Phase functions for potential scattering in optics

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(Submitted 12 April 1993)
Usp. Fiz. Nauk **163**, 85–92 (July 1993)

Equations for the phase functions are presented in a form convenient for analyzing the solutions of both the Schrödinger equation and the problem of electromagnetic wave propagation in inhomogeneous media. It is shown how the problem of electromagnetic wave propagation in media with a real-valued dielectric constant (and, hence, the problem of above- and below-barrier transmission) reduces to one of calculating the phase for the potential scattering. One can then obtain not only such integrated characteristics as the coefficients of transmission and reflection but also exact expressions for the solution of the wave equation, in the form of quadratures containing the current ("instantaneous") value of the phase. The problem simplifies substantially for a layer symmetric with respect to the coordinate. It is shown that the method of phase functions gives an exact description of two opposite limiting cases, viz., the short-wavelength limit and Fresnel reflection, through a single simple analytical formula. A detailed discussion is given for above- and below-barrier reflection near the edge of the barrier.

1. INTRODUCTION

Many problems in quantum mechanics and the theory of electromagnetic wave propagation, including optics, reduce to solving a one-dimensional time-independent wave equation.[1,2] One of the most effective methods of qualitative study, which is based on the Liouville–Green representation (1838), was originally formulated in acoustics and optics and was then put in its modern form in quantum mechanics, where it is known as the quasiclassical (or WKBJ) approximation (see, e.g., Ref. 3). A number of exactly solvable problems in quantum mechanics, particularly those involving the transmission of particles through potential barriers, are intimately related to analogous exact solutions of optical problems,[1,2] although the physical interpretation of the same resulting formulas is, of course, different.[4] A typical example is the so-called nonreflecting Einstein layer. In optics a transmission coefficient of unity is interpreted as an analog of brightening through the use of a quarter-wave plate that is in phase for all wavelengths. In quantum mechanical problems of particle transmission above a potential well having one or several discrete levels, the same effect is explained as being due to quasiresonant scattering on a discrete level (to slowing of the motion of the particle above the well), which leads to quenching of the reflected wave.[4] From a mathematical standpoint these problems are simply identical: the reflection of a particle above a barrier (well) corresponds to the optics of transparent media, while below-barrier transmission corresponds to the physics of a plasma with "cold" electrons.

Meanwhile, the efficient methods that have been developed over the years in quantum mechanics can find natural application in optics as well. One such method is the variable phase approach[5–8] (which is called the "method of phase functions" in the Russian literature), by which one can most simply investigate the problem of potential scattering, with quantitatively accurate results achievable by extremely modest computational efforts.

Our goal in this article is to show how the problem of electromagnetic wave propagation in media with a real-valued dielectric constant (and, hence, the problem of above- and below-barrier transmission) reduces to one of calculating the phase for the potential scattering.[9,10] Here one can obtain not only such integrated characteristics as the coefficients of transmission and reflection but also an exact expression for the solution of the wave equation at all values of the coordinate in the form of quadratures containing the current ("instantaneous") value of the phase. The problem simplifies substantially for a layer that is symmetric with respect to the coordinate: in this case the total reflection (transmission) coefficient is expressed solely in terms of the difference of the asymptotic values of the phases, much as an element of the potential scattering matrix is expressed in terms of the asymptotic value of the phase. It is shown that the method of phase functions gives an exact description of two opposite limiting cases, the short-wavelength limit and Fresnel reflection, through a single simple analytical formula. A number of problems of importance for applications do not at present have exact solutions. We will give an exact solution for one of these: the problem of above- or below-barrier transmission near the edge of a barrier.

The subsequent exposition involves the solution of the second-order differential equation

$$(\mathrm{d}^2/\mathrm{d}x^2+p^2(x))y=0. \tag{1}$$

In quantum mechanical problems

 1063-7869/93/070621-07$10.00

$$p^2=(2m/\hbar^2)(E-U(x))=k^2-2V(x), \tag{2}$$

where E and U are the kinetic and potential energies, m is the reduced mass of the particle, and $\hbar$ is Planck's constant. In problems of electromagnetic wave propagation, Eq. (1) describes a monotonic wave with linear polarization perpendicular to the x axis:

$$p^2(x)=(\omega/c)^2\varepsilon(x,\omega)=k^2\varepsilon(x,\omega); \tag{3}$$

where ω is the frequency, c is the speed of light in vacuum, and ε is the dielectric function.

