WKB METHOD FOR THREE-DIMENSIONAL PROBLEMS

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The quasiclassical expression for the wave function in a three-dimensional analytic potential is examined near the caustics, where the quasiclassical approximation breaks down. A function is constructed which approximates the exact solution of the Schrödinger equation in a finite region of space including a caustic. The amplitude in a scattering problem is found in the neighborhood of the caustic, where the ordinary quasiclassical cross section diverges.

1. A very important question for three-dimensional problems is that of the violations of the quasiclassical approximation in space. In cases in which the quasiclassical wave function is good in a large region of space the approximation makes it possible to derive important results.[1,2] For example, in the problem of scattering by a spherically symmetric potential for $E \gg U$,[2] when the classical limiting angle $\theta_{0\max}$ is small, one can get an analytic expression for the amplitude in the entire range of angles that is of interest in practice. In the neighborhood of $\theta_{0\max}$ the approximation is no longer applicable. Here the scattering angle as function of the impact parameter, $\theta_0(\rho)$, has a maximum, and the classical differential cross section $d\sigma/d\Omega$ goes to infinity.

As will be shown in what follows, the extrema of the function $\theta_0(\rho)$ correspond to caustics, where the radius of the wave surface goes to zero. Such singular points, where $d\theta_0(\rho)/d\rho = 0$, can occur not only on the boundary between classically accessible and inaccessible angles, but also inside each of these regions. Therefore it can happen that the usual quasiclassical expression for the wave function[1] is of little practical use (for example, if $\theta_{0\max}$ is not small and there are several caustics). We can, however, use a knowledge of the asymptotic form of the wave function in the direction toward a caustic to construct the exact function in its neighborhood, and then construct an approximation in a finite region of space by means of Airy functions. This procedure (the WKB method in the three-dimensional case) can be carried out independently of the boundary conditions of the quantum-mechanical problem and gives a corrected wave function where caustics invalidate the usual quasiclassical approximation.

In the present paper we expound the three-dimensional WKB method and apply it to the treatment of the scattering problem.

2. The quasiclassical solution of the Schrödinger equation with arbitrary boundary conditions can be written in the form[1,3]

$$\Psi = \sum_n A_n e^{iS_n/\hbar}. \tag{1}$$

Here S_n are particular solutions of the Hamilton-Jacobi equation

$$(\nabla S_n)^2 = 2m(E - U(\mathbf{r})) \equiv p^2(\mathbf{r}) \tag{2}$$

with the boundary conditions of the corresponding classical problem [E is the energy of the particles, and $U(\mathbf{r})$ is the potential in which they move]. Analogously, the amplitudes A_n are solutions of the equation

$$2(\nabla S_n \nabla A_n) + A_n \Delta S_n = 0. \tag{3}$$

The summation in (1) is taken over all of the particular solutions of Eq. (2) that exist at the given point $\mathbf{r}$.[1]

Let the manifold of characteristic lines of Eq. (2) which satisfy the boundary conditions be given in the usual form:

$$S = S(\mathbf{r}, \alpha, \beta), \quad S_\alpha \equiv \frac{\partial}{\partial \alpha} S(\mathbf{r}, \alpha, \beta) = 0, \quad S_\beta \equiv \frac{\partial}{\partial \beta} S(\mathbf{r}, \alpha, \beta) = 0, \tag{4}$$

where α and β are the parameters that define the manifold.[1)] As will be seen from what follows, in the problem considered it suffices to take into account in (1) only those solutions of (2) that correspond to different α and β. Generally speaking, however, there may be more than one solution corresponding to particular values α and β.[1] Accordingly, we set $S_n = S(\mathbf{r}, \alpha_n(\mathbf{r}), \beta_n(\mathbf{r}))$, where $\alpha_n(\mathbf{r})$ and $\beta_n(\mathbf{r})$ are real or complex solutions of the system of equations

$$S_\alpha(\mathbf{r}, \alpha, \beta) = 0, \qquad S_\beta(\mathbf{r}, \alpha, \beta) = 0. \tag{5}$$

In the construction of (1) we need take into account only those of the nonphysical roots of (5) that do not violate the boundary conditions of the quantum-mechanical problem under consideration. For example, one of a pair of complex-conjugate roots of (5) may give an exponentially large term in (1), since for these roots $\operatorname{Im} S_1 = -\operatorname{Im} S_2$. Roots for which $\operatorname{Im} S_n < 0$ are not to be included in (1). Moreover, we need retain in the sum (1) only the terms with the smallest values of $\operatorname{Im} S_n$, since inclusion of the others would exaggerate the accuracy.

It is easy to calculate the amplitude A_n if we go over to curvilinear coordinates S, α, and β by means of (4) and use the identities

$$\nabla S \nabla S_\alpha = 0, \qquad \nabla S \nabla S_\beta = 0, \tag{6}$$

obtained by differentiating $(\nabla S)^2 = p^2$ with respect to α and β. Then

$$\Delta S = {}^1/_2(\nabla S \nabla \ln J), \tag{7}$$

where

$$J = (\nabla S)^2 [\mathbf{r}_\alpha \mathbf{r}_\beta]^2 = (\nabla S)^2 \frac{(S_{\alpha^2} S_{\beta^2} - S_{\alpha\beta}^2)^2}{[\nabla S_\alpha \nabla S_\beta]^2} \tag{8}*$$

[1)] Here and in what follows lower indices α, β will denote the corresponding partial derivatives with respect to α, β for constant $\mathbf{r}$ (indices α^2, . . . indicate second, . . . derivatives), and the symbol ∇ means that the gradient is taken for fixed α, β.

