REFLECTION FROM A BARRIER IN THE QUASI-CLASSICAL APPROXIMATION

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The asymptotic expression for the coefficient of reflection from a one-dimensional potential barrier has been found for the case when the wavelength is much smaller than the characteristic dimensions of the barrier.

1. STATEMENT OF THE PROBLEM

THE determination of the reflection coefficient for the case when the de Broglie wavelength λ is commensurable with the characteristic dimensions of the potential barrier is a very complicated mathematical problem, which has been solved only in rare cases. For short wavelengths the Schrödinger equation is usually solved using the well-known Wentzel-Kramers-Brillouin (WKB) method, which in general gives no reflection.

The task of this paper is to find an asymptotic expression for the reflection coefficient for small wavelengths. We consider only the one-dimensional case.

The problem consists in solving the Schrödinger equation:

$$\alpha^2 \frac{d^2\psi}{d\xi^2} + k^2(\xi)\psi = 0, \tag{1.1}$$

where

$$\alpha = \lambda\!\!\!^{-}/a; \quad \xi = x/a; \quad k^2(\xi) = 1 - U(\xi)/E; \tag{1.1a}$$

$\lambda\!\!\!^{-}$ is the de Broglie wavelength of the free particle; a denotes the extent of the region where $U(\xi)$ changes significantly; E is the energy of the particle. Our fundamental assumption is

$$\alpha \ll 1. \tag{1.2}$$

In the following we shall always restrict ourselves to the case $E > U(\xi)$ on the entire ξ axis.

According to the familiar WKB method, the solution of Eq. (1.1) is sought in the form

$$\psi = e^{S/\alpha} \tag{1.3}$$

and S is expanded into a power series in α. The zeroth and first approximations give

$$\psi = \frac{1}{\sqrt{k}} \exp\left\{\frac{i}{\alpha}\int^{\xi} k\,d\xi\right\}. \tag{1.4}$$

The next corrections are small quantities of higher order in α and change the phase and the amplitude of solution (1.4) only insignificantly. For $\xi \to \pm\infty$ solution (1.4) goes over into $A_{\pm}\exp\{ik_{\pm}\xi/\alpha\}$ asymptotically, i.e., into a plane wave going in only one direction at both ends of the straight line ($k_{\pm} = \lim k(\xi)$, $\xi \to \pm\infty$).

In the WKB approximation the quantum effect of the reflection from a potential barrier is thus completely absent.

The reason for this lies in the fact that in the WKB method the function S is expanded into an asymptotic series in powers of α, and the method by its very nature, cannot take into account the reflection effect, which, for small α, has an amplitude of order $\exp(-A/\alpha)$ $(A > 0)$. In order to find the reflection of the wave we must therefore change the method.

We introduce the variable t:

$$\alpha t = \int^{\xi} k\,d\xi \tag{1.5}$$

and make the transformation

$$\psi = y/\sqrt{k}. \tag{1.6}$$

Equation (1.1) takes the form

$$\frac{d^2y}{dt^2} + (1 + \alpha^2 q(\alpha t))\,y = 0, \tag{1.7}$$

where q is determined by k through the relation

$$q = \frac{3(k')^2 - 2kk''}{4k^4}. \tag{1.8}$$

(The prime denotes differentiation with respect to ξ.)

We formally apply to Eq. (1.7) the perturbation theory for the continuous spectrum. It turns out that all the terms in the perturbation expansion have the same order of smallness in α.

2. CALCULATION OF THE REFLECTION COEFFICIENT

Our task is to find the amplitude for transition from the eigenstate of the Hamiltonian $H_0 = d^2/dt^2$ with momentum 1 to the state with momentum -1. This amplitude is expressed with the help of the well-known perturbation expansion

$$R = \frac{1}{2i}\left[V_{-1,1} + \frac{1}{2\pi}\int \frac{V_{-1,k}V_{k,1}}{1-k^2}\,dk + \frac{1}{(2\pi)^2}\iint \frac{V_{-1,k_1}V_{k_1,k_2}V_{k_2,1}}{(1-k_1^2)(1-k_2^2)}\,dk_1\,dk_2 + \ldots\right], \tag{2.1}$$

where $V_{k,k'}$ is the matrix element of the "perturbation" $V = \alpha^2 q$. The path of integration over k_i in formula (2.1) is taken along the real axis, circumventing the singular points $k_i = -1$ and $k_i = 1$ above and below the axis respectively. It will be shown in the Appendix that only a slight error is introduced if the path of integration is taken along the real axis without the by-passes.