In both cases (2) and (3) the wave number is related to the wavelength (in vacuum) as $k=2\pi/\lambda$. In cases when it should be noted that we are discussing the radial Schrödinger equation, we will use the notation r for the independent variable.

2. PHASE EQUATION IN THE THEORY OF POTENTIAL SCATTERING

Let us give the derivations of the phase function method[5–8] that are required for our discussion; for simplicity we restrict consideration to s-wave scattering. The solution of the radial Schrödinger equation for $k^2\geqslant 0$ is constructed in the form

$$y(r)=\frac{A(r)}{k^{1/2}}\sin(kr+\delta(r)), \tag{4}$$

where $y(r)$ is the solution that is regular at the origin and the functions $A(r)$ and $\delta(r)$ are the current values of the amplitude and phase. For unique separation of the two functions we impose the following condition on the derivative of solution (4):

$$y'(r)=k^{1/2}A(r)\cos(kr+\delta(r)), \tag{5}$$

which, together with Eq. (1), leads to separate equations for the amplitude and phase:

$$A'/A=(V(r)/k)\sin(2kr+2\delta(r)), \tag{6}$$

$$\begin{aligned}&\delta'(r)=-(2V(r)/k)\sin^2(kr+\delta(r)),\\&\delta(0)=0.\end{aligned} \tag{7}$$

The amplitude equation (6) can be integrated in an elementary manner if the solution of the phase equation (7) is known, and the boundary condition (at zero) for the amplitude can, in principle, be arbitrary. The scattering matrix element and the partial amplitude are expressed through the relation

$$\begin{aligned}&S_\infty(k)=\exp(2i\delta(\infty)),\\&f_\infty=\frac{S_\infty(k)-1}{2ik},\end{aligned} \tag{8}$$

where $\delta(\infty)=\delta(k;r\to\infty)$ is the asymptotic value of the solution of phase equation (7). In the derivation of equations (6) and (7) it was assumed that $V(r)\to 0$ as $r\to\infty$. If the potential does not change sign the solution of phase equation (7) is a monotonic function, decaying in a repulsive field and increasing in an attractive field.

A notable property of the phase $\delta(r)$ is its stepped behavior for low-energy scattering of a particle above a potential well in which there are bound states. If the part of the well from the origin of coordinates (or from the left-hand turning point) to the value $r=r_1$ can accomodate a bound state, then in the immediate vicinity of this point the phase increases by π while remaining continuous. The next such increase occurs in the neighborhood of the next point $r=r_2$, corresponding to the second level in the well $V(r\leqslant r_2)$, etc. In the limit $k\to 0$ the asymptotic value of the phase is

$$\delta(k\to 0,\ r\to\infty)=\pi N, \tag{9}$$

where N is the total number of levels in the well (the Levinson theorem).[7,8]

The generalization of Eq. (7) for the case of orbital quantum numbers $l>0$ (Ref. 6) does not alter the above-listed properties of the solutions. Detailed studies with numerous examples are found in the monographs by Babikov[7] and Calogero.[8]

3. PROPAGATION OF ELECTROMAGNETIC WAVES IN INHOMOGENEOUS MEDIA

For this problem the boundary conditions are different from the case of potential scattering, and the approach must be modified accordingly. We assume that the dielectric function $\varepsilon(x,\omega)$ is real-valued and write the solution of equation (1) in the form

$$y(x)=p^{-1/2}[a(x)\exp(-iS(x))-b(x)\exp(iS(x))], \tag{10}$$

where the classical action

$$S(x)=\int_{x_i}^{x}p(z)\mathrm{d}z. \tag{11}$$

Imposing on the derivative y' the condition

$$\begin{aligned}y'(x)=-ip^{1/2}[&a(x)\exp(-iS(x))\\&+b(x)\exp(iS(x))],\end{aligned} \tag{12}$$

we obtain a linear system of first-order differential equations[11]