*$[\mathbf{r}_\alpha \mathbf{r}_\beta] \equiv \mathbf{r}_\alpha \times \mathbf{r}_\beta$

and[1]

$$A_n = \varphi_n J^{-1/2}(\mathbf{r}, \alpha_n(\mathbf{r}), \beta_n(\mathbf{r})). \quad (9)$$

The factor φ_n is determined by the boundary conditions and the relation

$$\nabla S_n \nabla \varphi_n = 0. \quad (10)$$

For what follows it is convenient to bring into the treatment the set of trajectories with parameters α and β determined by Eq. (5). It is obvious that these trajectories satisfy the boundary conditions of the corresponding classical problem. To a set of solutions $\alpha = \alpha_n(\mathbf{r})$, and $\beta = \beta_n(\mathbf{r})$, n = 1, 2, ..., will correspond a group of trajectories, real or unreal, for example complex, passing through the given point $\mathbf{r}$.

It can be seen from (6) that the trajectories are orthogonal to the wave surfaces S_n = const, and consequently the unit vector tangent to the n-th trajectory is

$$\mathbf{l}_n = p^{-1}\nabla S_n. \quad (11)$$

Then the condition (10) means that φ is constant along a trajectory.

Finally, in the language of trajectories we can give a more intuitive formulation to the principle of construction of (1): the summation in (1) is taken over all trajectories passing through the point $\mathbf{r}$, except those that lead to a violation of the boundary conditions of the quantum-mechanical problem or go beyond the permissible accuracy.[1]

3. Let us now consider the condition of applicability of the quasiclassical approximation in the three-dimensional case.

On using (7), (11), and a relation known from differential geometry,

$$\operatorname{div} \mathbf{l} = 2H, \qquad H = {}^1/_2(R_1^{-1} + R_2^{-1})$$

(H is the mean curvature of the wave surface), we get

$$\frac{\hbar \Delta S}{(\nabla S)^2} = \frac{1}{2}\frac{\lambda(\mathbf{l}\nabla J)}{J} = -\mathbf{l}\nabla\lambda + \frac{\lambda}{R_1} + \frac{\lambda}{R_2}, \qquad \lambda = \frac{\hbar}{p(\mathbf{r})}. \quad (12)$$

From this it can be seen in particular that at the one-dimensional turning points, which arise when one separates the variables in (2), there is no breakdown of the approximation (1), since only the total momentum $p(\mathbf{r})$ is involved in the condition (12).

It follows from (12), and also from (9), that the approximation breaks down near J = 0. Here, owing to the identities

$$\nabla S_a \nabla S_b + \nabla S \nabla S_{ab} = 0, \qquad (a, b) \in (\alpha, \beta), \quad (13)$$

obtained from (6) by differentiation with respect to α and β, we have

$$[\nabla S_\alpha \nabla S_\beta]^2 = (\nabla S)^2((\mathbf{l}\nabla S_{\alpha^2})(\mathbf{l}\nabla S_{\beta^2}) - (\mathbf{l}\nabla S_{\alpha\beta})^2)^{1/2}$$

and the factor $(\nabla S)^2$ in J, Eq. (8), does not give an independent singularity. Finally, the geometrical locus of the singular points is determined by the equation

$$[\mathbf{r}_\alpha \mathbf{r}_\beta]^2_{\alpha_n(\mathbf{r}), \beta_n(\mathbf{r})} = 0. \quad (14)$$

At these points H and A_n go to infinity [cf. (9), (12)], and the cross section df = $|[\mathbf{r}_\alpha \times \mathbf{r}_\beta]|d\alpha d\beta$ of the bundle of trajectories goes to zero.

The condition (14) is satisfied either at points where $|[\nabla S_\alpha \times \nabla S_\beta]| = \infty$, which occurs, for example, along lines of concentration of the curvilinear coordinate system in which (2) was solved, or else at points where

$$S_{\alpha^2}S_{\beta^2} - S_{\alpha\beta}^2 \equiv \Phi(\mathbf{r}, \alpha, \beta) = 0. \quad (15)$$

This last condition, together with the system of equations (5), defines the caustics, which will be investigated in what follows.

It follows from the definition that on a caustic two solutions of (5) become equal. Depending on whether the coincident roots are real or complex, we shall distinguish between real and complex caustics. They can take different forms in real space; they may be surfaces or lines, or they may have no trace at all in real space. In six-dimensional complex space both types give four-dimensional regions. The difference between the two types of caustics is the same as that between real and complex turning points of a one-dimensional problem. (As will be shown later, a caustic of a three-dimensional problem is analogous to a linear turning point of a one-dimensional problem.)

In order to have an intuitive geometrical interpretation, let us consider the case of real trajectories, a manifold of which in real space forms a curvilinear congruence. Then by definition a caustic will be the envelope of the congruence of trajectories; in other words, it will bound the classical motion in a direction perpendicular to it. A caustic can be regarded as a surface consisting of singular solutions of the classical equations of motion, envelopes of certain one-parameter manifolds of trajectories. Each of the singular solutions is the locus of limiting positions of points of intersection of two infinitesimally contiguous trajectories. Accordingly, in the neighborhood of any point of the caustic there exist on one side of it two real and infinitesimally different roots of the system (5), and on the other side these roots become complex conjugates; that is, on passage through the caustic the number of real roots of the system (5) decreases by two. At points of the caustic it is impossible to distinguish the two "different" trajectories, since they have identical directions $\mathbf{l}_1 = \mathbf{l}_2$, and here the principle of superposition of trajectories, on which (1) is based, loses its meaning. It is reestablished at a certain distance from the caustic, when the angle between $\mathbf{l}_1$ and $\mathbf{l}_2$ becomes larger than the quantum-mechanical uncertainty in the angles.