We calculate the matrix element $V_{k,k'}$. We have

$$V_{k,k'} = -\alpha \int_{-\infty}^{\infty} \exp\left\{\frac{i}{\alpha}(k'-k)\tau\right\} q(\tau)\,d\tau. \tag{2.2}$$

We investigate the singularities of the function $q(\tau)$ in the complex plane τ. It follows from (1.8) that the singularities of $q(\tau)$ coincide with the roots and singularities of the function $k^2(\xi)$. We restrict ourselves to the case where the singular point τ_0 whose imaginary part has the smallest absolute value corresponds to a simple root. Clearly, this situation holds precisely for not too large energies E. The case where the term making the main contribution to the reflection coefficient involves a simple pole of $k^2(\xi)$ is treated analogously and leads to the same result.

Let ξ_0 be the simple root of $k^2(\xi)$. Near ξ_0 the function $k(\xi)$ has the form

$$k(\xi) = A\sqrt{\xi - \xi_0}. \tag{2.3}$$

The function $q(\xi)$, in the neighborhood of ξ_0, is of the form

$$q(\xi) = \frac{5}{16A^2(\xi-\xi_0)^3}\left[1 + O(\xi - \xi_0)\right]. \tag{2.4}$$

The leading term in $q(\xi)$, as is seen from (2.2), contains the constant A, which is determined by the form of the function $k(\xi)$. However, after transformation to the variable $\tau = \int^{\xi} k\,d\xi$ the point ξ_0 goes over into the point $\tau_0 = \int^{\xi_0} k\,d\xi$, in the vicinity of which $q(\tau)$ has the form

$$q(\tau) = \frac{5}{36(\tau-\tau_0)^2}\left[1 + O(\tau-\tau_0)^{2/3}\right]. \tag{2.5}$$

We see that the leading term in $q(\tau)$ does not depend on the form of the function $k(\xi)$ in the neighborhood of τ_0.

We now apply the theory of residues to the integral (2.2). Here we consider only the pole τ_0, as the contributions from the remaining singularities are exponentially small compared with the contribution of the point τ_0. We assume here that the different singular points of $q(\tau)$ are not too close to each other. With these assumptions, the calculation gives

$$V_{k,k'} = 2\pi\frac{5}{36}|k-k'|\exp\left\{\frac{i}{\alpha}(k'-k)\rho - \frac{1}{\alpha}|k-k'|\sigma\right\} \times (1 + O(\alpha^{2/3})), \tag{2.6}$$

where $\tau_0 = \rho + i\sigma\ (\sigma > 0)$. We note that the leading term in the coefficient of the exponential in $V_{k,k'}$ does not depend on the form of function $k(\xi)$.

In particular, we have

$$V_{-1,1} = \frac{5}{36}\pi e^{2i\tau_0/\alpha}(1 + O(\alpha^{2/3})). \tag{2.7}$$

We show that in all the other corrections of the perturbation theory the leading terms are also proportional to the same exponential $\exp(2i\tau_0/\alpha)$, whose coefficients are universal constants independent of the form of the function $k(\xi)$. We examine the general term in the series (2.1):

$$\begin{aligned} J_n &= \frac{1}{(2\pi)^n}\int\ldots\int dk_1\ldots dk_n\,\frac{V_{-1,k_1}V_{k_1,k_2}\ldots V_{k_n,1}}{(1-k_1^2)(1-k_2^2)\ldots(1-k_n^2)} \\ &= 2\pi\left(\frac{5}{36}\right)^{n+1} e^{2i\rho/\alpha}\int\ldots\int dk_1 dk_2\ldots dk_n \\ &\times \frac{|1+k_1|\,|k_2-k_1|\ldots|1-k_n|}{(1-k_1^2)\ldots(1-k_n^2)} \\ &\times \exp\left\{-\frac{\sigma}{\alpha}(|1+k_1| + \ldots + |1-k_n|)\right\}. \end{aligned} \tag{2.8}$$