$$a'(x)=-q(x)\exp(2iS(x))b(x), \tag{13a}$$

$$b'(x)=-q(x)\exp(-2iS(x))a(x), \tag{13b}$$

where we have used the notation

$$q(x)=p'/2p=\varepsilon'/4\varepsilon. \tag{14}$$

For real values of x and $p^2(x)\geqslant 0$ the symmetry properties of this system imply the flux conservation law

$$|a(x)|^2-|b(x)|^2=\text{const}, \tag{15}$$

where the constant is zero in the potential scattering problem: the amplitudes of the incident and reflected waves are equal in modulus. In the wave propagation problem we will use a normalization in terms of the transmitted wave (from right to left), which corresponds to the following initial conditions at the point $-x_0$ ($-x_0>-\infty$):

$$|a(-x_0)|=1, \quad b(-x_0)=0. \tag{16}$$

In this case the constant on the right-hand side of relation (15) is equal to unity. As the new independent variable we introduce the reflection function

$$R(x)=b(x)/a(x); \tag{17}$$

which satisfies the Riccati equation[12]

$$R'(x)=-q(x)\exp(-2iS(x)) + q(x)\exp(2iS(x))R^2(x), \tag{18}$$

$$R(-x_0)=0. \tag{19}$$

We now obtain a phase equation and express the solution of the problem in terms of the phase function. We note that for the partial solutions of equation (18) it has the form

$$R^{(1)}=\exp(2i\theta(x)), \tag{20}$$

which leads to the phase equation

$$\theta'(x)=q(x)\sin(2S(x)+2\theta(x)). \tag{21}$$

A natural initial condition is

$$\theta(x_i)=0, \tag{22}$$

where x_i is the lower limit in the integral for the eikonal (11), i.e., one has $S(x_i)=0$. This is essential in the case when there is a turning point $p^2(x_i)=0$, and it simplifies the analysis in all the remaining cases, for which the choice of the point x_i can be arbitrary.

Phase equation (21) is distinguished from the standard phase equation (7) both in its outward appearance and in a number of important properties (rapid convergence of the solutions, the absence of jumps in phase[9,10]). However, the substitution

$$k\,\mathrm{tg}(S(x)+\theta(x))=p(x)\mathrm{tg}(kx+\delta(x)) \tag{23}$$

brings (21) to the form (7) and *vice versa*. Thus Eq. (21) is one of the forms of the phase equations of potential scattering theory. Its coefficients are the logarithmic derivative of the refractive index $[p(x)=kn(x)=k(\varepsilon(x))^{1/2}]$ and the eikonal.

The solution of the equation for the reflection function (18) with boundary condition (19) can be written in the form

$$R(x)=z^{-1}(x)+\exp(2i\theta(x)), \quad R(-x_0)=0, \tag{24}$$

which, upon substitution into (18) gives a linear first-order differential equation that can be solved in quadratures. After some rather simple calculations we obtain

$$R(x)=-\frac{(\mathrm{sh}\,f(x)-iJ(x))\exp(i\theta(x))}{(\mathrm{ch}\,f(x)+iJ(x))\exp(-i\theta(x))}=\frac{b(x)}{a(x)}, \tag{25}$$

where

$$f(x)=\int_{x_0}^{x} q(u)\cos(2S(u)+2\theta(u))\mathrm{d}u, \tag{26}$$

$$J(x)=\exp(-f(x)) \times \int_{-x_0}^{x} \exp(2f(u))q(u)\sin(2S(u) +2\theta(u))\mathrm{d}u. \tag{27}$$

Here θ is a solution of phase equation (21). The reflection function (26) is written in a form in which the denominator is the incident (transmitted) wave and the numerator is the reflected wave. For $\varepsilon(x)>0$ we easily find from (25) that

$$|a(x)|^2-|b(x)|^2=1$$

in accordance with the flux conservation law (15). Thus the phase function $\theta(x)$ yields a complete description of the solution of wave equation (1) in the problem of electromagnetic wave propagation in plane-layered media.

A phase equation of the type (21) has been used in mathematical papers[13] on the study of the positions of the zeros of the partial solutions of linear differential equations (1) with $p^2(x)>0$. The equation for the current in a circuit consisting of series-connected resistor and superconductor with a tunneling contact[14] is of the same type as (21).