4. Let $\alpha_1(\mathbf{r})$, $\beta_1(\mathbf{r})$ and $\alpha_2(\mathbf{r})$, $\beta_2(\mathbf{r})$ be the two solutions of (5) which coincide at the corresponding caustic. Then

$$\alpha_1(\mathbf{R}) = \alpha_2(\mathbf{R}) = \alpha(\mathbf{R}), \qquad \beta_1(\mathbf{R}) = \beta_2(\mathbf{R}) = \beta(\mathbf{R})$$

at points $\mathbf{R}$ where by definition $\Phi(\mathbf{R}, \alpha(\mathbf{R}), \beta(\mathbf{R})) = 0$. We shall assume that there are no other singularities of the wave function (1) near the caustic in question. Then to find the form of (1) in this part of space it suffices to consider in the sum (1) the terms with the corresponding indices n = 1, 2. Let us find their expansion in Taylor's series in the neighborhood of the point $M_0(\mathbf{R}_0, \alpha_0, \beta_0)$, where $\alpha_0 = \alpha(\mathbf{R}_0)$, $\beta_0 = \beta(\mathbf{R}_0)$ and $\mathbf{R}_0$ is an arbitrary point of our caustic, i.e., $\Phi(M_0) = 0$. This can be done except at points where the first integral $S(\mathbf{r}, \alpha, \beta)$ of (2) is singular as a function of $\mathbf{r}$, α, or β. It is obvious that such singularities are due to singularities of the Hamilton-Jacobi equation, and not to the condition (15), although coincidences are indeed possible. Cases of coincidence are not considered here.

In the expansion we keep in the amplitudes $A_{1,2}$ only the first, main, term, in analogy with the linear approximation in the case of a one-dimensional turning point, so that we must neglect all derivatives of $S(\mathbf{r}, \alpha, \beta)$ of order higher than the third, and also the gradient of the potential. In fact, according to (8), (9), and (15), the main term of the expansion of $A_{1,2}$ in the neighborhood of M_0 is given by

$$A_n = \varphi_n C(M_0) / \sqrt{\Delta\Phi_n}, \quad n = 1, 2, \tag{16}$$

where

$$\Delta\Phi_n = (\alpha_n - \alpha_0)\Phi_\alpha(M_0) + (\beta_n - \beta_0)\Phi_\beta(M_0) + ((\mathbf{r} - \mathbf{R}_0)\nabla\Phi(M_0)),$$
$$C(M_0) = (p^{-2}(\mathbf{R}_0)[\nabla S_\alpha(M_0)\nabla S_\beta(M_0)]^2)^{1/4}.$$

Since in (16) we have dropped terms containing second-order partial derivatives of $\Phi(\mathbf{r}, \alpha, \beta)$, which in our approximation are given by

$$\Phi_{ab} = S_{a\alpha^2}S_{b\beta^2} + S_{b\alpha^2}S_{a\beta^2} - 2S_{a\alpha\beta}S_{b\alpha\beta},$$
$$\nabla\Phi_a = S_{a\alpha^2}\nabla S_{\beta^2} + S_{a\beta^2}\nabla S_{\alpha^2} - 2S_{a\alpha\beta}\nabla S_{\alpha\beta}, \tag{17}$$

where $(a, b) \in (\alpha, \beta)$, we shall also regard the corresponding combinations of third derivatives as small.

To supplement (6) and (13) we give a number of exact relations derived in similar ways:

$$(\nabla S\nabla)\nabla S = -\nabla U, \quad (\nabla S_a\nabla)\nabla S + (\nabla S\nabla)\nabla S_a = 0;$$
$$(\nabla S_a\nabla S_{bc}) + (\nabla S_b\nabla S_{ca}) + (\nabla S_c\nabla S_{ab}) = -(\nabla S\nabla S_{abc}), \tag{18}$$

$$(\nabla S_{ab}\nabla S_{cd}) + (\nabla S_{ac}\nabla S_{bd}) + (\nabla S_{ad}\nabla S_{bc}) = -(\nabla S_a\nabla S_{dbc})$$
$$- (\nabla S_b\nabla S_{adc}) - (\nabla S_c\nabla S_{abd}) - (\nabla S_d\nabla S_{abc}) - (\nabla S\nabla S_{abcd}); \tag{19}$$

with $(a, b, c, d) \in (\alpha, \beta)$. It can be seen from (13) and (19) that we must neglect the quantities $\nabla S_{ab}\nabla dc$ and $(\nabla S_a\nabla S_b)^2$, and it follows from (17) that we must also neglect $\mathbf{K}^2$, where

$$\mathbf{K} = \nabla S_\alpha\Phi_\beta - \nabla S_\beta\Phi_\alpha. \tag{20}$$

In fact, in this case

$$S_{ab^2} = (S_a S_{b^2}^2)^{1/3}, \quad \Phi_a = S_{a^2}^{1/3}(S_{b^2}^{1/2}S_{a^3}^{1/3} - S_{a^2}^{1/2}S_{b^3}^{1/3})$$

and we have

$$(S_{a^2}^2)\mathbf{K}^2 = \Phi_a(\nabla\Phi_a) \approx 0. \tag{21}$$

But when we regard $\mathbf{K}^2$ and $(\nabla S_{ab})^2$ as negligibly small we must obviously also drop $\mathbf{K}\nabla S_{ab}$, and then, noting (23) (sic), we see that $\nabla S_a\nabla S_{bc}$ is also to be neglected.