We separate the region of integration into the n-dimensional "tetrahedron" $-1 \le k_1 \le k_2 \ldots \le k_n \le 1$ and the whole remaining space. Inside the "tetrahedron" the exponent of the exponential in the integral (2.8) is equal to $-2\sigma/\alpha$; in the remaining region of integration it is everywhere smaller than this quantity, and therefore the latter region gives to the integral a contribution which is small in comparison with the contribution of the "tetrahedron" (of order $2^n\alpha/n!$). We can thus restrict the integration to the "tetrahedron," with the result

$$J_n = ({}^5/_{36})^{n+1}\,2\pi A_n e^{2i\tau_0/\alpha}(1 + O(\alpha^{2/3})), \tag{2.9}$$

where

$$A_n = \int_{-1}^{1} dk_1 \int_{k}^{1} dk_2 \ldots \int_{k_{n-1}}^{1} dk_n \frac{(1+k_1)(k_2-k_1)\ldots(1-k_n)}{(1-k_1^2)(1-k_2^2)\ldots(1-k_n^2)}. \tag{2.10}$$

We thus convince ourselves that the coefficients A_n indeed do not depend on the form of the function $k(\xi)$. Hence the amplitude of the reflection coefficient has the form

$$R = -i\pi e^{2i\tau_0/\alpha} \sum_{n=0}^{\infty} A_n \left(\frac{5}{36}\right)^{n+1}, \tag{2.11}$$

where $A_0 = 2$. It is not necessary to compute the sum in formula (2.11), since its value does not depend on the form of the function $k(\xi)$, and can thus be determined using any known exact solution of the Schrödinger equation.

A number of cases is known where the Schrödinger equation (1.1) admits of an exact solution.[1,2] The asymptotic expression for the reflection coefficient leads in all these cases to the formula

$$R = -ie^{2i\tau_0/\alpha} = -i \exp\left\{\frac{2i}{\alpha}\int^{\xi_0} k d\xi\right\}. \tag{2.12}$$

Consequently, formula (2.12) gives the leading term in the reflection coefficient for arbitrary form of the potential.*

3. RANGE OF APPLICABILITY

The formula for the coefficient for barrier reflection (2.12) obtained in the preceding section is valid only in the case where the singular points of the plane τ are separated from each other by distances much greater than α. Otherwise the expression (2.5) for the function $q(\tau)$ becomes incorrect.

We investigate, what limitations on the range of parameters of the problem follow from this requirement.

1. Region of high energies: $U_0/E \ll 1$. (U_0 denotes the maximal value of the potential U). In this case the root of $k^2 = 1 - U/E$ is clearly located in the vicinity of the singularity of U.

The criterion for the applicability of formula (2.12) depends essentially on the kind of singularity of U. We examine the case where the singularity of U is a simple pole. Near the pole ξ_1 the function U has the form

$$U = U_0 A/(\xi - \xi_1), \tag{3.1}$$

where A is a quantity of order unity. The function $k^2(\xi)$ near ξ_1 is of the form

$$k^2(\xi) = (\xi - \xi_0)/(\xi - \xi_1), \tag{3.2}$$

where $\xi_0 = \xi_1 + AU_0/E$. For the corresponding values of τ_0, τ_1 we find

$$\tau_0 - \tau_1 = \int_{\xi_1}^{\xi_0} \sqrt{\frac{\xi - \xi_0}{\xi - \xi_1}}\, d\xi = \frac{i\pi}{2}(\xi_0 - \xi_1) = \frac{i\pi}{2} A \frac{U_0}{E}. \tag{3.3}$$

Hence the required criterion is

$$U_0/E\alpha \gg 1. \tag{3.4}$$

We note that in the case $U_0/E \ll 1$ the usual perturbation theory is applicable.