Exact analytical solutions of phase equations (21) and (7) are easily obtained if the dielectric function (or the potential energy) is a set of rectangular wells and barriers, and also in the case $\varepsilon(x)=Dx^{-2}$, where D is a constant. In this case the functions $p^2(x)=k^2\varepsilon(x)$ can be positive, negative, or complex.

Since the functions $\theta(x)$ in (21) and $\delta(x)$ in (7) are the phases of regular wave functions in the problem of potential scattering, it follows from the definitions in Eqs. (10)–(12) for $|a(x)|=|b(x)|$ and from Eqs. (4) and (5) that

$$\theta(x)=\mathrm{arctg}(p(x)y(x)/y'(x))-S(x), \tag{28}$$

$$\delta(x)=\mathrm{arctg}(ky(x)/y'(x))-kx. \tag{29}$$

Thus the phase θ is the difference between the exact phase of the wave function and the eikonal (i.e., the value of the phase in the WKBJ approximation), while the phase δ contains the entire difference from the plane wave. In cases when the solutions of equation (1) can be expressed in well-known special functions, formulas (28) and (29) yield exact values of the phases, a circumstance which is especially important in the neighborhood of singular points in the complex plane. In the remaining cases Eqs. (7) and (21) must be solved by numerical methods, as can be done very simply nowadays.

Let us consider two limiting cases in the problem of electromagnetic wave propagation. In the short-wavelength limit, $k\gg 1$, it is natural to treat the dielectric function as an analytical function in the complex plane $z=x+iy$. It is well known[2] that the coefficient of reflection in this case is exponentially small, and the correct value of the exponent follows directly from the Riccati equation (18) already in the first approximation. The problem here is the pre-exponential factor, which is easily determined

only in the case of isolated singularities. For example, in the presence of only one zero of order α in the z plane,

$$p(z)\approx(z-z_0)^\alpha \quad \text{for } |z-z_0|\ll 1, \tag{30}$$

formula (26) with $-x_0=-\infty$, $x=+\infty$, taken jointly with Eq. (28), leads to the following result:

$$|R(+\infty)|=2\sin\frac{\pi\alpha}{2(1+\alpha)}\times\exp\left(-2\,\mathrm{Im}\int_0^{z_0}p(z)\mathrm{d}z\right), \tag{31}$$

which agrees with the known result,[7] which is a generalization of the Pokrovskiĭ–Khalatnikov formula. In the case of more than two singularities of the function $p(z)$ (if they cannot be treated as isolated) there are at present no systematic rigorous analytical or numerical results. We will consider the solution of this problem in Sec. 5.

In the long-wavelength limit $k^{-1}\gg d_0$, where d_0 is the characteristic distance for changes in the refractive index, we arrive at Fresnel reflection. Suppose that the dielectric function has the following step-like behavior:

$$\varepsilon(x,k)=\varepsilon_1=\text{const} \quad \text{for } x\leqslant x_\mathrm{i},$$

$$\varepsilon(x,k)=\varepsilon_2=\text{const} \quad \text{for } x\geqslant x_\mathrm{i}+\Delta x,$$

$$k(\varepsilon_1^{1/2}+\varepsilon_2^{1/2})\Delta x\ll 1,$$

i.e.,

$$\int_{x_\mathrm{i}}^{x_\mathrm{i}+\Delta x} p\,\mathrm{d}x\to 0,$$

and that inside the interval Δx the derivative of the function $p(x)$ exists and can have an arbitrarily large amplitude (in absolute value). In this case, phase equation (21) has the form

$$\theta'(x)=(p'/2p)\sin(2S(x_\mathrm{i})+2\theta(x)), \tag{32}$$

and its exact solution is

$$\mathrm{tg}(S(x_\mathrm{i})+\theta(x))=(p(x)/p(x_\mathrm{i}))\times\mathrm{tg}(S(x_\mathrm{i})+\theta(x_\mathrm{i})). \tag{33}$$

If the eikonal and phase are measured from the point x_i (i.e., $S(x_\mathrm{i})=0$, $\theta(x_\mathrm{i})=0$), we obtain $\theta(x_\mathrm{i}+\Delta x)=0$. Then the integral J in (27) is zero, and the reflection coefficient (25) takes the form

$$R(x_\mathrm{i}+\Delta x)=-\mathrm{th}\int_{x_\mathrm{i}}^{x_\mathrm{i}+\Delta x}\frac{p'(x)}{2p(x)}\mathrm{d}x=\frac{\varepsilon_1^{1/2}-\varepsilon_2^{1/2}}{\varepsilon_1^{1/2}+\varepsilon_2^{1/2}}=\frac{n_1-n_2}{n_1+n_2}, \tag{34}$$

which agrees with the Fresnel formula for normal incidence. It is important to note that in this derivation the quantity $\theta(x)$ can be real or complex.