Let us now consider the expansion of $S(\mathbf{r}, \alpha, \beta)$ to and including third derivatives:

$$S(M) = S(M_0) + S^{(1)} + S^{(2)} + S^{(3)}; \tag{22}$$

here

$$S^{(1)} = \mathbf{r}'\nabla S + \alpha' S_\alpha + \beta' S_\beta = \mathbf{r}'\nabla S$$

[since at the point M_0 we have $S_\alpha(M_0) = S_\beta(M_0) = 0$],

$$S^{(2)} = \frac{\alpha'^2}{2}S_{\alpha^2} + \alpha'\beta' S_{\alpha\beta} + \frac{\beta'^2}{2}S_{\beta^2} + \alpha'(\mathbf{r}'\nabla S_\alpha)$$
$$+ \beta'(\mathbf{r}'\nabla S_\beta) + \frac{1}{2}\mathbf{r}'(\mathbf{r}'\nabla)\nabla S,$$
$$S^{(3)} = \frac{\alpha'^3}{6}S_{\alpha^3} + \frac{\alpha'^2\beta'}{2}S_{\alpha^2\beta} + \frac{\alpha'\beta'^2}{2}S_{\alpha\beta^2} + \frac{\beta'^3}{6}S_{\beta^3}$$
$$+ \frac{\alpha'^2}{2}(\mathbf{r}'\nabla S_{\alpha^2}) + \frac{\beta'^2}{2}(\mathbf{r}'\nabla S_{\beta^2}) + \alpha'\beta'(\mathbf{r}'\nabla S_{\alpha\beta})$$
$$+ \frac{\beta'}{2}(\mathbf{r}'(\mathbf{r}'\nabla)\nabla S_\beta) + \frac{\alpha'}{2}(\mathbf{r}'(\mathbf{r}'\nabla)\nabla S_\alpha) + \frac{1}{6}\sum x_i' x_j' x_k' \frac{\partial^3 S}{\partial x_i\,\partial x_j\,\partial x_k}.$$
$$\mathbf{r}' = \mathbf{r} - \mathbf{R}_0, \quad \alpha' = \alpha - \alpha_0, \quad \beta' = \beta - \beta_0.$$

Since for the linear approximation in the three-dimensional WKB method we can confine ourselves to the expansion of $S_n(\mathbf{r}, \alpha_n, \beta_n)$ to second order in $|\mathbf{r} - \mathbf{R}_0|$, we neglect the last three terms in $S^{(3)}$. Then we must drop the last term in $S^{(2)}$, since its coefficients, according to (18), are equal to quantities which we are neglecting.

Having determined $S(\mathbf{r}, \alpha, \beta)$, we then get from (22) the system of equations (5). Solving it by successive approximations to first order in $|\mathbf{r} - \mathbf{R}_0|$, we find that near the caustic

$$\alpha_n - \alpha_0 = \sqrt{S_{\beta^2}}(D_n - M) - \Phi_\beta L + O(|\mathbf{r}'|^{3/2}),$$
$$\beta_n - \beta_0 = -\sqrt{S_{\alpha^2}}(D_n - M) + \Phi_\alpha L + O(|\mathbf{r}'|^{3/2}), \tag{23}$$

where n = 1, 2. Here, using (15) and (20), we have introduced the following notations:

$$D_n = e^{i\pi(n-1)}[2((\mathbf{r} - \mathbf{R}_0)\mathbf{N}) / d]^{1/2},$$
$$M = ((\mathbf{r} - \mathbf{R}_0)\nabla\Phi) / d, \quad L = ((\mathbf{r} - \mathbf{R}_0)\mathbf{K}) / d^2,$$
$$\mathbf{N} = \sqrt{S_{\alpha^2}}\nabla S_\beta - \sqrt{S_{\beta^2}}\nabla S_\alpha, \quad d = \Phi_\alpha\sqrt{S_{\beta^2}} - \Phi_\beta\sqrt{S_{\alpha^2}}. \tag{24}$$

Accordingly the two solutions that coincide on the caustic are the two branches of the root (24). With the given choice of indices, the first solution corresponds to a wave incident on the caustic, the second to a reflected wave.

After this (16), (22), and (23) allow us to determine the explicit form of the amplitudes:

$$A_n = \varphi_n C(M_0) / \sqrt{D_n d} \tag{25}$$

and also S_n, with accuracy to $|\mathbf{r} - \mathbf{R}_0|^2$:

$$S_n = S(M_0) + (\mathbf{r} - \mathbf{R}_0)\nabla S - \frac{D_n^3}{3}d - \frac{((\mathbf{r} - \mathbf{R}_0)\nabla\Phi)((\mathbf{r} - \mathbf{R}_0)\mathbf{N})}{d}$$
$$- \frac{1}{2}\frac{((\mathbf{r} - \mathbf{R}_0)\mathbf{K})^2}{d^2}. \tag{26}$$

Here, taking (21) into account, we can neglect the last term.