For the "Gaussian" potential $U = U_0 \exp(-\xi^2)$ the criterion for the applicability of the quasi-classical approximation (2.12) is much less stringent, namely

$$\frac{U_0}{E} e^{\alpha^{-2}} \gg 1. \tag{3.5}$$

It is interesting to note that in this case the region of applicability of perturbation theory lies outside the region (3.5):

$$U_0 e^{\alpha^{-2}}/E \ll 1.$$

2. Region of energies close to U_0. In this case the two roots ξ_0, ξ_0^* of the function $k^2(\xi)$ lie close to one another (they are also close to the point ξ_m where $U(\xi)'$ takes its maximum). From the condition that the distance between corresponding points τ_0, τ_0^* must be larger than α we obtain the criterion

$$(E - U_0)/U_0\alpha \gg 1. \tag{3.6}$$

In the region $(E - U_0)/U_0\alpha \lessgtr 1$ the amplitude of reflection may be obtained by other means (see, e.g., Refs. 4 and 5). We note that the expression for the reflection amplitude (66) of the paper of Fock,[5] obtained under the assumption $(E - U_0)/U_0\alpha \lessgtr 1$, may be extrapolated into the region $(E - U_0)/U_0\alpha \gg 1$, as this work shows.

In closing the authors express their sincere gratitude to L. D. Landau for valuable advice leading to significant simplifications of the mathematical calculations.

APPENDIX

The asymptotic expression (2.6) for the matrix element $V_{k,k'}$, obtained in Sec. 2, becomes incorrect for $|k - k'| \lesssim \alpha$. However, for the absolute value of the matrix element $V_{k,k'}$ there exists a simple estimate, which is valid for arbitrary $|k - k'|$:

$$|V_{k,k'}| \leqslant \alpha \int_{-\infty}^{\infty} |q(\tau)|\, d\tau = M\alpha, \tag{A.1}$$

where M is a quantity of order unity.

Consider, for example, the integral

*The formula for the reflection coefficient obtained in Ref. 3 proves to be wrong; it takes into account only the first term in the series (2.11).

$$J_1 = \int \frac{V_{-1,k} V_{k1}}{1-k^2}\, dk. \qquad (A.2)$$

The integral along the real axis of k, by-passing the singularities $k = \pm 1$, is broken up in the following way:

$$J_1 = \int\limits_{-\infty}^{-1-\alpha} + \int\limits_{-1+\alpha}^{1-\alpha} + \int\limits_{1+\alpha}^{\infty} + \int\limits_{\Gamma_1} + \int\limits_{\Gamma_2}, \qquad (A.3)$$

where Γ_1 and Γ_2 are semicircles of radius α about the singular points. Making an error of order α in comparison with the leading term, we replace the exact values $V_{k,k'}$ by their asymptotic expressions (2.6) in the integrals along the straight lines, and extend the second integral to an interval from -1 to 1. The integrals over the semicircles are estimated with the help of (A.1). They give a contribution of order α as compared to the leading term.

In an analogous manner one can justify the application of formulae (2.9), (2.10) for the general term in the iteration series.

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RADIATION COOLING OF AIR. I. GENERAL DESCRIPTION OF THE PHENOMENON AND THE WEAK COOLING WAVE

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We consider non-stationary radiation cooling of a large volume of air heated to a high temperature (on the order of tens and hundreds of thoudands degrees) by a strong explosion. It is shown that, owing to the strong temperature dependence of light absorption in the air, the cooling involves the propagation of a sharp temperature jump, i.e., of a cooling wave. Cooling from the initial high temperature to that at which the air becomes almost transparent and ceases to radiate occurs in a narrow wave front. A system of equations is derived, which permits an investigation of the internal structure of the cooling wave and leads to a connection between its parameters and the propagation velocity. A weak wave with a small temperature difference is considered.

1. QUALITATIVE DESCRIPTION OF THE PROCESS OF COOLING HEATED AIR

THE problem of a strong explosion in air was considered by Sedov[1] (see also Ref. 2). A strong shock wave heats the air irreversibly to a very high temperature, so that a large mass of very hot air is produced after the explosion, when the pressure returns to atmospheric.

Imagine a large mass of air with linear dimensions on the order of several hundreds of meters, heated to a high temperature — above 100,000° at the center; the temperature towards the periphery drops to below 1,000°. How is such a mass cooled? Obviously, the molecular heat conduction does not play any role at all: with a heat-diffusion coefficient