Let us add one more step in the dielectric function:

$$\varepsilon(x,k)=\varepsilon_3 \quad \text{for } x>x_\mathrm{f}+\Delta x,$$

$$x_\mathrm{f}-x_\mathrm{i}=l.$$

In passing through the point x_f the phase increment (33) is not equal to zero, since $S(x_\mathrm{f})\neq 0$. The transition J in formula (25) is also nonzero for arbitrary values of ε_2 on the segment l. Since all the results in the case of two (or more) steps are expressed as before in elementary form, one can verify directly that the coefficient of reflection goes to zero, $R(x_\mathrm{f}+\Delta x)=0$, when the following two conditions hold:

$$\varepsilon_2=(\varepsilon_1\varepsilon_3)^{1/2},\quad 2\varepsilon_2^{1/2}kl=\pi(1+2N),\quad N=0,1,2,\ldots.$$

The second condition is usually written in the form

$$l=(1+2N)\lambda_2/4,$$

where $\lambda_2=\lambda/n_2$ is the wavelength in medium ε_2. Consequently, we have an exact description of optical brightening through the use of a quarter-wave plate.

It is interesting to note that the results[9,10] presented here differ from the results obtained using a simple interpolation formula[12] (see also Ref. 2) only in that the exact value is obtained for the pre-exponential factor in formula (31). This is an additional consequence of the fact that the phase θ, which was neglected completely in Ref. 12, is ordinarily small compared to the eikonal.

For a symmetric layer, when $\varepsilon(-x)=\varepsilon(x)$, the natural origin for the eikonal and phase is the point $x_\mathrm{i}=0$. In this case, for transmission through the entire layer, i.e., over the interval $[-x_0,x_0]$ ($|x_0|\leqslant\infty$), integral (26) goes to zero, and formula (25) becomes[10]

$$R(x_0)=\frac{iJ(x_0)}{1+iJ(x_0)}\exp(2i\theta(x_0)), \tag{35}$$

where $J(x_0)$ is determined by integral (27) with an upper limit of x_0. This formula is useful for making analytical estimates, since the exact solutions of phase equation (21) are not subject to the Stokes phenomenon near singular points of the eikonal, unlike the asymptotic series of the WKBJ method, which are obtained far from any singularities.[15] However, for a symmetric layer the following approach is a more interesting one.

4. SYMMETRIC LAYER

For a symmetric layer

$$\varepsilon(-x,k)=\varepsilon(x,k),\quad \varepsilon'(-x,k)=-\varepsilon'(x,k)$$

we consider reflection on the interval $[-x_0,x_0]$ ($|x_0|\leqslant\infty$) with the initial condition $R(-x_0)=0$, and we measure the eikonal and the phase from the origin. In this case the eikonal (11) and phase (21) are odd functions:

$$S(-x)=-S(x),\quad \theta(-x)=-\theta(x). \tag{36}$$

Together with (20), we introduce a second partial solution of the Riccati equation (18):

$$R^{(1)}=\exp(2i\theta(x)),\qquad R^{(2)}=-\exp(2i\phi(x)), \tag{37}$$

and obtain two independent phase equations

$$\theta'(x)=q(x)\sin(2S+2\theta),\quad \theta(0)=0, \tag{38a}$$

$$\phi'(x)=-q(x)\sin(2S+2\phi),\quad \phi(0)=0, \tag{38b}$$

where

$$q=p'/2p=\varepsilon'/4\varepsilon,$$

which have different solutions under the given initial conditions.