It follows from this expansion that near an arbitrary caustic the main term of the asymptotic formula (1) depends on a single (complex) variable $\eta \sim (\mathbf{r} - \mathbf{R}_0)\mathbf{N}$; that is, the problem in six-dimensional space can be reduced to a problem on the plane of η. The only thing that is different for different characters (real or complex) of the caustic is the orientation of the η plane relative to real space. Obviously the form of the exact solution of the Schrödinger equation is as little dependent on the type of caustic as is the asymptotic form. Therefore for clarity we consider a real caustic, which is a surface in real space. [In our approximation this is the plane $(\mathbf{r} - \mathbf{R}_0)\mathbf{N}(\mathbf{M}_0) = 0$].

Let us introduce rectangular coordinates ξ, η, ζ so that

$$\mathbf{r} - \mathbf{R}_0 = \xi\mathbf{l}(\mathbf{R}_0) + \eta\mathbf{n}(\mathbf{R}_0) + \zeta\mathbf{b}(\mathbf{R}_0). \tag{27}$$

Here $\mathbf{l} = p^{-1}\nabla S$; $\mathbf{n}$ is the normal to the caustic; and $\eta > 0$ defines the region accessible to the trajectories; $\mathbf{b} = [\mathbf{ln}]$. To find $\mathbf{n}$ we differentiate the system $S_\alpha = S_\beta = \Phi = 0$ that defines the caustic $\mathbf{R} = \mathbf{R}(\alpha, \beta)$ with respect to α, β; then, after finding $\mathbf{R}_\alpha, \mathbf{R}_\beta$, we have

$$\mathbf{n} = \pm\frac{[\mathbf{R}_\alpha\mathbf{R}_\beta]}{|[\mathbf{R}_\alpha\mathbf{R}_\beta]|} = \pm\frac{\mathbf{N}}{|\mathbf{N}|}. \tag{28}$$

By definition the direction of $\mathbf{n}$ is found from the condition $(\mathbf{n}\cdot\mathbf{N})/d > 0$, since, according to (23) and (24), at points $((\mathbf{r} - \mathbf{R}_0)\cdot\mathbf{N})/d < 0$ the quantities α_n and β_n become complex.

Let us examine the geometrical meaning of the expression

$$\mathbf{N}N^2/d \equiv p^2\gamma\mathbf{n}, \quad \gamma > 0, \tag{29}$$

which appears in the main term $S_n - D_n^3 d$; to do so we select in the congruence (5) a one-parameter family of trajectories $\mathcal{H}$ which admits an envelope, and calculate its normal and curvature. We consider the congruence of trajectories in the following parametric representation, determined by the system (4): $\mathbf{r} = \mathbf{r}(S, \alpha, \beta)$; here S is the parameter that changes along a trajectory. Then the caustic is

$$\mathbf{R}(\alpha, \beta) = \mathbf{r}(S_0(\alpha, \beta), \alpha, \beta),$$

where $S_0(\alpha, \beta)$ is found from $\Phi(\mathbf{r}(S_0, \alpha, \beta), \alpha, \beta) = 0$; the manifold $\mathcal{H}$ is defined by

$$\mathbf{r}_{\mathcal{H}}(S, \beta) = \mathbf{r}(S, \alpha_0(\beta), \beta),$$

where $\alpha_0(\beta)$ is found from the condition that the vector $d\mathbf{R} = \mathbf{R}_\alpha d\alpha + \mathbf{R}_\beta d\beta$ be parallel to $\mathbf{l}(\mathbf{R})$. The envelope of $\mathcal{H}$ as a function of the parameter β is of the form

$$\mathbf{q}(\beta) = \mathbf{r}(S_0(\alpha, \beta), \alpha, \beta)\,|_{\alpha=\alpha_0(\beta)}.$$

After this, and after calculating the quantity

$$\frac{[\mathbf{q}_\beta[\mathbf{q}_\beta\mathbf{q}_\beta]]}{(\mathbf{q}_\beta\mathbf{q}_\beta)^2} = \nu_q\mathbf{n}_q,$$

we find

$$\gamma\mathbf{n} = \nu_t\mathbf{n}_t - \nu_q\mathbf{n}_q, \tag{30}$$

where ν_t (ν_q) is the normal curvature of the trajectory (envelope); and $\mathbf{n}_t$ ($\mathbf{n}_q$) is the principal normal to the trajectory, directed toward the center of curvature.

Finally, going over to the coordinates ξ, η, ζ in (25), (26) by means of (27) and using (13), (24), and (29), we find in our approximation the form of (1) far from the caustic:

$$\Psi = \Psi_s + \Psi_r;$$

$$\Psi_s = \frac{C(M_0)}{(3d^2\hbar)^{1/6}} \exp\left\{i\left(\frac{S(M_0)}{\hbar} + X\right)\right\} \frac{\varphi_1 e^{-iY} + \varphi_2 e^{-i\pi/2} e^{iY}}{Y^{1/6}}, \tag{31}$$

where

$$Y = \frac{d}{3\hbar}\sqrt{\frac{8((\mathbf{r}-\mathbf{R}_0)\mathbf{N})^3}{d^3}} = \frac{1}{3\lambda}\sqrt{\gamma(2\eta)^3},$$
$$X = \frac{1}{\lambda}(\xi - \xi\eta\gamma), \quad \lambda = \frac{\hbar}{p(R_0)}, \tag{32}$$

and

$$\Psi_r = \sum_{n\neq 1,\,2} A_n e^{iS_n/\hbar}$$

is regular in the neighborhood of $\mathbf{R}_0$.

