provides an elucidation of the structure of the series, it requires a knowledge of the answer for some particular case. The purpose of the present note is to present a much simpler and more regular method for getting the amplitude for above-barrier reflection (without requiring previous knowledge of the answer for any particular case).

The present method, like the so-called Zwaan method,[5,6] is based on an investigation of the behavior of the wave function in the complex plane. Let U(x) be an analytic function of x which has no singularities on the real axis, and such that the particle energy $E > U(x)$ for all real x. We shall assume that the particle is quasi-classical:

$$kd \gg 1, \qquad k = \sqrt{2mE}, \tag{1}$$

where d is a characteristic dimension of the potential U(x).

The Schrödinger equation

$$d^2\psi/dx^2 + p^2\psi = 0, \qquad p^2 = 2m(E - U) \tag{2}$$

has a solution ψ_0 that behaves asymptotically like e^{ip_+x} for $x \to +\infty$. Then for $x \to -\infty$ the function ψ_0 behaves like $ae^{ip_-x} + be^{-ip_-x}$, where $p_\pm^2 = \lim p^2(x)$ for $x \to \pm\infty$, and a and b are constants. The reflection amplitude A is the ratio b/a.

It is well known that in the quasi-classical approximation considered here the equation (2) has approximate solutions of the form[7]

$$\psi_\pm = \frac{1}{\sqrt{p}} \exp\Big(\pm i \int_{\bar{x}}^{x} p\,dx\Big), \tag{3}$$

where $\bar{x}$ is an arbitrary lower limit. The solutions $\psi_\pm$ can be interpreted as waves traveling in opposite directions. The general solution can be represented in the form

$$\psi = a\psi_+ + b\psi_-, \tag{4}$$

where a and b are constants. This way of writing the function has meaning, however, only in cases in which the two terms in the right member of Eq. (4) are of the same order of magnitude, since the solutions themselves are inexact and the separation into waves traveling in different directions is defined only to the fractional accuracy $\sim 1/kd$.

The coefficients a and b take on exact meanings only for $x \to \pm\infty$, where $p(x) \to p_\pm = \text{const}$. In the case considered we have for $x \to +\infty$

$$a = \exp\Big[i \int_{\bar{x}}^{\infty} (p - p_+)\,dx - ip_+\bar{x} \Big], \qquad b = 0.$$

According to what has been said, as we go along the real axis the coefficient a remains unchanged to accuracy 1/kd, and b is everywhere not larger than order of magnitude 1/kd. For real x ($|x| \lesssim d$), however, the exact value of b is not defined. Therefore we cannot determine the value of b for $x \to -\infty$ by moving along the real axis.

The idea of the method is to leave the real axis and move in the complex plane along a line L on which the two waves are of the same order of magnitude. First of all it is clear that the condition

$$\operatorname{Im} \int^{x} p\,dx = \text{const} \tag{5}$$

must hold on the line L, since otherwise one of the exponentials will increase and the other will decrease. Furthermore, this line must pass through zeroes or singularities of the function p^2. In fact, otherwise the solutions ψ_+ will be correct to accuracy $1/kd$ along the entire line L and all of the difficulties still remain.

Thus we can try to find the coefficient b in the following way. We continue the solution that behaves like e^{ip_+x} for $\operatorname{Re} x \to +\infty$ away from the real axis into the upper half-plane of x until we get to the first line L that satisfies the stated condition. This can always be done, because the potential vanishes for $|x| \to \infty$. We then move along L to a zero or singularity x_0 of the function p^2. Near x_0 the solution ψ_+ with which we came to the point will be irregular, and we must "join it on" to the solution of the approximate equation obtained from Eq. (2) by expanding p^2 in powers of $x - x_0$. We then make the passage around the point x_0 that is necessary to get to the branch of L that goes toward $\operatorname{Re} x \to -\infty$. By moving along this branch and then going down to the real axis we get the coefficient b.

Let us begin with the case $U/E \lesssim 1$. In this case the simplest and most likely situation is that x_0 is a simple root of the function p^2. In analogy with the case of below-barrier reflection we shall speak of a complex "turning point," since x_0 satisfies the equation

$$U(x_0) = E. \tag{6}$$

Near x_0 we can write approximately

$$p = C\sqrt{x - x_0}; \qquad \int_{x_0}^{x} p\,dx = \tfrac{2}{3} C (x - x_0)^{3/2}. \tag{7}$$