The functions $R^{(1)}$ and $R^{(2)}$ in (37) are the ratios of the partial solutions of the following system of linear first-order differential equations (13a) and (13b):

$$a_1=m\exp(-i\theta),\quad b_1=m\exp(i\theta), \tag{39a}$$

$$a_2=n\exp(-i\phi),\quad b_2=-n\exp(i\phi). \tag{39b}$$

In addition to the phase equations (38), system (13) also gives the amplitude equations

$$m'=-mq\cos(2S+2\theta),\quad m(0)=1, \tag{40a}$$

$$n'=nq\cos(2S+2\phi),\quad n(0)=1, \tag{40b}$$

the solutions of which are even functions:

$$m(-x)=m(x),\quad n(-x)=n(x). \tag{41}$$

The reflection function has the form

$$R(x)=\frac{b(x)}{a(x)}=\frac{b_1(x)+Cb_2(x)}{a_1(x)+Ca_2(x)}, \tag{42}$$

where the constant C is determined from the initial condition

$$|a(-x_0)|=1,\quad b(-x_0)=0. \tag{43}$$

For reflection from the entire symmetric layer, one obtains[9] by simple algebra

$$R(x_0)=-i\sin(\theta(x_0)-\phi(x_0))\times\exp(i\theta(x_0)+i\phi(x_0)). \tag{44}$$

The corresponding transmission coefficient is given by

$$T(-x_0)=a(-x_0)/a(x_0)=\cos(\theta(x_0)-\phi(x_0))\times\exp(i\theta(x_0)+i\phi(x_0)). \tag{45}$$

For transparent media we have

$$|R|^2+|T|^2=1. \tag{46}$$

There are two nontrivial conclusions of interest. First, the results of the electromagnetic wave propagation problem are expressed solely in terms of the asymptotic values of the phases, just as in potential scattering theory. Second, the reflection coefficient is zero when the phase difference satisfies

$$\theta(x_0)-\phi(x_0)=\pi N,\quad N=0,\pm1,\pm2,\pm3\ldots. \tag{47}$$

A study of phase equations (38) shows[9,10] that their solutions do not exceed $\pi/4$ in absolute value in transparent media, i.e., $N=0$ is the only possible value. The values $N=\pm1$ can arise at optical analogs of a turning point ($\varepsilon\to0$) and at singularities of the type $\varepsilon\to\infty$.

For analysis of the convergence of the procedure used for numerical solution of phase equations (38a) and (38b), the reflection coefficient was calculated[9] according to formula (44) in the case of a completely nonreflecting layer for all values of k at $x_0\to\infty$:

$$k^2\varepsilon(x,k)=p^2(x)=k^2+2B[\mathrm{ch}(\beta x)]^{-2}, \tag{48a}$$

$$B/\beta^2=[(2N+1)^2-1]/8,\quad N=1,2,3\ldots. \tag{48b}$$

This is what is called a symmetric Einstein layer.[4] Its quantum mechanical analog[1,4] is the reflection of a particle above a well (48a) containing discrete levels (48b). The results of the calculations[9] show that phase difference (47) converges rapidly and monotonically to zero for values of the dimensionless parameter $x_0\beta>5$. Thus only the whole layer ($x_0\to\infty$) is nonreflecting. Any finite part of it on a bounded interval $(-x_0,x_0)$ has a small but finite reflection. This is not very important for applications: for $0.1\leqslant k\leqslant1$ and $10\leqslant x_0\beta\leqslant20$ the coefficient of reflection from a layer cut off at points $\pm x_0$ does not exceed 10^{-5}.

Formulas (44) and (45) together with the phase equations (38) provide an extremely simple way of solving direct problems of electromagnetic wave propagation and above-barrier reflection in the symmetric case.