The nature of the main term Ψ_S shows that with regard to the variable η the situation is analogous to that at a linear turning point in the one-dimensional motion in a field $V = (\nabla Sn)^2/2 = p^2\gamma\eta$, and therefore to determine the exact wave function Ψ_C in the neighborhood of the caustic we carry out a procedure similar to the one-dimensional WKB method. We write the Schrödinger equation in variables X, Y, $Z = \zeta/\hbar$, using the fact that S_n has been calculated to second order in $\mathbf{r} - \mathbf{R}_0$:

$$p^2(1 - 2\eta\gamma)\Psi_{x^2} + 2\eta\gamma p^2\Psi_{Y^2} + \hbar p\sqrt{\frac{\gamma}{2\eta}}\Psi_Y + \Psi_{z^2} + p^2\Psi = 0.$$

The solution of this equation that has the asymptotic form Ψ_S far from the caustic is of the form

$$\Psi_c = \varphi_1 \frac{C(M_0)}{(3d^2\hbar)^{1/6}} \exp\left\{i\left(\frac{S(M_0)}{\hbar} + X - \frac{\pi}{12}\right)\right\} F(Y),$$

$$F(Y) = \sqrt{\frac{\pi}{2}}\, Y^{1/6}(H^{(1)}_{1/3}(Y) + H^{(2)}_{-1/3}(Y)); \tag{33}$$

$H^{(1,2)}_{\pm 1/3}$ are the Hankel functions of first and second kinds.

It follows from the boundary conditions that

$$\varphi_2 = \varphi_1. \tag{34}$$

In the case of a real caustic Eq. (34) is obtained if we require that for $\eta < 0$ the function Ψ_C contain no exponentially increasing term. This requirement is equivalent to the boundary conditions. In fact, beyond the caustic α_1 and α_2, β_1 and β_2, and consequently S_1 and S_2, become complex-conjugate pairs of quantities, and in accordance with what has been said Ψ_S contains only one term, for which $\operatorname{Im} S_n > 0$.

For a complex caustic the situation is somewhat different. At points on it a pair of complex roots of the system (5) coincide, and these roots are such that $\operatorname{Im} S(M_0)$ is positive for them; that is, Ψ_S is exponentially small in this neighborhood. Therefore here terms are admissible in Ψ_C which increase exponentially as we go away from the caustic, but only far enough so that the quantity $\operatorname{Im} S(M_0) > 0$ is balanced out. The points where this occurs, in other words the points where an imaginary term in S_n first appears, are the real caustics. Accordingly, if in the real space we introduce the Stokes surfaces $\operatorname{Re} Y = 0$ [Eq. (32)], two of them go out to corresponding real caustics. Along them Ψ_C will increase exponentially from $\exp(-\operatorname{Im} S_0)$ to a quantity of the order of unity. Along the third Stokes surface, which goes out to infinity, there must be a further exponential decrease of Ψ_C, and this is the required boundary condition for Ψ_C.

The case we have considered is not the most general one; for example, all three Stokes surfaces can end on other complex caustics, but the character of the solution will be the same.

5. Using the results that have been given, one can easily construct, just as in the one-dimensional case, a unique function which approximates the exact solution both in the neighborhood of the caustic and at finite distances from it:

$$\Psi_a = \exp\left\{i\frac{S_1+S_2}{2\hbar} - i\frac{\pi}{12}\right\}\sqrt{\frac{\pi}{2}\frac{(S_2-S_1)}{2\hbar}}$$
$$\times\left[A_1 H^{(2)}_{-1/3}\left(\frac{S_2-S_1}{2\hbar}\right) + A_2 e^{i\pi/2} H^{(1)}_{1/3}\left(\frac{S_2-S_1}{2\hbar}\right)\right], \tag{35}$$

with $\varphi_1 = \varphi_2$ [Eq. (34)].

Near the caustic

$$S_1 = S_0 + \hbar(X - Y), \quad S_2 = S_0 + \hbar(X + Y)$$

and $\Psi_a \to \Psi_C$ [Eq. (33)]. At finite distances from the caustic ($|S_2 - S_1| \gg 2\hbar$)

$$\Psi_a \to \sum_{n=1,\,2} A_n e^{iS_n/\hbar}.$$

It is clear that in the vicinity of another caustic one can approximate the appropriate pair of terms in the sum (1) in precisely the same way.

6. As a practical application of these results let us consider the concrete quantum-mechanical problem of the scattering of particles in a potential $U(\mathbf{r})$.

Suppose that the trajectories satisfying the boundary conditions of the corresponding classical problem are known.[10] Then

$$S_n(\mathbf{r}) = \int^{\mathbf{r}} (p\mathbf{l}_n - \mathbf{p}_0)\,d\mathbf{r} + \mathbf{p}_0\mathbf{r}. \qquad (36)$$

Here $\mathbf{p}_0$ is the initial momentum of the particles; the integration in (36) is taken from a point $\mathbf{R}$, with $\mathbf{p}_0 \cdot \mathbf{R} \to -\infty$.

According to (9), the amplitude A_n is

$$A_n = \left(\frac{J_0}{J}\right)^{1/4}_{\alpha=\alpha_n(\mathbf{r}),\ \beta=\beta_n(\mathbf{r})} = \sqrt{\frac{p_0}{p}\frac{df_0}{df}}\Big|_{\alpha=\alpha_n,\ \beta=\beta_n}, \qquad (37)$$

where

$$df_n = \sqrt{[\mathbf{r}_\alpha \mathbf{r}_\beta]^2}\,d\alpha\,d\beta = \sqrt{\frac{J_n}{p^2}}\,d\alpha\,d\beta$$

is the cross section of a bundle of trajectories located in the neighborhood $d\alpha d\beta$ of the n-th trajectory. $J_0(df_0)$ is the value of $J_n(df_n)$ obtained by moving along the n-th trajectory to the point $\mathbf{p}_0\mathbf{R} = -\infty$.