It is obvious that the lines $\operatorname{Im} \int_{x_0}^{x} p\,dx$ go out from the point x_0 at angles of $2\pi/3$ with each other. Two of them are the branches of the curve L, as is shown in Fig. 1, which represents schematically the level lines of $\operatorname{Im} \int_{x_0}^{x} p\,dx$. Near x_0 Eq. (2) is of the form

$$\psi'' + C^2 (x - x_0)\,\psi = 0. \tag{8}$$

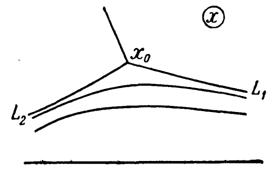

FIG. 1

The solution of this equation that goes over into the wave traveling "to the right" on the "right" branch L_1 takes the form

$$\psi = C\sqrt{x - x_0}\,H^{(1)}_{1/3}\left(\tfrac{2}{3} C (x - x_0)^{3/2}\right). \tag{9}$$

Using the well known asymptotic formulas for the Hankel functions, one can show that for $C(x - x_0)^{3/2} \gg 1$ the function (9) has the form

$$C\sqrt{x - x_0}\,H^{(1)}_{1/3}\left(\frac{2}{3} C (x - x_0)^{3/2}\right) \to \frac{1}{\sqrt{p}} \exp\left(i \int_{x_0}^{x} p\,dx - i\,\frac{5\pi}{12}\right). \tag{10}$$

This solution differs from ψ_0 by a constant factor. Since we are concerned only with the ratio $A = b/a$, the value of this factor is of no importance for what follows.

Let us now go over to the branch L_2; to do so we make a rotation by the angle $-2\pi/3$ and express the function $H^{(1)}_{1/3}$ on the branch L_2 in terms of its value and that of $H^{(2)}_{1/3}$ on L_1. To do so we use the relation (cf., e.g., reference 8)

$$H^{(1)}_{1/3}(e^{-i\pi} z) = H^{(1)}_{1/3}(z) + e^{-i\pi/3} H^{(2)}_{1/3}(z). \tag{11}$$

Using the asymptotic formulas for $H^{(1)}_{1/3}(z)$ and $H^{(2)}_{1/3}(z)$ for large positive z, we get on L_2

$$\psi = C\sqrt{x - x_0}\,H^{(1)}_{1/3}\left(\tfrac{2}{3} C (x - x_0)^{3/2}\right) \to \frac{1}{\sqrt{p}}\Big[\exp\left(-i \int_{x_0}^{x} p\,dx - i\,\frac{5\pi}{12}\right) + e^{-i\pi/3} \exp\left(i \int_{x_0}^{x} p\,dx + i\,\frac{5\pi}{12}\right)\Big]. \tag{12}$$

We see that on L_2 the two waves in fact are of the same order of magnitude and therefore can be distinguished. Their coefficients remain the same also for $\operatorname{Re} x \to -\infty$.

We still have to go over from functions of the type $\exp(\pm i \int_{x_0}^{x} p\,dx)$ to functions that behave like $\exp(\pm i p_- x)$ for $x \to -\infty$. To do this we use the obvious relations

$$\int_{x_0}^{x} p\,dx = p_- x - \varphi_0, \qquad \varphi_0 = \int_{-\infty}^{x_0} (p - p_-)\,dx + p_- x_0, \tag{13}$$

and thus get from Eq. (12)

$$\psi \to \frac{1}{\sqrt{p}}\left[e^{ip_- x} e^{-i(\varphi_0 + 5\pi/12)} + e^{-i\pi/3} e^{-ip_- x} e^{i(\varphi_0 + 5\pi/12)}\right]. \tag{14}$$

We emphasize that the coefficient of $\exp\left(i\int_{x_0}^{x} p\,dx\right)$ is not changed, since in the passage below the point x_0

$$\exp\left(i\int_{x_0}^{x} pdx\right) \gg \exp\left(-i\int_{x_0}^{x} pdx\right).$$

From Eq. (14) we find

$$A = b/a = -ie^{2i\varphi_0}. \tag{15}$$

It is not hard to extend this result to the case in which p^2 has at x_0 a singularity or zero of the form $p^2 = C^2(x-x_0)^{2\beta-2}$ (with $\beta > 0$). In this case the solution of the equation

$$\psi'' + C^2(x-x_0)^{2\beta-2}\psi = 0,$$

that goes over into a wave running to the right on L_1 has the form[8]

$$\psi = H^{(1)}_{1/2\beta}\left(\frac{C}{\beta}(x-x_0)^{\beta}\right) \to \frac{1}{\sqrt{p}}\exp\left\{i\int_{x_0}^{x} pdx - \frac{i\pi}{4}\left(\frac{1}{\beta}+1\right)\right\}.$$

The level lines of $\operatorname{Im}\int_{x_0}^{x} p\,dx = 0$ go out from x_0 at angles π/β with each other. Therefore in this case the passage from L_1 to L_2 is equivalent to a change of the argument of $(x-x_0)^{\beta}$ by $-\pi$. Using the general formula for rotation by $-\pi$

$$H^{(1)}_{\nu}(e^{-i\pi}z) = \frac{\sin 2\nu\pi}{\sin \nu\pi} H^{(1)}_{\nu}(z) + e^{-\nu\pi i} H^{(2)}_{\nu}(z)$$

and the asymptotic formulas for $H^{(1),(2)}(z)$, we get

$$A = -i\left(\sin\frac{\pi}{\beta} \Big/ \sin\frac{\pi}{2\beta}\right)e^{2i\varphi_0},$$

where φ_0 is defined by Eq. (13). For $\beta = 3/2$ we get the result already known.