5. TRANSMISSION OF A PARTICLE THROUGH A SYMMETRIC POTENTIAL BARRIER

From a mathematical standpoint this problem is equivalent to the problem of electromagnetic wave propagation. For modern applications[16] the situation in which the kinetic energy of the particle is close to the height of the barrier is of greatest interest. This gives rise to two closely spaced zeros of the function $p^2(x)$ in (2)—turning points on the real axis x in the case of below-barrier transmission or two complex conjugate zeros for above-barrier transmission. These zeros of $p(x)$ coalesce when the kinetic energy is exactly equal to the potential energy. To calculate the transmission coefficient in this case a parabolic layer (an "inverted" linear oscillator)[4] is used, which permits description of a situation with two closely spaced and coalescing zeros. If the kinetic energy of the particle is specified, it is necessary to cut off the parabolic layer with respect to height. That this leads to unsatisfactory results has long been noted in optics (see Ref. 2), especially for a thin layer (the results of the previous Section show that the reflecting layer can also turn out to be extremely sensitive to the procedure for cutting off the layer with respect to width, and to obtain an accurate result it is necessary to take a rather wide interval $(-x_0,x_0)$; this cannot be done for a parabolic layer at a specified kinetic energy). To sum up what we have said, we note that both the well-known quasiclassical solution of Kemble[4,15] and the comparison-equation method with a parabolic layer[2,4] give the following values for the transmission and reflection coefficients

$$|T|^2=|R|^2=1/2, \tag{49}$$

if the kinetic energy of the particle is equal to the barrier height. The known exact solution of the problem for a symmetric barrier,[1,4]

$$p^2(x)=k^2-2B[\mathrm{ch}(\beta x)]^{-2}, \tag{50}$$

demonstrates that result (49) is applicable if

$$k^2/\beta^2=2B/\beta^2\gg 1, \tag{51}$$

i.e., if the conditions of quasiclassical motion are satisfied.

This conclusion is based on the behavior of the function

$$S(x)=\int^x p\mathrm{d}x$$

in the complex plane. Under the quasiclassical conditions the analytical singularities of the action (eikonal), i.e., branch points at zeros and poles of the function $p^2(x)$, are isolated and can be considered separately. Two coalescing zeros (or poles) can still be treated by modifications of the WKBJ method.[15,17] This is just the case corresponding to the parabolic layer approximation. When there are three such singularities (two turning points and a pole in the complex plane) the WKBJ method is applicable only in the quasiclassical region. For larger numbers of closely spaced singular points the quasiclassical approximation does not apply, and there are no comparison equations solvable in known special functions (the hypergeometric equation of Gauss corresponds to three singular points[3,4]).

To study such problems we use the method of phase equations, which we shall solve numerically. We note beforehand that the phase functions (38a) and (38b) used in the symmetric case have imaginary-valued functions for the action $S(x)$ and phase $\theta(x)$ and $\phi(x)$; this is unimportant for the overall analysis but causes certain difficulties in numerical calculations. Taking into account that the turning points $p^2(x)=0$ are generally not singular points of the initial wave equation (1), we make the change of phase variables (23):

$$k\,\mathrm{tg}(S(x)+\theta(x))=p(x)\mathrm{tg}(kx+\delta(x)), \tag{52a}$$

$$k\,\mathrm{ctg}(S(x)+\phi(x))=p(x)\mathrm{ctg}(kx+\gamma(x)), \tag{52b}$$

i.e., we go over to the standard phases for potential scattering (7). Substituting (52) into (38), we obtain

$$\delta'(x)=-(2V(x)/k)\sin^2(kx+\delta(x)),\quad \delta(0)=0, \tag{53a}$$

$$\gamma'(x)=-(2V(x)/k)\cos^2(kx+\gamma(x)),\quad \gamma(0)=0, \tag{53b}$$

where

$$-2V(x)=p^2(x)-k^2,\quad k^2>0,$$

i.e., equations with real coefficients over the entire domain of definition, including below-barrier transmission. Repeating steps (39)–(43) with allowance for (6) and (7), we arrive at expressions for the coefficients of transmission and reflection in the case of a symmetric barrier:

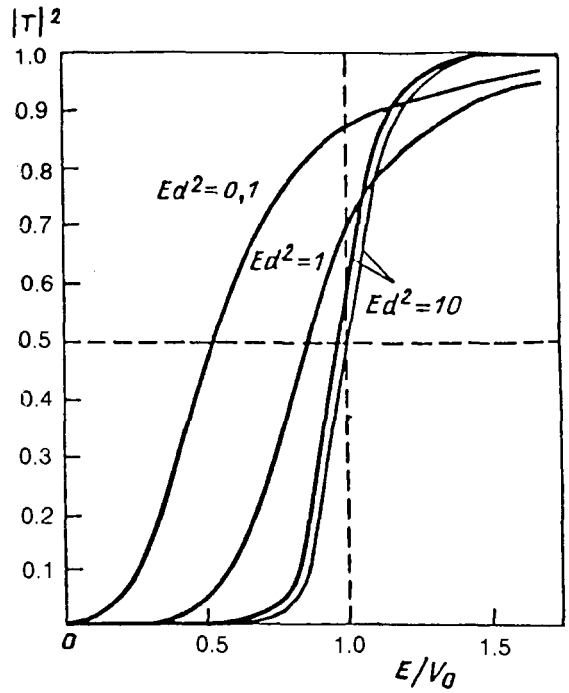

FIG. 1. Coefficient of transmission of the potential barrier given above Eq. (56) as a function of the particle energy E (in units of the barrier height V_0) for various values of Ed^2. The curve drawn with a fine line is the result calculated by the Kemble formula (57).

$$T(-x_0)=\cos(\delta(x_0)-\gamma(x_0))\times\exp(i\delta(x_0)+i\gamma(x_0)), \tag{54}$$

$$R(x_0)=-i\sin(\delta(x_0)-\gamma(x_0))\times\exp(i\delta(x_0)+i\gamma(x_0)), \tag{55}$$

with

$$|R|^2+|T|^2=1.$$

We note that formulas (54) and (55) are equivalent to the results (44) and (45), as follows, in particular, from an analysis of formulas (28) and (29).

Let us discuss the results of a demonstrational calculation for the potential

$$V(x)=V_0d^2/(x^2+d^2).$$

The coefficient of equation (1) is given by

$$p^2(x)=k^2-2V_0\,d^2(x^2+d^2)^{-1} \tag{56}$$

and has four singular points (for the WKBJ method): poles $x_p=\pm id$ and zeros $kx_i=\pm(2V_0-k^2)^{1/2}d$, which lie on the real axis in the case of below-barrier transmission and on the imaginary axis in the above-barrier region. When the kinetic energy is equal to the barrier height the zeros coalesce at the origin.

Phase equations (53), which do not have any singularities, were solved by the Runge–Kutta method. The results of the calculation for the transmission coefficient for an infinite interval ($x_0\to\infty$) are shown in Fig. 1. It is seen

that even at extremely large values of the parameter $ka(V_0/E) \gg 1$ the Kemble formula for the below-barrier region and up to the edge of the barrier,

$$|T|^2 = \left[1 + \exp\left(2\,\mathrm{Im} \int_{-x_i}^{x_i} p(x)\mathrm{d}x\right)\right]^{-1}, \qquad (57)$$

which is the same result as for the parabolic layer model,[3,4,7] appreciably understates the exact value. This is also true for the above-barrier case, where the Kemble approximation and the solution of comparison equations also have well-known forms[2,3,4,17] which we will not give here. At lower energies the model approximations describe the exact results only in the two limiting cases $|T|^2 \to 0$ and $|T|^2 \to 1$ and differ substantially from them everywhere else, including on approach to the edge of the barrier, $k^2 \approx 2V_0$. We note that in this region the exact values are always larger than the values calculated in the Kemble approximation.

In barrier problems the absence of any sort of phase jumps like those established by the Levinson theorem greatly simplifies making direct numerical calculations.

6. CONCLUSION

The above treatment indicates that the method of phase functions is promising for applications in regions where it has not traditionally been employed. The procedure for such applications is extremely simple: problems involving the solutions of linear second-order differential equations reduce to the problem of potential scattering, for which the phase equation that is formulated is easily solved by numerical methods. The forms of the phase equations can be different, but they are all interrelated by identity transformations that follow simply from the equation of continuity of the logarithmic derivative of the solution of the initial equation. The phase equations are a particular case of Riccati equations to which the initial linear differential equation reduces. Nonlinear equations are generally more informative in this case: they enable one to establish the general form of the desired solution, which is extremely stable against changes in the physical parameters. The approach described here can be used to analyze the propagation of electromagnetic waves in absorbing (or amplifying) media and also barrier problems with a complex potential.

One of the authors (L. P. P.) wishes to thank V. L. Ginzburg and I. I. Sobel'man for their interest in this field of study and for some stimulating discussions. Both authors thank the participants in the seminars led by V. L. Ginzburg, I. L. Fabelinskiĭ, and N. B. Delone for constructive discussions.

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Translated by Steve Torstveit