The wave function (1) resulting from this construction can be obtained by the method of steepest descents from the exact solution, if the latter can be written as a superposition of some particular solutions of the Schrödinger equation. Then the saddle points correspond to the solutions of the system (5), and consequently the caustics will be loci where two saddle points come together.

The advantage of the trajectory method over the method of steepest descents is that the class of potentials in which the Hamilton-Jacobi equation separates is much wider than the class in which the Schrödinger equation separates. This question will be discussed further in later papers.

Let us consider Eq. (1) for the scattering problem for $r \to \infty$. It is obvious that among the trajectories that pass through the point (r, θ, φ), where $r \to \infty$, there is one real rectilinear trajectory that corresponds to the term $\exp(i\mathbf{p}_0 \cdot \mathbf{r}/\hbar)$. The others will be trajectories of particles which have undergone scattering in the direction (θ, φ). For them

$$d\mathbf{f}_n \to \frac{\mathbf{r}}{r}df_n = \frac{\mathbf{r}}{r}r^2 d\Omega_n, \quad A_n \to \frac{1}{r}\sqrt{\frac{df_0}{d\Omega_n}}, \quad r \to \infty. \qquad (38)$$

Here $\mathbf{df}_n$ is the vector cross section of a bundle of the n-th trajectory, and $d\Omega_n$ is its solid angle.

Let us find out what the caustic is in the scattering problem. It follows from (38) that

$$\nabla S_a \to \frac{1}{r}\left(S_{a\theta}\mathbf{e}_\theta + \frac{S_{a\varphi}}{\sin\theta}\mathbf{e}_\varphi\right) \equiv \frac{\nabla_\Omega S_a}{r}, \qquad (39)$$

where $\mathbf{e}_\theta$ and $\mathbf{e}_\varphi$ are unit vectors of the spherical coordinate system, and $a = (\alpha, \beta)$.

By means of (5) we introduce the scattering angles on the sphere of radius r as functions of the parameters α and β:

$$\theta = \theta(r, \alpha, \beta), \quad \varphi = \varphi(r, \alpha, \beta). \qquad (40)$$

Then (15), (8), and (9) can be written in the form

$$\Phi(r, \alpha, \beta) = \frac{\partial(\theta, \varphi)}{\partial(\alpha, \beta)} \to \frac{\partial(S_\theta S_\varphi)}{\partial(\alpha, \beta)},$$
$$[\nabla S_\alpha \nabla S_\beta] \to \frac{\mathbf{r}}{r^3 \sin\theta}\frac{\partial(S_\theta S_\varphi)}{\partial(\alpha, \beta)},$$
$$A \to \left[\frac{\sqrt{J_0}}{r^2 \sin\theta\,\partial(\theta, \varphi)/\partial(\alpha, \beta)}\right]^{1/2}_{\alpha=\alpha_n,\ \beta=\beta_n} \qquad (41)$$

where α_n and β_n are roots of (40). It follows from this that the caustic is determined by the condition $j = \partial(\theta, \varphi)/\partial(\alpha, \beta) = 0$, together with the system (40). Letting $r \to \infty$, we get

$$\theta = \theta_0(\alpha, \beta), \quad \varphi = \varphi_0(\alpha, \beta), \quad j_0 = \partial(\theta_0, \varphi_0)/\partial(\alpha\beta) = 0. \qquad (42)$$

Accordingly, at large distances the caustics that are of interest in the scattering problem asymptotically approach the conical surfaces (42). Furthermore complex caustics may have no trace in real space, but approach it asymptotically for $r \to \infty$; then the actual caustics in real space are surfaces which bound the beam of trajectories. In particular, for $E > U(r)$, when there exists a classically inaccessible region of scattering angles, its boundary will be one of the real caustics. Naturally the inaccessible region, unlike the accessible region, will contain no further real caustics. But there can be complex caustics in it, and if the cross section falls off exponentially in this region they must be taken into account.

The system (42) takes a simple form for azimuthally symmetric scattering. Here we can assume that

$$\theta_0 = \theta_0(\beta), \quad \varphi_0 = \alpha.$$

Then $j_0 = \theta_0'(\beta)$, and the caustics are determined by an extremum of the scattering angle.

Let us find the form of the scattering function for $r \to \infty$ near a real isolated caustic. Writing $\eta/R_0 = \Delta\chi$ and using (24), (32), and (39), we have

$$Y = (a/\lambda)(\Delta\chi)^{3/2}, \qquad (43)$$

where a is a finite quantity given by

$$a = \frac{2}{3p_0}\left[2(\nabla_\Omega S_\gamma)^2 \frac{\mathbf{n}\nabla_\Omega S_\gamma}{d}\right]^{1/2}, \quad \frac{\partial}{\partial\gamma} = \sqrt{S_{\beta^2}}\frac{\partial}{\partial\alpha} - \sqrt{S_{\alpha^2}}\frac{\partial}{\partial\beta}.$$