If on the single line L there are not one but several singularities (on zeroes) $x_1, x_2, \ldots$ of the function p^2, their contributions to A are additive if the condition

$$\left|\int_{x_i}^{x_{i+1}} pdx\right| \gg 1 \tag{16}$$

is satified. If, on the other hand, the condition (16) is not satisfied, it is necessary to treat the equation with close-space singularities.

If we abstract from accidental coincidences, the situation with two close-spaced zeroes arises in the case of small values of the ratio $(E-U)/E$. In this case the energy of the particle is not much above the barrier, and near the point on the real axis of x at which U takes its maximum value there are two closely spaced complex conjugate roots of p^2. Here, however, there is no need to go off into the complex plane, since the line L

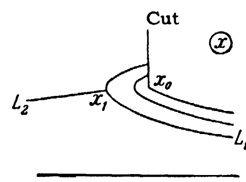

FIG. 2

coincides with the real axis. Physically this is associated with the fact that in this case the reflection coefficient is not small. This situation has been treated in detail earlier (cf. e.g., reference 6).

A zero and a pole are close together for small values of the ratio U/E. In fact, the potential U takes large values equal to E only in the complex plane near a singularity. Let us consider the case of a simple pole x_0, near which U(x) has the form

$$U(x) = U_0x_0/(x-x_0). \tag{17}$$

Then the root x_1 of the function $p^2 = 2m(E-U)$ is determined from the equation

$$x_1 = x_0(1 + U_0/E). \tag{18}$$

The condition for the zero and pole to be close together is

$$\left|\int_{x_1}^{x} pdx\right| \sim \left|\frac{U_0}{E}kx_0\right| \lesssim 1. \tag{19}$$

Near x_0 and x_1 we have

$$p^2 = k^2(x-x_1)/(x-x_0), \tag{20}$$

$$\int_{x_1}^{x} pdx = k\left[\sqrt{(x-x_0)(x-x_1)} - \frac{U_0x_0}{2E}\ln\left(\frac{x-x_0-(U_0x_0/2E)+\sqrt{(x-x_0)(x-x_1)}}{-U_0x_0/2E}\right)\right]. \tag{21}$$

The position of the level lines of $\operatorname{Im}\int^{x} p\,dx$ near x_0 and x_1 is shown schematically in Fig. 2. A cut is taken through the point x_0, which is a singular point of the Eq. (2). As L one can take, for example, the line $\operatorname{Im}\int_{x_1}^{x} p\,dx = 0$.* Its two branches L_1, L_2 are shown in Fig. 2. Obviously for $|x-x_0| \gg |x_1-x_0|$ the passage from L_1 to L_2 corresponds to a rotation through the angle $-\pi$.†

*At first glance it seems natural to take for L the line $\operatorname{Im}\int_{x_0}^{x} p\,dx = 0$. Unfortunately, however, this line has only one branch and does not go to infinity in one of the directions (cf. Fig. 2).

†We emphasize that in the case of the pole the results of going around above and below are not the same, since in going around above we cross the cut. In the case in which the point x_0 was a simple zero of p^2 the results of going around above and below coincided, since a simple zero of p^2 is not a singular point of the equation (2).

The solutions of the approximate equation*

$$\psi'' + k^2[(x - x_1)/(x - x_0)]\psi = 0 \quad (22)$$

are of the form

$$\psi = W_{\pm\lambda, 1/2}(\pm z), \qquad \lambda = -\tfrac{1}{2} ikx_0U_0/E,$$
$$z = -2ik(x - x_0), \quad (23)$$

where $W_{\lambda,\mu}$ are the Whittaker functions (cf. reference 8). The asymptotic formulas for the Whittaker functions for large $|z|$ are of the form

$$W_{\mu,\lambda} \sim e^{-z/2}z^{\lambda} \qquad (|\arg z| < \pi). \quad (24)$$

We see that for large values of $k(x - x_0)$ on the branch L_1

$$W_{\lambda,1/2}(z) \to E^{1/4}\exp\left(\lambda \ln\frac{\lambda}{e} + i\int_{x_1}^{x} pdx\right) \qquad \left(\arg z = -\frac{\pi}{2}\right). \quad (25)$$

On L_2 the second solution $W_{-\lambda,\frac{1}{2}}$ has the asymptotic formula

$$W_{-\lambda,1/2}(-z) \to E^{1/4}\exp\left(-\lambda \ln\frac{-\lambda}{e} - i\int_{x_1}^{x} pdx\right), \quad (26)$$

and we shall set $-\lambda = e^{-i\pi}\lambda$, $-z = e^{-i\pi}z$.

Equation (22) is noninvariant under change of sign of $(x - x_0)$, and therefore there is no linear connection between $W_{\lambda,\mu}(-z)$ and $W_{\pm\lambda,\mu}(\pm z)$. Equation (22) is, however, invariant under rotation through 2π around the point x_0. Therefore there does exist a linear connection between $W_{\lambda,\mu}(e^{-2\pi i}z)$ and $W_{\pm\lambda,\mu}(\pm z)$ (cf. reference 10):

$$W_{\lambda,\mu}(e^{-2\pi i}z) = e^{-2\pi i\lambda}W_{\lambda,\mu}(z) - \frac{2\pi i e^{-i\pi\lambda}}{\Gamma(1/2 + \mu - \lambda)\Gamma(1/2 - \mu - \lambda)}W_{-\lambda,\mu}(-z). \quad (27)$$

On L_2 the argument of z is $-3\pi i/2$. Therefore in the right member of Eq. (27) we have $\arg(\pm z) = \pm i\pi/2$. Using the asymptotic formulas (24) and going over, as in the case of the simple zero, to solutions that behave like $\exp(\pm ip_-x)$ for $x \to -\infty$, we get

$$A = F(\lambda)\exp\left\{2i\left[\int_{-\infty}^{x_1}(p - p_-)\,dx + p_-x_1\right]\right\}, \quad (28)$$

$$F(\lambda) = 2\pi i e^{-2\lambda\ln(-\lambda/e)}/\Gamma(-\lambda)\Gamma(1 - \lambda). \quad (29)$$

If $|\lambda| \sim U/\hbar v \gg 1$, then $F(\lambda) \approx -i$, and Eq. (28) goes over into Eq. (15). In the opposite case with $U/\hbar v \ll 1$ we have $F(\lambda) \approx -2\pi i\lambda$, and Eq. (28) gives the Born approximation:

$$A = -2\pi i\lambda e^{2ip_-x_0}. \quad (30)$$

Taking the square of the absolute value of the scattering amplitude (28), we get the reflection coefficient

$$R = |A|^2 = |F(\lambda)|^2\exp\left\{4i\,\mathrm{Im}\int_{-\infty}^{x_1} pdx\right\}. \quad (31)$$

In the one-dimensional case the formulas of Gol'dman and Migdal[3] and of Saxon and Schiff[4] give the same result

$$A = -2\pi i\lambda\exp\left\{2i\left[\int_{-\infty}^{x_1}(p - p_-)\,dx + p_-x_1\right]\right\}.$$

This differs from Eq. (28) by the replacement of the function $F(\lambda)$ by the quantity $-2\pi i\lambda$. As we have shown, this is correct only in the Born case $U/\hbar v \ll 1$. In the case $U/\hbar v \sim 1$ the results of references 3 and 4 are correct only in order of magnitude.

In conclusion the writers express their deep gratitude to L. D. Landau for helpful discussions.

*An analogous equation has been considered by Denisov[9] in connection with a different problem; in Denisov's case, however, unlike the present problem, the zero and pole were on the real axis, which decidedly alters the situation.

1 Pokrovskii, Savvinykh, and Ulinich, JETP **34**, 1272, 1629 (1958), Soviet Phys. JETP **7**, 879, 1119 (1958).

2 L. I. Schiff, Phys. Rev. **103**, 443 (1956).

3 I. I. Gol'dman and A. B. Migdal, JETP **28**, 394 (1954), Soviet Phys. JETP **1**, 304 (1955).

4 D. S. Saxon and L. I. Schiff, Nuovo cimento **6**, 614 (1957).

5 E. C. G. Stueckelberg, Helv. Phys. Acta **5**, 369 (1932).

6 E. C. Kemble, Phys. Rev. **48**, 549 (1935).

7 L. D. Landau and E. M. Lifshitz, Квантовая механика (Quantum Mechanics), Vol. 1, Gostekhizdat 1948, pp. 192-193. [Transl., Pergamon, 1958].

8 I. M. Ryzhik and I. S. Gradshteĭn, Таблицы интегралов (Tables of Integrals), Gostekhizdat, 1951.

9 N. G. Denisov, Радиотехника и электроника (Radio Engineering and Electron Physics) **4**, 388 (1959).

10 Higher Transcendental Functions, Bateman Manuscript Project, McGraw-Hill, 1953. H. Buchholz, Die confluente hypergeometrische Function, Springer-Verlag, 1953.

Translated by W. H. Furry
292