Finally, the value of Ψ on a sphere R_0 (sic!) in the neighborhood of an arbitrary point of the caustic R_0, θ_0, φ_0 is given by

$$\Psi = \Psi_r + \frac{\exp(ip_0R_0/\hbar)}{R} f(\theta - \theta_0, \varphi - \varphi_0),$$
$$f = \left[\frac{\sqrt{J_0}}{p_0 \sin\theta_0}\frac{\partial(S_\theta S_\varphi)}{\partial(\alpha, \beta)}(3\hbar d^2\lambda^{-1})^{1/3}\right]^{1/2}$$
$$\times \exp\left\{\frac{i}{\hbar}(S(\mathbf{R}_0) - p_0R_0) - i\frac{\pi}{12}\right\}F\left(\frac{a}{\lambda}(\Delta\chi)^{3/2}\right), \qquad (44)$$

since for $R_0 \to \infty$ we have $\xi \to 0$ for points of the sphere R_0. It can be seen from this that the scattering cross section near the caustic is finite, in contrast with the classical case, where it goes to infinity as $Y^{-1/3} \sim (\Delta\chi)^{-1/2}$.

Beyond the caustic the amplitude falls off exponentially:

$$f \sim (\Delta\chi)^{1/2}K_{1/3}\left(\frac{a}{\lambda}|\Delta\chi|^{3/2}\right)$$

and is of interest only if the caustic bounds a classically accessible region and if the potential is such that the further cross section will be exponentially small.

The amplitude for this sort of case (spherically symmetric even potential) has been derived in[2] for $U_0/E \ll 1$ in the range of angles $\theta \gg (U_0/E)^{1/4}$. For smaller angles $\theta \lesssim (U_0/E)^{1/4}$ to the classically accessible region the explicit form of the amplitude is unknown. Equation (44), having been obtained from the exact solution of the Schrödinger equation in the neighborhood of the caustic ($\theta_0 \sim U_0/E$), gives the amplitude for the range of angles $|\theta - \theta_0| < (\lambda_0/a)^{2/3}$. For large angles it does not go over

into the result of[2]. This question will be considered in more detail in a separate paper.

7. Finally, let us compare the approximating function (35) with the exact function for the scattering problem in a field $U(r) = \alpha/r$. In this case all of the quasiclassical quantities can be calculated exactly, and the results for S_n and A_n are

$$\frac{2E}{\alpha p_0} S_n = \varepsilon_r(\xi - \varepsilon_n\sqrt{\eta(\eta-2)}) + \\ + \ln\frac{[1+2\xi(\eta-1+\varepsilon_n\sqrt{\eta(\eta-2)}]^{(\varepsilon_r+1)/2}}{4(rE/\alpha)[2\xi+\eta-1-\varepsilon_n\sqrt{\eta(\eta-2)}\,]^{\varepsilon_r}}, \quad (45)$$

where

$$\xi = \frac{r}{\alpha/E}(1+\cos\theta), \quad \eta = \frac{r}{\alpha/E}(1-\cos\theta),$$
$$\varepsilon_n = e^{i\pi(n-1)}, \quad n = 1, 2;$$

the quantity ϵ_r being -1 on the part of the trajectory between $p_0 \cdot r \to -\infty$ and r_0, the radial turning point, and having the value $\epsilon_r = +1$ on the symmetrical part of the range; and

$$A_n = \left(\frac{\eta - 1 + \varepsilon_n\sqrt{\eta(\eta-2)}}{\varepsilon_n\sqrt{\eta(\eta-2)}}\right)^{1/2}. \quad (46)$$

Here the caustic is the paraboloid of revolution $\eta = 2$; $\eta = 0$ ($\theta = 0$) is the line of concentration of the spherical coordinate system.

The function (35), which approximates the expression (1) in the neighborhood of the caustic, is given by

$$\Psi_a = \frac{G_a}{[4\eta(\eta-2)]^{1/4}}\exp\left\{i\frac{\xi-1-\ln 2\gamma}{2\gamma} + i\left(\delta_0 - \frac{\pi}{12}\right)\right\},$$
$$G_a = \sqrt{\frac{\pi y}{2}}[H^{(1)}_{1/3}(y)(\eta - 1 + \varepsilon_2\sqrt{\eta(\eta-2)})^{1/2} \\ + H^{(2)}_{-1/3}(y)(\eta - 1 + \varepsilon_1\sqrt{\eta(\eta-2)})^{1/2}]. \quad (47)$$

Here

$$y = \frac{S_2 - S_1}{2\hbar} = \frac{1}{2\gamma}[\sqrt{\eta(\eta-2)} - \ln(\eta - 1 + \sqrt{\eta(\eta-2)})],$$
$$\delta_0 = \frac{1}{2\gamma}\ln\frac{\lambda}{r},$$

and $\gamma = \lambda E/\alpha$ is the quasiclassical small parameter. The distance at which Ψ_a goes over into (1) is determined, in terms of the smallness of γ, by the condition $(\eta-2)^{3/2}/\gamma \gg 1$.

The asymptotic form of the exact solution

$$\Psi = e^{-\pi/4\gamma}\Gamma\left(1 + \frac{i}{\gamma}\right)e^{i(\xi-\eta)/2\gamma}F\left(-\frac{i}{2\gamma}, 1, \frac{i\eta}{\gamma}\right)$$

for $\gamma \to 0$ is given by Eq. (47) if we replace G_a with G_F, where

$$G_F = \sqrt{\frac{\pi}{2}}y[H'_{1/3}(y) + H^{(2)}_{-1/3}(y)] + O(\gamma^{5/6}). \quad (48)$$

A difference between G_a and G_F appears as we go further from the caustic, and begins with terms of order $(\eta-2)^{1/2}$.

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